



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:54 PM GMT

PDB ID : 1YWH
Title : crystal structure of urokinase plasminogen activator receptor
Authors : Llinas, P.; Le Du, M.H.; Gardsvoll, H.; Dano, K.; Ploug, M.; Gilquin, B.;
Stura, E.A.; Menez, A.
Deposited on : 2005-02-18
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

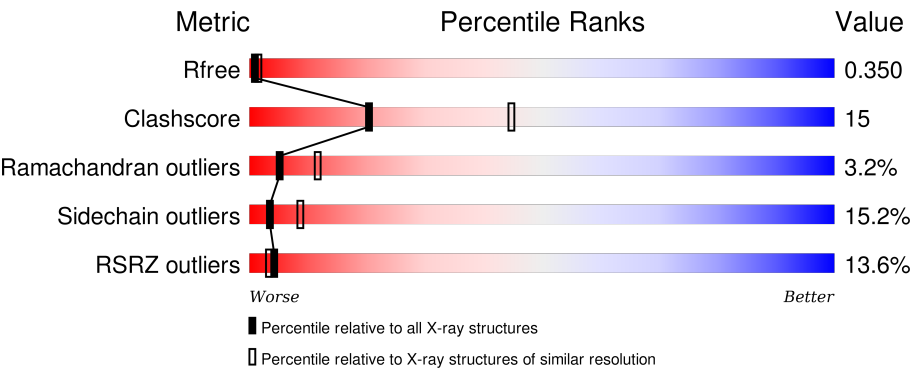
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	313	
1	C	313	
1	E	313	
1	G	313	
1	I	313	

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Mol	Chain	Length	Quality of chain
1	K	313	
1	M	313	
1	O	313	
2	B	13	
2	D	13	
2	F	13	
2	H	13	
2	J	13	
2	L	13	
2	N	13	
2	P	13	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SO4	K	810	-	-	X	-
3	FUC	A	316	X	-	-	-
3	NAG	C	331	X	-	-	-
3	FUC	C	336	X	-	-	-
3	FUC	E	316	X	-	-	-
3	FUC	K	316	X	-	-	-
5	NAG	A	321	X	-	-	-
5	NAG	C	316	X	-	-	-
5	NAG	C	321	X	-	-	-
6	FUC	C	315	X	-	-	-
6	FUC	E	326	X	-	-	X
6	FUC	G	315	X	-	-	X
6	FUC	I	315	X	-	-	-
6	FUC	I	336	X	-	-	-
6	FUC	M	315	X	-	-	-
6	FUC	O	315	X	-	-	X
8	FUC	G	336	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18552 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2040	1222	377	407	34			
1	C	259	Total	C	N	O	S	0	0	0
			1985	1188	368	395	34			
1	E	262	Total	C	N	O	S	0	0	0
			2006	1202	370	400	34			
1	G	258	Total	C	N	O	S	0	0	0
			1978	1186	363	395	34			
1	I	264	Total	C	N	O	S	0	0	0
			2008	1201	372	401	34			
1	K	257	Total	C	N	O	S	0	0	0
			1969	1180	363	392	34			
1	M	263	Total	C	N	O	S	0	0	0
			2016	1204	374	404	34			
1	O	258	Total	C	N	O	S	0	0	0
			1970	1180	362	394	34			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLN	ASN	CONFLICT	UNP Q9UMV0
C	200	GLN	ASN	CONFLICT	UNP Q9UMV0
E	200	GLN	ASN	CONFLICT	UNP Q9UMV0
G	200	GLN	ASN	CONFLICT	UNP Q9UMV0
I	200	GLN	ASN	CONFLICT	UNP Q9UMV0
K	200	GLN	ASN	CONFLICT	UNP Q9UMV0
M	200	GLN	ASN	CONFLICT	UNP Q9UMV0
O	200	GLN	ASN	CONFLICT	UNP Q9UMV0

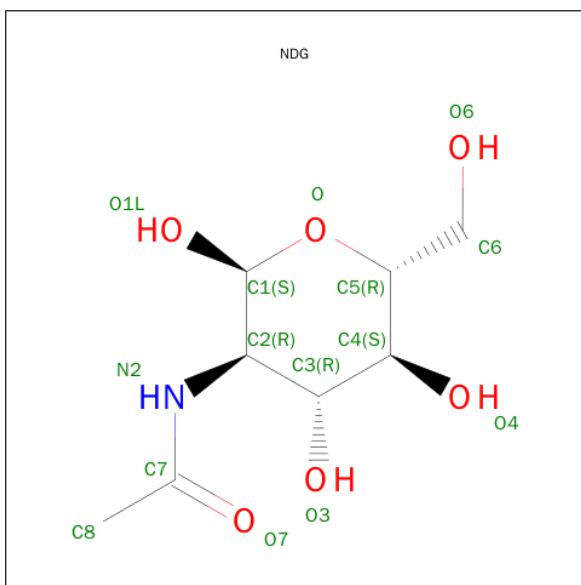
- Molecule 2 is a protein called antagonist peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	D	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	F	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	H	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	J	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	L	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	N	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	P	13	Total	C	N	O	0	0	0
			116	78	17	21			

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

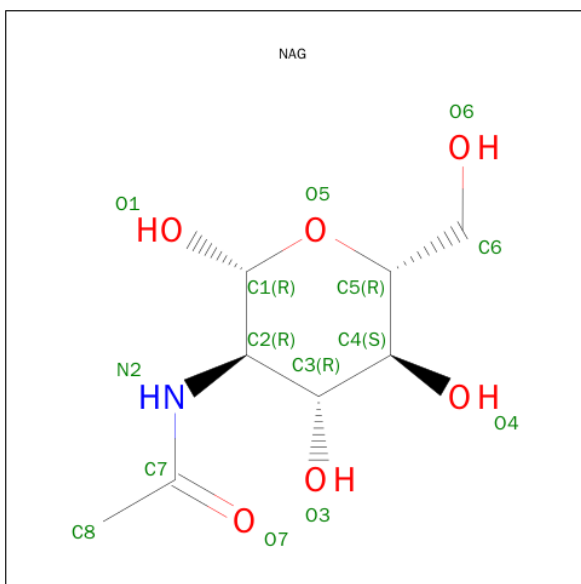
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			38	22	2	14		
3	C	3	Total	C	N	O	0	0
			38	22	2	14		
3	E	3	Total	C	N	O	0	0
			38	22	2	14		
3	K	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	2	Total	C	N	O	0	0
			24	14	1	9		
6	E	2	Total	C	N	O	0	0
			24	14	1	9		
6	G	2	Total	C	N	O	0	0
			24	14	1	9		
6	I	2	Total	C	N	O	0	0
			24	14	1	9		
6	I	2	Total	C	N	O	0	0
			24	14	1	9		
6	M	2	Total	C	N	O	0	0
			24	14	1	9		
6	O	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	2	Total	C	N	O	0	0
			28	16	2	10		
7	M	2	Total	C	N	O	0	0
			28	16	2	10		

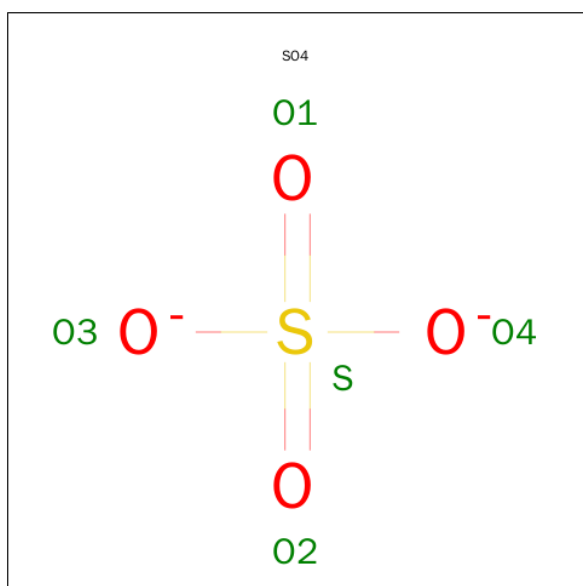
- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	I	5	Total	C	N	O	0	0
			61	34	2	25		
9	K	5	Total	C	N	O	0	0
			61	34	2	25		
9	M	5	Total	C	N	O	0	0
			61	34	2	25		
9	O	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	G	1	Total	O	S	0	0
			5	4	1		
10	K	1	Total	O	S	0	0
			5	4	1		
10	I	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total O S 5 4 1	0	0
10	E	1	Total O S 5 4 1	0	0
10	G	1	Total O S 5 4 1	0	0
10	I	1	Total O S 5 4 1	0	0
10	K	1	Total O S 5 4 1	0	0
10	M	1	Total O S 5 4 1	0	0
10	O	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0
10	E	1	Total O S 5 4 1	0	0
10	G	1	Total O S 5 4 1	0	0
10	G	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0
10	M	1	Total O S 5 4 1	0	0
10	E	1	Total O S 5 4 1	0	0
10	I	1	Total O S 5 4 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	81	Total O 81 81	0	0
11	B	5	Total O 5 5	0	0
11	C	85	Total O 85 85	0	0

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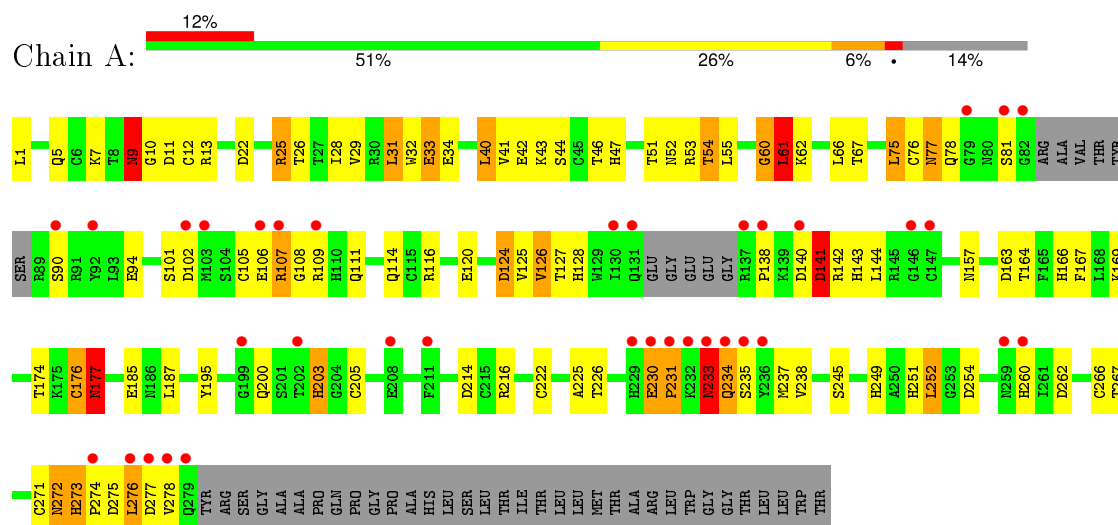
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total 2	O 2	0	0
11	E	98	Total 98	O 98	0	0
11	F	8	Total 8	O 8	0	0
11	G	88	Total 88	O 88	0	0
11	H	4	Total 4	O 4	0	0
11	I	87	Total 87	O 87	0	0
11	J	3	Total 3	O 3	0	0
11	K	83	Total 83	O 83	0	0
11	L	2	Total 2	O 2	0	0
11	M	91	Total 91	O 91	0	0
11	N	1	Total 1	O 1	0	0
11	O	106	Total 106	O 106	0	0
11	P	5	Total 5	O 5	0	0

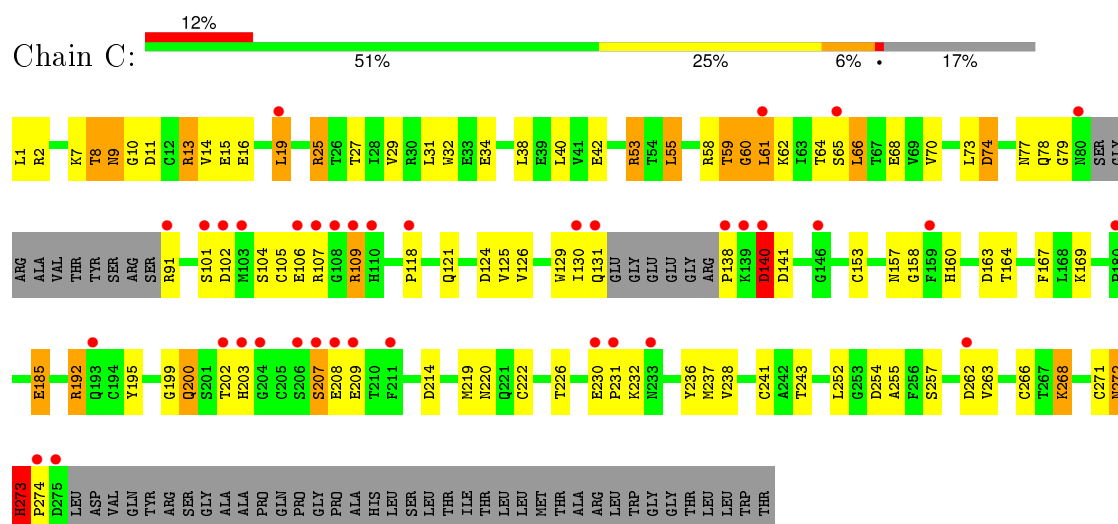
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Urokinase plasminogen activator surface receptor

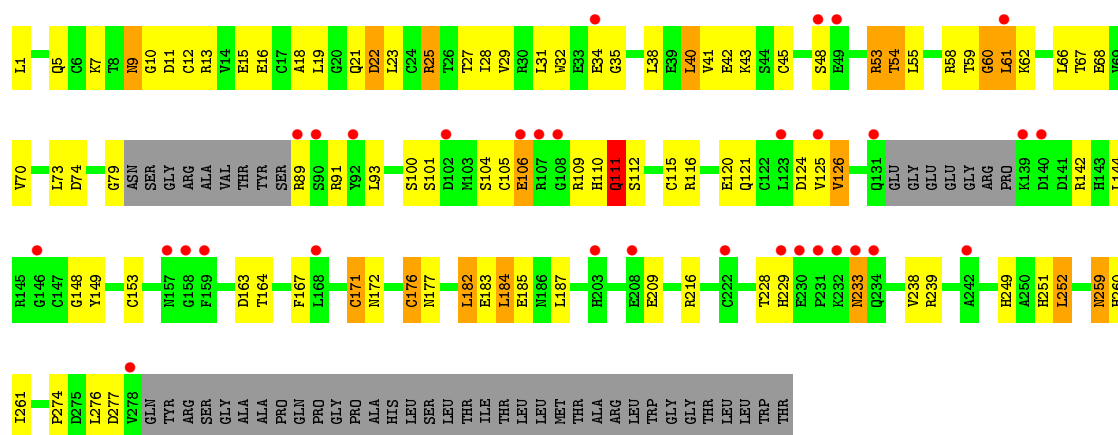


- Molecule 1: Urokinase plasminogen activator surface receptor



- Molecule 1: Urokinase plasminogen activator surface receptor



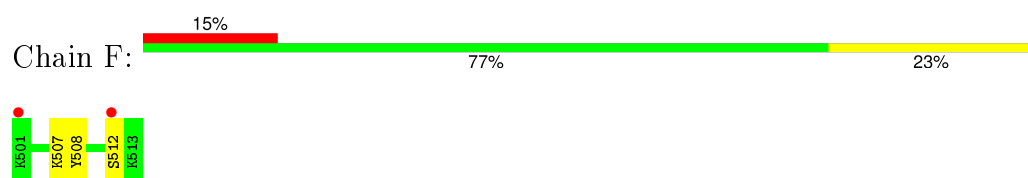




- Molecule 2: antagonist peptide



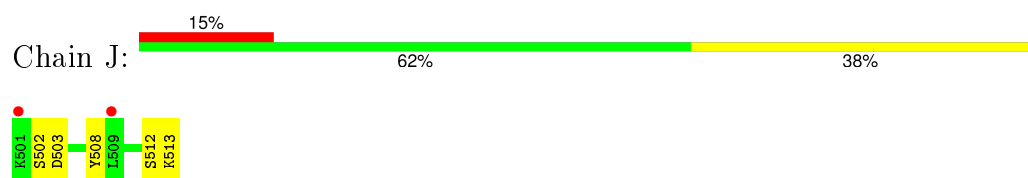
- Molecule 2: antagonist peptide



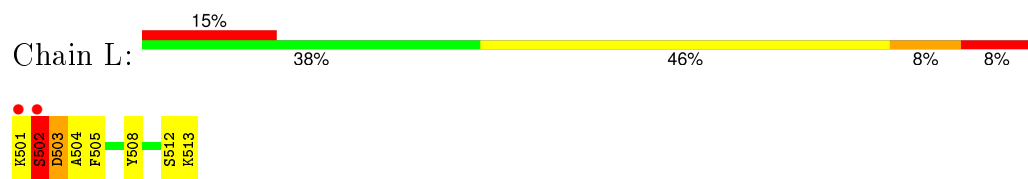
- Molecule 2: antagonist peptide



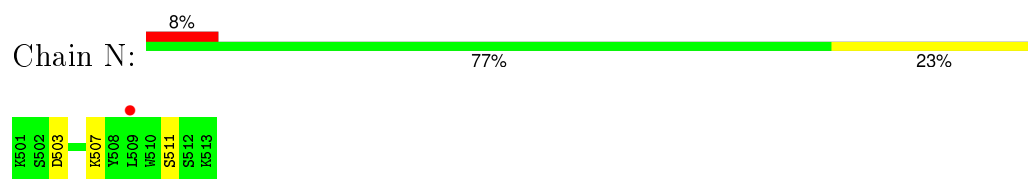
- Molecule 2: antagonist peptide



- Molecule 2: antagonist peptide



- Molecule 2: antagonist peptide



- Molecule 2: antagonist peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.93Å 136.83Å 140.54Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	24.85 – 2.70 24.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (24.85-2.70) 97.2 (24.85-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.245 , 0.315 0.281 , 0.350	Depositor DCC
R_{free} test set	5332 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 106877 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18552	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, ALC, NDG, DSN, SO4, DLY, MAN, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.55	2/2072 (0.1%)	0.87	11/2791 (0.4%)
1	C	0.62	3/2016 (0.1%)	0.87	10/2713 (0.4%)
1	E	0.54	0/2037	0.85	4/2742 (0.1%)
1	G	0.54	0/2009	0.90	10/2704 (0.4%)
1	I	0.53	1/2039 (0.0%)	0.85	9/2746 (0.3%)
1	K	0.60	1/2000 (0.1%)	0.85	6/2693 (0.2%)
1	M	0.52	0/2047	0.87	7/2755 (0.3%)
1	O	0.50	0/2001	0.82	7/2695 (0.3%)
2	B	0.63	0/91	0.86	1/116 (0.9%)
2	D	0.56	0/91	0.82	1/116 (0.9%)
2	F	0.61	0/91	0.82	0/116
2	H	0.67	0/91	0.88	1/116 (0.9%)
2	J	0.71	0/91	0.96	1/116 (0.9%)
2	L	0.54	0/91	0.86	0/116
2	N	0.56	0/91	0.92	1/116 (0.9%)
2	P	0.49	0/91	0.84	0/116
All	All	0.55	7/16949 (0.0%)	0.86	69/22767 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	E	0	1
1	G	0	1
1	I	0	1
1	K	0	2
3	A	2	0
3	C	3	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	2	0
3	K	2	0
6	C	2	0
6	E	2	0
6	G	2	0
6	I	4	0
6	M	2	0
6	O	2	0
8	G	2	0
All	All	25	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	268	LYS	CE-NZ	14.47	1.85	1.49
1	C	273	HIS	CE1-NE2	13.68	1.64	1.32
1	C	273	HIS	CG-ND1	11.19	1.63	1.38
1	A	233	ASN	CG-ND2	6.80	1.49	1.32
1	I	268	LYS	CE-NZ	5.75	1.63	1.49
1	C	273	HIS	CG-CD2	5.33	1.44	1.35
1	A	233	ASN	CG-OD1	5.20	1.35	1.24

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	141	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	102	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	262	ASP	CB-CG-OD2	6.68	124.31	118.30
1	I	141	ASP	CB-CG-OD2	6.54	124.19	118.30
2	H	503	ASP	CB-CG-OD2	6.45	124.10	118.30
1	I	124	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	141	ASP	CB-CG-OD2	6.30	123.97	118.30
1	G	22	ASP	CB-CG-OD2	6.27	123.94	118.30
1	E	124	ASP	CB-CG-OD2	6.18	123.87	118.30
1	K	275	ASP	CB-CG-OD2	6.16	123.84	118.30
1	C	124	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	138	PRO	N-CA-CB	6.08	110.60	103.30
1	C	262	ASP	CB-CG-OD2	6.05	123.75	118.30
1	E	176	CYS	CA-CB-SG	-6.05	103.11	114.00
1	O	22	ASP	CB-CG-OD2	6.04	123.73	118.30
1	M	141	ASP	CB-CG-OD2	6.03	123.72	118.30
1	I	138	PRO	N-CA-CB	6.02	110.53	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	74	ASP	CB-CG-OD2	6.00	123.70	118.30
1	G	102	ASP	CB-CG-OD2	5.97	123.67	118.30
2	N	503	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	31	LEU	CA-CB-CG	5.88	128.83	115.30
1	G	212	LEU	CA-CB-CG	5.88	128.82	115.30
1	C	74	ASP	CB-CG-OD2	5.84	123.56	118.30
1	K	214	ASP	CB-CG-OD2	5.76	123.48	118.30
1	O	163	ASP	CB-CG-OD2	5.70	123.43	118.30
1	M	124	ASP	CB-CG-OD2	5.69	123.42	118.30
1	O	214	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	163	ASP	CB-CG-OD2	5.66	123.40	118.30
1	K	102	ASP	CB-CG-OD2	5.63	123.37	118.30
1	G	141	ASP	CB-CG-OD2	5.63	123.37	118.30
1	G	140	ASP	CB-CG-OD2	5.61	123.35	118.30
1	O	124	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	214	ASP	CB-CG-OD2	5.58	123.32	118.30
1	O	254	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	273	HIS	CG-ND1-CE1	-5.57	98.47	105.70
1	G	254	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	163	ASP	CB-CG-OD2	5.49	123.24	118.30
1	I	102	ASP	CB-CG-OD2	5.47	123.23	118.30
1	M	163	ASP	CB-CG-OD2	5.47	123.22	118.30
1	C	254	ASP	CB-CG-OD2	5.47	123.22	118.30
1	K	163	ASP	CB-CG-OD2	5.46	123.22	118.30
1	I	275	ASP	CB-CG-OD2	5.46	123.21	118.30
2	J	503	ASP	CB-CG-OD2	5.46	123.21	118.30
1	E	74	ASP	CB-CG-OD2	5.46	123.21	118.30
1	K	141	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	22	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	102	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	9	ASN	CB-CA-C	-5.35	99.69	110.40
1	C	140	ASP	CB-CG-OD2	5.34	123.11	118.30
1	M	275	ASP	CB-CG-OD2	5.33	123.10	118.30
1	I	214	ASP	CB-CG-OD2	5.32	123.09	118.30
1	E	277	ASP	CB-CG-OD2	5.31	123.08	118.30
1	M	25	ARG	NE-CZ-NH1	-5.31	117.65	120.30
2	B	503	ASP	CB-CG-OD2	5.29	123.06	118.30
1	G	25	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	O	262	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	124	ASP	CB-CG-OD2	5.25	123.02	118.30
1	M	74	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	277	ASP	CB-CG-OD2	5.21	122.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	55	LEU	CA-CB-CG	5.20	127.26	115.30
1	G	214	ASP	CB-CG-OD2	5.19	122.97	118.30
1	I	11	ASP	CB-CG-OD2	5.15	122.94	118.30
2	D	503	ASP	CB-CG-OD2	5.12	122.91	118.30
1	G	124	ASP	CB-CG-OD2	5.11	122.90	118.30
1	M	22	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	214	ASP	CB-CG-OD2	5.09	122.89	118.30
1	G	163	ASP	CB-CG-OD2	5.08	122.87	118.30
1	K	254	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	254	ASP	CB-CG-OD2	5.03	122.83	118.30

All (25) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	316	FUC	C5,C1
6	C	315	FUC	C5,C1
3	C	331	NAG	C1
3	C	336	FUC	C5,C1
3	E	316	FUC	C5,C1
6	E	326	FUC	C5,C1
6	G	315	FUC	C5,C1
8	G	336	FUC	C5,C1
6	I	315	FUC	C5,C1
6	I	336	FUC	C5,C1
3	K	316	FUC	C5,C1
6	M	315	FUC	C5,C1
6	O	315	FUC	C5,C1

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	GLU	Peptide
1	A	272	ASN	Peptide
1	A	61	LEU	Peptide
1	E	61	LEU	Peptide
1	G	208	GLU	Peptide
1	I	80	ASN	Peptide
1	K	102	ASP	Peptide
1	K	61	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2040	0	1885	59	0
1	C	1985	0	1840	72	0
1	E	2006	0	1864	66	0
1	G	1978	0	1836	62	0
1	I	2008	0	1850	67	0
1	K	1969	0	1825	65	0
1	M	2016	0	1868	56	0
1	O	1970	0	1823	55	0
2	B	116	0	112	9	0
2	D	116	0	112	7	0
2	F	116	0	112	3	0
2	H	116	0	112	3	0
2	J	116	0	112	2	0
2	L	116	0	112	7	0
2	N	116	0	112	2	0
2	P	116	0	112	6	0
3	A	38	0	34	0	0
3	C	38	0	34	0	0
3	E	38	0	34	0	0
3	K	38	0	34	0	0
4	A	14	0	13	0	0
4	K	14	0	13	0	0
4	O	14	0	13	0	0
5	A	14	0	13	0	0
5	C	28	0	26	0	0
5	E	14	0	13	0	0
5	G	14	0	13	0	0
5	I	14	0	13	0	0
5	K	14	0	13	0	0
5	M	14	0	13	0	0
6	C	24	0	22	0	0
6	E	24	0	22	1	0
6	G	24	0	22	0	0
6	I	48	0	44	1	0
6	M	24	0	22	1	0
6	O	24	0	22	0	0
7	G	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	28	0	25	0	0
8	G	24	0	22	0	0
9	I	61	0	52	1	0
9	K	61	0	52	1	0
9	M	61	0	52	1	0
9	O	61	0	52	1	0
10	A	15	0	0	1	0
10	C	15	0	0	1	0
10	E	15	0	0	0	0
10	G	20	0	0	1	0
10	I	15	0	0	1	0
10	K	10	0	0	3	0
10	M	10	0	0	1	0
10	O	5	0	0	0	0
11	A	81	0	0	2	0
11	B	5	0	0	0	0
11	C	85	0	0	1	0
11	D	2	0	0	1	0
11	E	98	0	0	4	0
11	F	8	0	0	1	0
11	G	88	0	0	3	0
11	H	4	0	0	0	0
11	I	87	0	0	1	0
11	J	3	0	0	0	0
11	K	83	0	0	4	0
11	L	2	0	0	1	0
11	M	91	0	0	4	0
11	N	1	0	0	0	0
11	O	106	0	0	5	0
11	P	5	0	0	1	0
All	All	18552	0	16400	500	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (500) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:268:LYS:NZ	1:K:268:LYS:CE	1.85	1.38
1:C:273:HIS:HB3	1:C:274:PRO:HD3	1.11	1.10
1:C:273:HIS:HB3	1:C:274:PRO:CD	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:LEU:HB3	1:C:66:LEU:HD23	1.35	1.04
1:G:55:LEU:HD23	1:G:123:LEU:HD12	1.46	0.97
1:M:29:VAL:HB	1:M:66:LEU:HD13	1.45	0.96
1:M:4:MET:CE	1:M:75:LEU:HD22	2.00	0.91
1:C:273:HIS:CB	1:C:274:PRO:HD3	2.01	0.90
1:G:195:TYR:H	1:G:272:ASN:HD21	1.13	0.90
1:G:32:TRP:CE2	1:G:62:LYS:HB3	2.06	0.90
1:G:198:LYS:NZ	10:G:817:SO4:O2	2.05	0.90
1:O:32:TRP:CD1	1:O:62:LYS:HB3	2.08	0.89
1:G:55:LEU:HD23	1:G:123:LEU:CD1	2.05	0.87
1:K:27:THR:HG23	1:K:68:GLU:HG2	1.53	0.87
1:E:184:LEU:HD22	1:E:216:ARG:HD3	1.55	0.87
1:C:8:THR:HG21	1:E:12:CYS:H	1.40	0.86
1:C:32:TRP:CE2	1:C:62:LYS:HB3	2.09	0.86
1:G:7:LYS:HG3	1:G:9:ASN:HD21	1.42	0.84
1:A:32:TRP:CD1	1:A:62:LYS:HB3	2.12	0.84
1:I:4:MET:H	1:I:77:ASN:HD21	1.23	0.83
1:O:9:ASN:ND2	11:O:916:HOH:O	2.11	0.83
1:M:4:MET:HE2	1:M:75:LEU:HD22	1.58	0.83
1:C:8:THR:CG2	1:E:12:CYS:H	1.91	0.83
1:G:205:CYS:HB3	1:G:237:MET:HE2	1.61	0.82
1:E:91:ARG:NH1	1:E:116:ARG:HE	1.77	0.81
1:M:29:VAL:HB	1:M:66:LEU:CD1	2.11	0.80
2:P:508:TYR:HA	2:P:512:SER:HB3	1.63	0.80
1:I:32:TRP:CE2	1:I:62:LYS:HB3	2.17	0.80
1:E:32:TRP:CD1	1:E:62:LYS:HB3	2.16	0.80
1:C:195:TYR:H	1:C:272:ASN:HD21	1.25	0.80
1:E:54:THR:HG21	1:E:120:GLU:OE1	1.83	0.78
1:K:32:TRP:CD1	1:K:62:LYS:HB3	2.19	0.78
1:C:8:THR:HG21	1:E:12:CYS:N	1.99	0.77
2:F:508:TYR:HA	2:F:512:SER:HB3	1.65	0.77
2:B:508:TYR:HA	2:B:512:SER:HB3	1.67	0.77
1:I:239:ARG:HD3	1:I:272:ASN:HB3	1.67	0.75
1:C:268:LYS:HD3	1:C:268:LYS:H	1.51	0.75
1:M:123:LEU:HD22	1:M:170:CYS:HB3	1.69	0.75
1:K:157:ASN:ND2	1:K:245:SER:OG	2.20	0.75
1:M:195:TYR:H	1:M:272:ASN:HD21	1.36	0.74
1:O:29:VAL:HB	1:O:66:LEU:HD13	1.69	0.74
1:I:161:ASN:ND2	1:I:164:THR:H	1.85	0.74
1:I:123:LEU:HD22	1:I:170:CYS:HB3	1.70	0.73
1:M:98:CYS:HA	1:M:103:MET:HE3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASP:O	1:A:276:LEU:HB2	1.88	0.73
1:A:75:LEU:C	1:A:77:ASN:H	1.90	0.73
2:J:508:TYR:CD2	2:J:512:SER:HB3	2.23	0.73
1:G:246:MET:HE2	1:G:252:LEU:HG	1.71	0.72
1:A:9:ASN:ND2	1:C:11:ASP:OD1	2.20	0.72
1:M:9:ASN:HD21	1:M:11:ASP:HB3	1.54	0.71
1:O:259:ASN:HD21	2:P:501:LYS:N	1.89	0.71
1:G:105:CYS:O	1:G:109:ARG:HG3	1.90	0.71
1:I:200:GLN:H	1:I:203:HIS:HD2	1.39	0.71
1:G:205:CYS:HB3	1:G:237:MET:CE	2.21	0.71
1:O:157:ASN:HA	1:O:243:THR:HG21	1.73	0.71
1:E:34:GLU:O	11:E:836:HOH:O	2.08	0.71
1:I:157:ASN:HA	1:I:243:THR:HG21	1.73	0.71
1:O:239:ARG:HD3	1:O:272:ASN:O	1.92	0.70
1:O:195:TYR:HB2	1:O:272:ASN:HB2	1.74	0.70
1:I:200:GLN:H	1:I:203:HIS:CD2	2.10	0.70
1:G:126:VAL:HG13	1:G:167:PHE:HB3	1.74	0.70
1:C:192:ARG:HD2	1:C:220:ASN:O	1.90	0.70
1:M:188:PRO:O	1:M:216:ARG:O	2.09	0.70
1:K:243:THR:HG22	1:K:246:MET:HG2	1.73	0.69
1:G:246:MET:CE	1:G:252:LEU:HG	2.23	0.69
1:G:274:PRO:C	1:G:276:LEU:H	1.96	0.69
1:M:184:LEU:HD22	1:M:216:ARG:HG3	1.73	0.69
10:K:810:SO4:O1	11:K:823:HOH:O	2.11	0.69
1:M:32:TRP:CE2	1:M:62:LYS:HB3	2.28	0.69
1:C:61:LEU:CA	1:O:61:LEU:CA	2.70	0.69
1:G:272:ASN:HD22	1:G:272:ASN:H	1.41	0.68
1:C:8:THR:HG22	11:E:822:HOH:O	1.91	0.68
1:A:53:ARG:NH1	1:A:251:HIS:HB3	2.09	0.68
1:A:230:GLU:HG2	1:A:233:ASN:H	1.57	0.68
1:E:9:ASN:ND2	1:G:11:ASP:OD1	2.22	0.67
1:C:268:LYS:CD	1:C:268:LYS:H	2.06	0.67
1:C:25:ARG:NH2	1:C:42:GLU:OE1	2.25	0.67
1:O:192:ARG:HG3	1:O:269:SER:HB3	1.77	0.66
1:C:10:GLY:O	11:C:860:HOH:O	2.12	0.66
1:G:25:ARG:NH2	1:G:42:GLU:OE1	2.24	0.66
1:I:195:TYR:HB2	1:I:272:ASN:HB2	1.78	0.65
1:C:157:ASN:HA	1:C:243:THR:HG21	1.79	0.65
1:K:109:ARG:O	1:K:110:HIS:HB2	1.97	0.65
1:M:226:THR:HG22	1:M:262:ASP:HB3	1.79	0.65
1:I:190:ASN:ND2	1:I:192:ARG:H	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:HIS:HE1	1:G:216:ARG:H	1.46	0.65
1:I:273:HIS:CD2	1:I:275:ASP:H	2.16	0.64
1:G:55:LEU:CD2	1:G:123:LEU:HD12	2.26	0.64
1:A:25:ARG:HG2	1:A:46:THR:HB	1.80	0.63
1:K:66:LEU:HD23	2:L:505:PHE:CD1	2.33	0.63
1:K:197:CYS:SG	1:K:239:ARG:HD2	2.38	0.63
1:G:7:LYS:HG3	1:G:9:ASN:ND2	2.13	0.63
1:E:185:GLU:CD	1:E:185:GLU:H	2.00	0.63
1:I:190:ASN:HD22	1:I:192:ARG:H	1.47	0.63
1:G:68:GLU:OE2	11:G:822:HOH:O	2.15	0.63
1:I:29:VAL:HB	1:I:66:LEU:HD13	1.80	0.63
1:C:2:ARG:HD3	1:C:74:ASP:OD1	1.98	0.63
1:M:104:SER:O	1:M:108:GLY:N	2.28	0.63
1:I:8:THR:HG22	1:K:10:GLY:O	1.99	0.63
10:A:801:SO4:O3	1:C:13:ARG:NH1	2.31	0.62
1:A:67:THR:OG1	1:A:81:SER:HB3	1.99	0.62
1:O:195:TYR:HB2	1:O:272:ASN:CB	2.28	0.62
1:K:246:MET:HE2	1:K:252:LEU:HD13	1.81	0.62
2:L:508:TYR:HA	2:L:512:SER:HB3	1.81	0.62
1:M:25:ARG:NH1	1:M:42:GLU:OE1	2.25	0.62
1:E:43:LYS:NZ	1:E:79:GLY:H	1.98	0.61
1:I:7:LYS:NZ	11:I:834:HOH:O	2.19	0.61
1:O:207:SER:C	1:O:209:GLU:H	2.04	0.61
1:M:246:MET:HE1	1:M:252:LEU:HG	1.81	0.61
1:I:13:ARG:HD2	10:I:804:SO4:O4	1.99	0.61
1:G:60:GLY:O	1:K:61:LEU:O	2.18	0.61
1:C:129:TRP:HZ3	1:C:140:ASP:O	1.83	0.61
1:M:25:ARG:HG2	1:M:26:THR:N	2.15	0.61
1:O:104:SER:O	1:O:108:GLY:HA3	2.01	0.61
1:O:247:CYS:HA	1:O:263:VAL:CG2	2.30	0.61
1:A:225:ALA:HB3	1:A:238:VAL:HG12	1.83	0.61
1:I:243:THR:HG22	1:I:246:MET:HG2	1.83	0.60
1:G:101:SER:OG	2:H:513:LYS:O	2.13	0.60
1:G:61:LEU:CA	1:K:61:LEU:CA	2.79	0.60
1:K:117:SER:HB2	1:K:120:GLU:HG3	1.82	0.60
1:I:116:ARG:O	1:I:117:SER:HB3	2.02	0.60
1:M:254:ASP:O	2:N:507:DLY:HE3	2.00	0.60
1:A:105:CYS:O	1:A:109:ARG:HG3	2.02	0.60
1:M:185:GLU:H	1:M:185:GLU:CD	2.04	0.60
1:A:10:GLY:O	1:G:8:THR:HG22	2.02	0.59
1:I:17:CYS:HB3	1:I:21:GLN:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:O	1:A:111:GLN:HB2	2.03	0.59
1:C:272:ASN:H	1:C:272:ASN:HD22	1.51	0.59
1:C:160:HIS:CE1	1:C:241:CYS:HB2	2.38	0.58
1:K:210:THR:HG21	1:K:274:PRO:HG3	1.84	0.58
1:G:205:CYS:CB	1:G:237:MET:HE2	2.33	0.58
1:C:9:ASN:HD22	1:C:9:ASN:H	1.49	0.58
1:K:192:ARG:HH11	1:K:269:SER:HB2	1.69	0.58
1:E:54:THR:HG22	1:E:148:GLY:HA2	1.86	0.58
1:A:28:ILE:HG12	1:A:41:VAL:HG22	1.86	0.58
1:C:226:THR:HG23	1:C:237:MET:HB3	1.85	0.58
2:D:501:LYS:HG3	1:E:13:ARG:NH2	2.19	0.58
1:C:59:THR:HG21	1:C:64:THR:OG1	2.04	0.58
1:G:225:ALA:HB3	1:G:238:VAL:HG12	1.86	0.58
1:M:5:GLN:HB2	1:M:15:GLU:HG2	1.86	0.58
1:E:104:SER:HB3	1:E:106:GLU:HG3	1.86	0.57
2:D:508:TYR:CD2	2:D:512:SER:HB3	2.39	0.57
1:A:114:GLN:O	1:A:116:ARG:NH1	2.36	0.57
1:E:121:GLN:HB3	1:E:171:CYS:O	2.03	0.57
1:O:243:THR:HG23	1:O:245:SER:HB2	1.85	0.57
1:E:182:LEU:HD21	1:E:187:LEU:HD21	1.85	0.57
1:K:27:THR:HG23	1:K:68:GLU:CG	2.30	0.57
1:C:164:THR:HG21	10:C:818:SO4:O1	2.04	0.57
1:O:160:HIS:CE1	1:O:215:CYS:HA	2.38	0.57
1:C:268:LYS:N	1:C:268:LYS:HD3	2.18	0.57
1:E:34:GLU:HG3	1:E:35:GLY:H	1.69	0.57
1:G:251:HIS:CE1	1:G:252:LEU:HD13	2.39	0.57
2:F:507:DLY:HE3	11:F:421:HOH:O	2.03	0.57
1:G:192:ARG:HG3	1:G:220:ASN:O	2.05	0.57
1:I:207:SER:OG	1:I:274:PRO:HG3	2.05	0.57
1:K:9:ASN:HD22	1:K:10:GLY:N	2.03	0.56
1:A:195:TYR:HB2	1:A:272:ASN:HB2	1.87	0.56
1:M:246:MET:CE	1:M:252:LEU:HG	2.35	0.56
1:O:247:CYS:HA	1:O:263:VAL:HG23	1.86	0.56
1:E:105:CYS:O	1:E:109:ARG:HG3	2.05	0.56
1:C:32:TRP:CD2	1:C:62:LYS:HB3	2.40	0.56
1:M:9:ASN:ND2	1:M:11:ASP:HB3	2.20	0.56
1:E:251:HIS:HB3	11:E:908:HOH:O	2.06	0.56
1:G:75:LEU:C	1:G:77:ASN:H	2.08	0.56
1:A:176:CYS:SG	1:A:177:ASN:N	2.79	0.55
1:A:106:GLU:O	1:A:107:ARG:HB3	2.06	0.55
1:K:121:GLN:HB3	1:K:171:CYS:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:C	1:A:77:ASN:N	2.60	0.55
2:B:501:LYS:HE3	1:C:13:ARG:HH22	1.70	0.55
1:E:228:THR:HG21	1:E:233:ASN:ND2	2.22	0.55
1:K:149:TYR:C	1:K:150:LEU:HD12	2.27	0.55
1:A:273:HIS:HB3	1:A:274:PRO:HD3	1.88	0.55
1:A:200:GLN:HG3	1:A:203:HIS:HD2	1.70	0.55
1:O:121:GLN:HB3	1:O:171:CYS:O	2.06	0.55
1:M:1:LEU:O	1:M:1:LEU:HD13	2.06	0.55
1:A:205:CYS:HB3	1:A:237:MET:HE2	1.87	0.55
1:M:126:VAL:HG13	1:M:167:PHE:HB3	1.89	0.55
1:K:275:ASP:OD2	1:K:276:LEU:N	2.40	0.55
1:K:192:ARG:NH1	1:K:269:SER:HB2	2.21	0.55
1:K:25:ARG:HD3	11:K:817:HOH:O	2.07	0.55
1:E:29:VAL:CG1	1:E:40:LEU:HB2	2.37	0.55
1:O:239:ARG:HD2	1:O:272:ASN:HB3	1.87	0.55
1:G:160:HIS:CE1	1:G:216:ARG:H	2.25	0.54
1:O:55:LEU:HD21	1:O:57:TYR:CE2	2.43	0.54
1:M:18:ALA:HB3	1:M:21:GLN:HE21	1.72	0.54
1:I:14:VAL:HG21	2:P:504:ALC:HE23	1.89	0.54
1:C:257:SER:HA	1:E:16:GLU:OE1	2.07	0.54
1:M:32:TRP:O	1:M:33:GLU:HB2	2.07	0.54
1:K:9:ASN:HD21	1:K:11:ASP:HB3	1.73	0.54
1:O:257:SER:OG	2:P:507:DLY:NZ	2.40	0.54
1:E:25:ARG:HH21	1:E:42:GLU:HG2	1.72	0.54
1:C:60:GLY:O	1:O:61:LEU:O	2.25	0.54
1:K:192:ARG:HH12	1:K:268:LYS:NZ	2.06	0.53
1:I:47:HIS:HB3	1:I:49:GLU:OE2	2.08	0.53
1:C:199:GLY:HA2	1:C:236:TYR:CZ	2.43	0.53
2:L:513:LYS:HD2	1:M:73:LEU:HD22	1.90	0.53
1:O:32:TRP:CG	1:O:62:LYS:HB3	2.41	0.53
1:E:43:LYS:HZ1	1:E:79:GLY:H	1.57	0.53
1:I:83:ARG:O	1:I:84:ALA:HB2	2.08	0.53
1:K:9:ASN:C	1:K:9:ASN:HD22	2.10	0.53
1:E:142:ARG:HG3	1:E:142:ARG:HH11	1.72	0.53
1:I:195:TYR:HB3	1:I:210:THR:HG22	1.89	0.53
1:O:245:SER:HB3	1:O:252:LEU:HD23	1.90	0.53
1:E:53:ARG:NH2	1:E:68:GLU:OE2	2.39	0.53
1:C:230:GLU:HB2	1:E:18:ALA:CB	2.38	0.53
1:M:122:CYS:O	1:M:170:CYS:HA	2.09	0.53
1:E:15:GLU:HG2	1:E:45:CYS:SG	2.49	0.53
1:A:9:ASN:HB3	1:A:11:ASP:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:227:GLY:HA2	1:M:260:HIS:O	2.09	0.52
1:A:126:VAL:HG13	1:A:167:PHE:HB3	1.90	0.52
1:K:160:HIS:HE1	1:K:216:ARG:H	1.57	0.52
1:C:130:ILE:O	1:C:131:GLN:HB2	2.10	0.52
1:K:207:SER:C	1:K:209:GLU:H	2.13	0.52
1:A:124:ASP:HB3	1:A:169:LYS:HG3	1.90	0.52
1:M:181:ILE:H	1:M:181:ILE:HD12	1.74	0.52
2:B:501:LYS:HD3	1:C:16:GLU:HB2	1.91	0.52
1:G:189:GLN:N	1:G:189:GLN:OE1	2.39	0.52
1:A:126:VAL:HB	1:A:143:HIS:HD2	1.74	0.51
1:G:182:LEU:HD11	1:G:187:LEU:HD21	1.91	0.51
2:L:501:LYS:O	2:L:502:SER:HB2	2.10	0.51
1:A:32:TRP:CG	1:A:62:LYS:HB3	2.45	0.51
1:O:38:LEU:HD12	11:O:828:HOH:O	2.10	0.51
1:G:123:LEU:HD23	1:G:170:CYS:HB3	1.91	0.51
1:I:30:ARG:NH1	1:I:39:GLU:OE1	2.44	0.51
1:O:230:GLU:HG3	1:O:231:PRO:HA	1.92	0.51
1:M:5:GLN:O	1:M:12:CYS:HA	2.11	0.51
1:G:131:GLN:HG2	1:G:132:GLU:H	1.75	0.51
1:G:9:ASN:ND2	1:G:9:ASN:H	2.09	0.50
1:E:121:GLN:HE22	1:E:153:CYS:HB3	1.76	0.50
1:C:91:ARG:HB2	1:C:118:PRO:HB3	1.92	0.50
1:K:18:ALA:H	1:K:21:GLN:HE21	1.60	0.50
1:C:9:ASN:HD22	1:C:9:ASN:N	2.08	0.50
1:E:142:ARG:HH12	2:F:512:SER:C	2.13	0.50
1:O:55:LEU:HD21	1:O:57:TYR:HE2	1.77	0.50
1:E:66:LEU:HD12	1:E:67:THR:N	2.27	0.50
1:G:162:ASN:HD22	7:G:316:NAG:H82	1.76	0.50
1:E:115:CYS:HB3	1:E:120:GLU:CG	2.42	0.50
1:I:29:VAL:HG13	1:I:40:LEU:HB3	1.93	0.50
1:G:274:PRO:C	1:G:276:LEU:N	2.64	0.50
1:K:251:HIS:HD2	11:K:823:HOH:O	1.93	0.50
1:E:110:HIS:O	1:E:111:GLN:HB2	2.10	0.50
1:C:200:GLN:HE21	1:C:203:HIS:HB2	1.77	0.50
1:O:259:ASN:ND2	2:P:501:LYS:N	2.60	0.50
1:I:256:PHE:HB2	1:I:261:ILE:HD11	1.94	0.50
1:I:161:ASN:HD21	1:I:164:THR:H	1.58	0.50
1:O:246:MET:HE1	1:O:252:LEU:HG	1.94	0.50
1:I:226:THR:HG22	1:I:262:ASP:HB3	1.94	0.50
1:E:32:TRP:CG	1:E:62:LYS:HB3	2.46	0.49
1:I:149:TYR:O	1:I:150:LEU:HD13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:508:TYR:HD2	2:J:512:SER:HB3	1.76	0.49
1:A:61:LEU:CA	1:I:61:LEU:CA	2.90	0.49
1:K:190:ASN:HB3	1:K:192:ARG:H	1.76	0.49
1:C:104:SER:OG	1:C:106:GLU:HG2	2.13	0.49
1:E:54:THR:CG2	1:E:120:GLU:OE1	2.59	0.49
1:K:207:SER:HA	1:K:210:THR:HG22	1.93	0.49
1:C:121:GLN:NE2	1:C:153:CYS:HB3	2.27	0.49
1:K:192:ARG:HH12	1:K:268:LYS:HZ3	1.60	0.49
1:C:268:LYS:O	1:C:271:CYS:SG	2.70	0.49
1:M:33:GLU:O	1:M:34:GLU:HB2	2.12	0.49
1:K:126:VAL:HG13	1:K:167:PHE:HB3	1.94	0.49
1:G:53:ARG:HG3	2:H:505:PHE:CE2	2.48	0.49
1:K:7:LYS:HD3	10:K:803:SO4:O4	2.12	0.49
1:O:190:ASN:HD21	1:O:217:GLY:N	2.11	0.49
1:I:204:GLY:O	1:I:209:GLU:HB3	2.13	0.49
1:I:108:GLY:O	1:I:111:GLN:HB2	2.12	0.49
1:K:157:ASN:HA	1:K:243:THR:HG21	1.95	0.49
1:O:29:VAL:HG13	1:O:40:LEU:HB2	1.94	0.49
1:C:9:ASN:H	1:C:9:ASN:ND2	2.10	0.49
1:M:73:LEU:O	1:M:74:ASP:C	2.51	0.49
1:E:22:ASP:OD2	1:E:48:SER:HA	2.12	0.49
1:G:158:GLY:N	1:G:246:MET:HE3	2.28	0.48
1:G:25:ARG:HA	1:G:69:VAL:O	2.13	0.48
9:M:316:NDG:H2	9:M:316:NDG:H8C1	1.60	0.48
1:A:60:GLY:O	1:I:61:LEU:O	2.31	0.48
1:K:63:ILE:HD11	1:K:113:LEU:HD21	1.94	0.48
1:I:247:CYS:HA	1:I:263:VAL:CG2	2.43	0.48
2:L:504:ALC:HE23	1:M:14:VAL:HG21	1.94	0.48
1:K:243:THR:HG23	1:K:245:SER:OG	2.13	0.48
1:A:231:PRO:HD3	1:C:19:LEU:HB2	1.96	0.48
1:A:251:HIS:CE1	1:A:252:LEU:HD22	2.48	0.48
1:A:51:THR:HG21	11:A:815:HOH:O	2.13	0.48
1:G:94:GLU:CD	1:G:175:LYS:HD2	2.34	0.48
1:C:230:GLU:HB2	1:E:18:ALA:HB2	1.95	0.48
1:A:51:THR:HG22	1:A:52:ASN:N	2.29	0.48
1:A:54:THR:HG21	1:A:120:GLU:OE1	2.14	0.48
1:C:55:LEU:HB3	1:C:66:LEU:CD2	2.25	0.48
1:I:246:MET:CE	1:I:252:LEU:HG	2.43	0.48
1:E:27:THR:OG1	1:E:68:GLU:HG3	2.13	0.48
1:M:8:THR:HG22	1:O:10:GLY:O	2.14	0.48
1:O:43:LYS:NZ	11:O:879:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:222:CYS:HB3	1:K:272:ASN:HB3	1.95	0.48
1:O:55:LEU:C	1:O:55:LEU:HD23	2.34	0.47
1:I:203:HIS:CG	1:I:204:GLY:N	2.82	0.47
2:B:501:LYS:HB3	1:C:16:GLU:OE2	2.14	0.47
1:K:268:LYS:HA	1:K:268:LYS:HD2	1.51	0.47
1:G:61:LEU:O	1:K:60:GLY:O	2.33	0.47
1:I:114:GLN:HB2	1:I:114:GLN:HE21	1.56	0.47
1:C:27:THR:OG1	1:C:68:GLU:HG2	2.13	0.47
1:K:190:ASN:ND2	1:K:219:MET:O	2.47	0.47
1:A:67:THR:OG1	1:A:81:SER:CB	2.63	0.47
1:E:176:CYS:SG	1:E:177:ASN:N	2.85	0.47
1:O:123:LEU:O	1:O:145:ARG:HA	2.14	0.47
1:M:251:HIS:CD2	1:M:252:LEU:HD13	2.50	0.47
1:I:104:SER:O	1:I:108:GLY:HA3	2.14	0.47
1:E:54:THR:HB	1:E:149:TYR:HB3	1.96	0.47
1:I:273:HIS:HD2	1:I:275:ASP:H	1.59	0.47
2:N:507:DLY:O	2:N:511:SER:HB2	2.15	0.47
1:I:56:SER:HB2	1:I:147:CYS:HB2	1.96	0.47
1:E:239:ARG:NH2	1:E:274:PRO:HA	2.30	0.47
1:C:53:ARG:HG3	2:D:505:PHE:CE2	2.50	0.47
1:G:218:PRO:O	1:G:243:THR:HG22	2.16	0.46
1:G:21:GLN:HG2	1:G:45:CYS:HB3	1.96	0.46
1:A:43:LYS:O	1:A:44:SER:HB3	2.15	0.46
1:I:2:ARG:HA	1:I:15:GLU:O	2.16	0.46
1:O:5:GLN:NE2	11:O:898:HOH:O	2.48	0.46
1:A:157:ASN:HD22	1:A:245:SER:CB	2.28	0.46
1:O:157:ASN:HD22	1:O:245:SER:CB	2.28	0.46
1:K:66:LEU:HD23	2:L:505:PHE:HD1	1.79	0.46
1:G:2:ARG:HA	1:G:15:GLU:O	2.16	0.46
1:M:100:SER:O	1:M:101:SER:C	2.54	0.46
1:A:249:HIS:HB2	1:A:252:LEU:HD23	1.97	0.46
1:G:32:TRP:CD2	1:G:62:LYS:HB3	2.49	0.46
1:C:8:THR:HG23	1:E:11:ASP:HA	1.97	0.46
1:G:122:CYS:O	1:G:170:CYS:HA	2.15	0.46
1:A:222:CYS:HB2	1:A:271:CYS:SG	2.56	0.46
1:G:239:ARG:NH2	1:G:274:PRO:HA	2.31	0.46
1:E:259:ASN:O	1:E:261:ILE:N	2.48	0.46
9:O:319:MAN:H62	11:O:814:HOH:O	2.15	0.46
1:C:8:THR:CG2	1:E:12:CYS:N	2.64	0.46
1:G:276:LEU:HD11	11:G:901:HOH:O	2.15	0.46
1:C:268:LYS:HG2	1:C:271:CYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:272:ASN:H	1:M:272:ASN:HD22	1.63	0.45
1:K:9:ASN:ND2	1:K:11:ASP:H	2.15	0.45
1:A:40:LEU:HD23	2:B:504:ALC:HZ2	1.97	0.45
1:A:34:GLU:O	11:A:834:HOH:O	2.21	0.45
1:C:29:VAL:HG13	1:C:66:LEU:CD1	2.46	0.45
1:K:53:ARG:HG2	1:K:68:GLU:HB2	1.97	0.45
1:C:266:CYS:HB2	1:C:268:LYS:HE2	1.98	0.45
2:L:503:ASP:HB3	11:L:745:HOH:O	2.15	0.45
1:I:246:MET:HE1	1:I:252:LEU:HG	1.98	0.45
1:G:255:ALA:HB2	2:H:510:TRP:CE2	2.52	0.45
1:M:169:LYS:HE2	1:M:169:LYS:HB3	1.78	0.45
1:K:123:LEU:HD22	1:K:123:LEU:HA	1.82	0.45
1:A:7:LYS:HB2	1:A:9:ASN:HB2	1.98	0.45
1:C:8:THR:HG23	1:E:10:GLY:O	2.16	0.45
1:E:34:GLU:HG3	1:E:35:GLY:N	2.31	0.45
1:E:7:LYS:HB2	1:E:9:ASN:HB2	1.98	0.45
1:M:243:THR:O	1:M:246:MET:HB2	2.16	0.45
1:I:25:ARG:HH22	1:I:42:GLU:CD	2.19	0.45
1:K:32:TRP:CG	1:K:62:LYS:HB3	2.52	0.45
1:E:249:HIS:HB3	1:E:251:HIS:CD2	2.51	0.45
1:A:33:GLU:HG2	1:C:78:GLN:O	2.16	0.45
1:A:230:GLU:HA	1:A:231:PRO:C	2.37	0.45
1:E:89:ARG:N	11:E:851:HOH:O	2.49	0.45
1:O:195:TYR:H	1:O:272:ASN:ND2	2.15	0.45
1:M:208:GLU:HG3	1:M:209:GLU:N	2.31	0.45
1:E:34:GLU:OE1	1:E:34:GLU:HA	2.17	0.45
1:C:192:ARG:CD	1:C:220:ASN:O	2.64	0.45
1:C:158:GLY:H	1:C:243:THR:HG22	1.82	0.45
1:A:25:ARG:HH21	1:A:42:GLU:HG2	1.83	0.45
1:K:223:LEU:HD12	1:K:265:CYS:SG	2.57	0.45
1:M:150:LEU:HB2	1:M:153:CYS:SG	2.57	0.45
1:O:246:MET:CE	1:O:252:LEU:HG	2.46	0.44
1:K:230:GLU:HA	1:K:231:PRO:HA	1.77	0.44
1:O:181:ILE:H	1:O:181:ILE:HG13	1.64	0.44
1:I:251:HIS:CD2	1:I:252:LEU:HD13	2.52	0.44
1:M:178:GLU:HB3	11:M:823:HOH:O	2.17	0.44
1:E:23:LEU:HB3	1:E:70:VAL:HG22	1.99	0.44
1:O:160:HIS:CE1	1:O:216:ARG:H	2.35	0.44
1:M:261:ILE:HG22	11:M:849:HOH:O	2.15	0.44
1:C:140:ASP:OD2	1:E:73:LEU:HD23	2.18	0.44
2:B:504:ALC:HE12	1:C:14:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:CYS:SG	1:I:145:ARG:HG3	2.57	0.44
1:I:239:ARG:HD3	1:I:272:ASN:CB	2.42	0.44
1:C:7:LYS:HB2	1:C:9:ASN:ND2	2.32	0.44
1:A:29:VAL:CG1	1:A:40:LEU:HB2	2.47	0.44
1:E:115:CYS:HB3	1:E:120:GLU:HG3	1.99	0.44
1:O:158:GLY:H	1:O:243:THR:CG2	2.31	0.44
1:O:243:THR:CG2	1:O:245:SER:HB2	2.46	0.44
1:O:207:SER:C	1:O:209:GLU:N	2.70	0.44
1:I:83:ARG:O	1:I:84:ALA:CB	2.65	0.44
1:I:198:LYS:HG2	1:I:236:TYR:CE1	2.53	0.44
1:O:225:ALA:HA	1:O:262:ASP:O	2.17	0.44
1:A:128:HIS:ND1	1:A:141:ASP:OD1	2.51	0.44
1:M:109:ARG:HB3	1:M:110:HIS:H	1.44	0.44
1:M:168:LEU:HD23	1:M:168:LEU:C	2.37	0.44
1:K:243:THR:CG2	1:K:245:SER:OG	2.66	0.44
1:I:161:ASN:HD22	1:I:164:THR:H	1.64	0.44
1:K:9:ASN:HD21	1:K:11:ASP:CB	2.30	0.44
1:E:5:GLN:O	1:E:12:CYS:HA	2.18	0.43
1:I:203:HIS:CD2	1:I:204:GLY:H	2.36	0.43
1:C:273:HIS:CB	1:C:274:PRO:CD	2.70	0.43
1:G:109:ARG:HH11	1:G:180:PRO:HA	1.83	0.43
9:I:316:NDG:H8C1	9:I:316:NDG:H2	1.69	0.43
1:I:122:CYS:O	1:I:170:CYS:HA	2.19	0.43
1:A:5:GLN:O	1:A:12:CYS:HA	2.19	0.43
1:G:145:ARG:HD3	1:G:177:ASN:O	2.18	0.43
1:E:28:ILE:HG12	1:E:41:VAL:HG22	1.99	0.43
1:K:109:ARG:O	1:K:110:HIS:CB	2.65	0.43
1:G:221:GLN:NE2	1:G:244:ALA:HB2	2.34	0.43
1:C:13:ARG:NH2	1:C:15:GLU:HA	2.34	0.43
1:A:28:ILE:O	1:A:66:LEU:HA	2.17	0.43
1:A:101:SER:N	2:B:513:LYS:O	2.51	0.43
1:O:167:PHE:HE2	1:O:169:LYS:HG3	1.83	0.43
2:B:508:TYR:CD2	2:B:512:SER:CB	3.01	0.43
1:O:158:GLY:CA	1:O:246:MET:HE3	2.49	0.43
1:K:55:LEU:O	1:K:66:LEU:N	2.42	0.43
1:M:223:LEU:HA	1:M:264:SER:O	2.19	0.43
1:A:75:LEU:O	1:A:77:ASN:N	2.51	0.43
6:M:314:NAG:O4	11:M:834:HOH:O	2.21	0.43
1:C:185:GLU:CD	1:C:185:GLU:H	2.22	0.43
1:O:1:LEU:HD23	1:O:74:ASP:OD1	2.19	0.43
1:K:32:TRP:CZ2	1:K:37:GLU:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:158:GLY:O	1:M:246:MET:HG3	2.19	0.43
2:D:505:PHE:O	2:D:506:DSN:C	2.66	0.43
1:I:126:VAL:HA	1:I:142:ARG:O	2.18	0.43
1:C:158:GLY:H	1:C:243:THR:CG2	2.32	0.43
2:D:501:LYS:NZ	11:D:350:HOH:O	0.58	0.43
1:E:228:THR:OG1	1:E:259:ASN:HB2	2.19	0.43
1:G:28:ILE:HG12	1:G:41:VAL:HG22	2.01	0.43
1:C:167:PHE:HE2	1:C:169:LYS:HB2	1.84	0.42
1:K:230:GLU:HG3	1:M:17:CYS:O	2.19	0.42
1:I:195:TYR:HA	1:I:211:PHE:O	2.19	0.42
1:K:54:THR:HB	1:K:149:TYR:HB3	2.01	0.42
1:A:53:ARG:CZ	1:A:251:HIS:HB3	2.49	0.42
1:C:222:CYS:HB2	1:C:271:CYS:SG	2.59	0.42
1:A:200:GLN:N	1:A:203:HIS:O	2.52	0.42
1:A:187:LEU:O	1:A:216:ARG:HD3	2.19	0.42
1:G:9:ASN:HD22	1:G:9:ASN:N	2.17	0.42
1:C:7:LYS:HB2	1:C:9:ASN:HD21	1.84	0.42
1:C:199:GLY:HA2	1:C:236:TYR:CE2	2.54	0.42
1:M:268:LYS:HE3	1:M:269:SER:H	1.84	0.42
1:C:255:ALA:HB2	2:D:510:TRP:CE2	2.54	0.42
1:K:150:LEU:HD23	1:K:251:HIS:CE1	2.55	0.42
1:E:251:HIS:CE1	1:E:252:LEU:HD13	2.55	0.42
7:G:316:NAG:H62	7:G:317:NAG:N2	2.35	0.42
9:K:317:NDG:H8C1	9:K:317:NDG:H2	1.67	0.42
1:C:272:ASN:N	1:C:272:ASN:HD22	2.13	0.42
1:I:123:LEU:CD2	1:I:170:CYS:HB3	2.45	0.42
1:K:251:HIS:CD2	11:K:823:HOH:O	2.70	0.42
1:A:127:THR:HG23	1:A:166:HIS:CE1	2.55	0.42
1:G:252:LEU:HA	1:G:252:LEU:HD12	1.90	0.42
1:O:222:CYS:O	1:O:265:CYS:HA	2.20	0.42
1:E:121:GLN:NE2	1:E:153:CYS:HB3	2.35	0.41
1:I:67:THR:HG21	1:I:84:ALA:HB1	2.01	0.41
1:I:161:ASN:ND2	1:I:163:ASP:H	2.18	0.41
1:O:252:LEU:HD12	1:O:252:LEU:HA	1.90	0.41
2:B:505:PHE:O	2:B:506:DSN:C	2.68	0.41
1:K:5:GLN:O	1:K:12:CYS:HA	2.19	0.41
1:A:94:GLU:HB3	1:A:174:THR:HG23	2.01	0.41
1:K:128:HIS:CD2	1:K:141:ASP:OD1	2.73	0.41
1:A:249:HIS:HB2	1:A:252:LEU:CD2	2.50	0.41
1:K:207:SER:O	1:K:208:GLU:HB3	2.20	0.41
1:G:139:LYS:HD3	11:G:899:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:ASN:OD1	6:E:321:NAG:O5	2.39	0.41
1:G:145:ARG:HB3	1:G:177:ASN:ND2	2.36	0.41
1:E:126:VAL:HG13	1:E:167:PHE:HB3	2.03	0.41
1:M:116:ARG:HD3	11:M:863:HOH:O	2.21	0.41
1:G:60:GLY:C	1:G:62:LYS:H	2.22	0.41
1:O:230:GLU:HA	1:O:231:PRO:C	2.41	0.41
1:M:258:MET:HG3	1:M:261:ILE:HD12	2.03	0.41
1:I:198:LYS:HG2	1:I:236:TYR:HE1	1.85	0.41
1:O:185:GLU:HG2	1:O:186:ASN:N	2.36	0.41
1:O:34:GLU:HB3	1:O:35:GLY:H	1.68	0.41
1:O:75:LEU:C	1:O:77:ASN:N	2.73	0.41
1:K:123:LEU:CD2	1:K:170:CYS:HB3	2.50	0.41
1:M:204:GLY:O	1:M:209:GLU:HB3	2.21	0.41
1:E:100:SER:O	1:E:101:SER:C	2.59	0.41
1:K:199:GLY:HA2	1:K:236:TYR:CE2	2.55	0.41
6:I:314:NAG:H2	6:I:314:NAG:H82	1.91	0.41
1:M:128:HIS:HD2	1:M:141:ASP:OD1	2.03	0.41
1:I:249:HIS:HB2	1:I:252:LEU:HD22	2.03	0.41
1:O:160:HIS:HE1	1:O:215:CYS:HA	1.85	0.41
1:I:247:CYS:SG	1:I:265:CYS:N	2.94	0.41
2:P:513:LYS:NZ	11:P:260:HOH:O	2.53	0.41
1:M:53:ARG:NH2	10:M:811:SO4:O3	2.54	0.41
1:A:142:ARG:NH2	1:A:144:LEU:HD22	2.35	0.41
1:O:197:CYS:CB	1:O:210:THR:HG22	2.51	0.41
1:I:208:GLU:OE1	1:I:209:GLU:HB2	2.21	0.41
1:K:250:ALA:N	10:K:810:SO4:O1	2.54	0.41
2:D:501:LYS:HB2	1:E:13:ARG:HH21	1.86	0.41
1:E:171:CYS:SG	1:E:172:ASN:N	2.90	0.41
1:C:200:GLN:H	1:C:200:GLN:CD	2.24	0.41
1:E:60:GLY:O	1:M:61:LEU:CA	2.68	0.41
1:A:47:HIS:CD2	1:A:47:HIS:H	2.39	0.41
1:A:5:GLN:OE1	1:A:13:ARG:HD2	2.21	0.40
1:M:268:LYS:O	1:M:271:CYS:SG	2.79	0.40
1:I:43:LYS:O	1:I:44:SER:HB3	2.20	0.40
1:I:239:ARG:CD	1:I:272:ASN:HB3	2.44	0.40
1:I:243:THR:O	1:I:246:MET:HB2	2.21	0.40
1:I:100:SER:O	1:I:101:SER:C	2.59	0.40
1:E:142:ARG:NH2	1:E:144:LEU:HG	2.35	0.40
1:E:53:ARG:HH11	1:E:251:HIS:HB3	1.86	0.40
1:G:182:LEU:HA	1:G:182:LEU:HD13	1.87	0.40
1:G:206:SER:O	1:G:207:SER:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:LEU:HD21	1:I:187:LEU:HD21	2.03	0.40
1:K:32:TRP:CH2	1:K:37:GLU:HG2	2.56	0.40
1:I:29:VAL:HB	1:I:66:LEU:CD1	2.50	0.40
1:G:182:LEU:CD1	1:G:187:LEU:HD21	2.52	0.40
1:K:95:CYS:O	1:K:113:LEU:N	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/313 (84%)	231 (88%)	16 (6%)	15 (6%)	2	3
1	C	253/313 (81%)	226 (89%)	16 (6%)	11 (4%)	3	7
1	E	256/313 (82%)	229 (90%)	22 (9%)	5 (2%)	9	24
1	G	252/313 (80%)	233 (92%)	16 (6%)	3 (1%)	16	39
1	I	258/313 (82%)	228 (88%)	23 (9%)	7 (3%)	6	16
1	K	251/313 (80%)	227 (90%)	20 (8%)	4 (2%)	12	30
1	M	257/313 (82%)	230 (90%)	15 (6%)	12 (5%)	3	5
1	O	252/313 (80%)	223 (88%)	20 (8%)	9 (4%)	4	9
2	B	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	D	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	F	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	H	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	J	8/13 (62%)	7 (88%)	0	1 (12%)	0	0
2	L	8/13 (62%)	7 (88%)	0	1 (12%)	0	0
2	N	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	P	8/13 (62%)	8 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2105/2608 (81%)	1884 (90%)	153 (7%)	68 (3%)	5	12

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	PRO
1	A	231	PRO
1	A	276	LEU
1	C	208	GLU
1	C	273	HIS
1	E	111	GLN
1	E	259	ASN
1	I	33	GLU
1	I	101	SER
1	M	101	SER
1	O	203	HIS
1	O	206	SER
1	O	208	GLU
1	O	232	LYS
1	A	61	LEU
1	A	177	ASN
1	C	109	ARG
1	C	207	SER
1	G	275	ASP
1	I	84	ALA
1	I	208	GLU
1	K	275	ASP
1	M	91	ARG
1	M	207	SER
1	M	276	LEU
1	O	109	ARG
1	A	234	GLN
1	A	235	SER
1	A	278	VAL
1	E	61	LEU
1	K	206	SER
1	M	60	GLY
1	M	105	CYS
1	M	106	GLU
1	M	208	GLU
1	M	274	PRO
1	A	90	SER

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Mol	Chain	Res	Type
1	A	107	ARG
1	A	273	HIS
1	C	61	LEU
1	C	231	PRO
1	G	207	SER
1	I	60	GLY
1	I	117	SER
1	K	231	PRO
1	M	109	ARG
1	O	204	GLY
1	A	75	LEU
1	C	34	GLU
1	C	60	GLY
1	C	79	GLY
1	C	101	SER
1	C	107	ARG
1	I	35	GLY
1	O	106	GLU
1	A	76	CYS
1	A	233	ASN
1	E	260	HIS
2	J	502	SER
2	L	502	SER
1	M	111	GLN
1	M	206	SER
1	O	60	GLY
1	O	274	PRO
1	E	60	GLY
1	G	108	GLY
1	K	60	GLY
1	A	60	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	234/273 (86%)	208 (89%)	26 (11%)	8 17
1	C	229/273 (84%)	192 (84%)	37 (16%)	3 7
1	E	232/273 (85%)	200 (86%)	32 (14%)	4 10
1	G	229/273 (84%)	188 (82%)	41 (18%)	2 5
1	I	230/273 (84%)	183 (80%)	47 (20%)	1 4
1	K	228/273 (84%)	194 (85%)	34 (15%)	4 9
1	M	234/273 (86%)	196 (84%)	38 (16%)	3 7
1	O	228/273 (84%)	198 (87%)	30 (13%)	5 12
2	B	10/10 (100%)	8 (80%)	2 (20%)	1 4
2	D	10/10 (100%)	10 (100%)	0	100 100
2	F	10/10 (100%)	10 (100%)	0	100 100
2	H	10/10 (100%)	8 (80%)	2 (20%)	1 4
2	J	10/10 (100%)	9 (90%)	1 (10%)	9 22
2	L	10/10 (100%)	8 (80%)	2 (20%)	1 4
2	N	10/10 (100%)	10 (100%)	0	100 100
2	P	10/10 (100%)	10 (100%)	0	100 100
All	All	1924/2264 (85%)	1632 (85%)	292 (15%)	3 9

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	9	ASN
1	A	25	ARG
1	A	26	THR
1	A	31	LEU
1	A	33	GLU
1	A	40	LEU
1	A	54	THR
1	A	55	LEU
1	A	77	ASN
1	A	78	GLN
1	A	125	VAL
1	A	126	VAL
1	A	140	ASP

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Mol	Chain	Res	Type
1	A	141	ASP
1	A	164	THR
1	A	176	CYS
1	A	177	ASN
1	A	185	GLU
1	A	203	HIS
1	A	226	THR
1	A	234	GLN
1	A	252	LEU
1	A	260	HIS
1	A	266	CYS
1	A	267	THR
2	B	502	SER
2	B	512	SER
1	C	1	LEU
1	C	8	THR
1	C	9	ASN
1	C	13	ARG
1	C	19	LEU
1	C	25	ARG
1	C	31	LEU
1	C	38	LEU
1	C	40	LEU
1	C	53	ARG
1	C	55	LEU
1	C	58	ARG
1	C	59	THR
1	C	65	SER
1	C	66	LEU
1	C	70	VAL
1	C	73	LEU
1	C	77	ASN
1	C	105	CYS
1	C	109	ARG
1	C	125	VAL
1	C	126	VAL
1	C	140	ASP
1	C	141	ASP
1	C	185	GLU
1	C	192	ARG
1	C	200	GLN
1	C	202	THR

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Mol	Chain	Res	Type
1	C	207	SER
1	C	209	GLU
1	C	219	MET
1	C	232	LYS
1	C	238	VAL
1	C	252	LEU
1	C	263	VAL
1	C	268	LYS
1	C	272	ASN
1	E	1	LEU
1	E	9	ASN
1	E	19	LEU
1	E	21	GLN
1	E	22	ASP
1	E	25	ARG
1	E	31	LEU
1	E	38	LEU
1	E	40	LEU
1	E	53	ARG
1	E	54	THR
1	E	55	LEU
1	E	58	ARG
1	E	59	THR
1	E	93	LEU
1	E	106	GLU
1	E	111	GLN
1	E	112	SER
1	E	125	VAL
1	E	126	VAL
1	E	163	ASP
1	E	164	THR
1	E	171	CYS
1	E	182	LEU
1	E	183	GLU
1	E	184	LEU
1	E	209	GLU
1	E	229	HIS
1	E	233	ASN
1	E	238	VAL
1	E	252	LEU
1	E	276	LEU
1	G	1	LEU

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Mol	Chain	Res	Type
1	G	2	ARG
1	G	8	THR
1	G	9	ASN
1	G	19	LEU
1	G	25	ARG
1	G	29	VAL
1	G	31	LEU
1	G	38	LEU
1	G	40	LEU
1	G	53	ARG
1	G	55	LEU
1	G	59	THR
1	G	65	SER
1	G	67	THR
1	G	77	ASN
1	G	93	LEU
1	G	107	ARG
1	G	116	ARG
1	G	125	VAL
1	G	126	VAL
1	G	130	ILE
1	G	131	GLN
1	G	140	ASP
1	G	164	THR
1	G	169	LYS
1	G	170	CYS
1	G	182	LEU
1	G	193	GLN
1	G	200	GLN
1	G	202	THR
1	G	203	HIS
1	G	205	CYS
1	G	210	THR
1	G	212	LEU
1	G	226	THR
1	G	234	GLN
1	G	238	VAL
1	G	252	LEU
1	G	272	ASN
1	G	276	LEU
2	H	502	SER
2	H	512	SER

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Mol	Chain	Res	Type
1	I	1	LEU
1	I	8	THR
1	I	19	LEU
1	I	21	GLN
1	I	29	VAL
1	I	34	GLU
1	I	38	LEU
1	I	49	GLU
1	I	53	ARG
1	I	54	THR
1	I	55	LEU
1	I	58	ARG
1	I	59	THR
1	I	69	VAL
1	I	70	VAL
1	I	73	LEU
1	I	77	ASN
1	I	107	ARG
1	I	111	GLN
1	I	114	GLN
1	I	116	ARG
1	I	117	SER
1	I	123	LEU
1	I	125	VAL
1	I	126	VAL
1	I	131	GLN
1	I	144	LEU
1	I	150	LEU
1	I	161	ASN
1	I	175	LYS
1	I	182	LEU
1	I	190	ASN
1	I	193	GLN
1	I	202	THR
1	I	203	HIS
1	I	206	SER
1	I	207	SER
1	I	210	THR
1	I	216	ARG
1	I	224	VAL
1	I	243	THR
1	I	252	LEU

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Mol	Chain	Res	Type
1	I	257	SER
1	I	261	ILE
1	I	263	VAL
1	I	267	THR
1	I	268	LYS
2	J	513	LYS
1	K	1	LEU
1	K	8	THR
1	K	9	ASN
1	K	19	LEU
1	K	25	ARG
1	K	31	LEU
1	K	36	GLU
1	K	40	LEU
1	K	54	THR
1	K	55	LEU
1	K	58	ARG
1	K	63	ILE
1	K	66	LEU
1	K	70	VAL
1	K	106	GLU
1	K	113	LEU
1	K	116	ARG
1	K	123	LEU
1	K	125	VAL
1	K	126	VAL
1	K	163	ASP
1	K	169	LYS
1	K	176	CYS
1	K	182	LEU
1	K	187	LEU
1	K	189	GLN
1	K	193	GLN
1	K	206	SER
1	K	212	LEU
1	K	235	SER
1	K	239	ARG
1	K	243	THR
1	K	258	MET
1	K	268	LYS
2	L	502	SER
2	L	503	ASP

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Mol	Chain	Res	Type
1	M	9	ASN
1	M	13	ARG
1	M	25	ARG
1	M	29	VAL
1	M	37	GLU
1	M	38	LEU
1	M	40	LEU
1	M	53	ARG
1	M	55	LEU
1	M	59	THR
1	M	69	VAL
1	M	70	VAL
1	M	91	ARG
1	M	102	ASP
1	M	103	MET
1	M	114	GLN
1	M	123	LEU
1	M	125	VAL
1	M	126	VAL
1	M	150	LEU
1	M	169	LYS
1	M	170	CYS
1	M	184	LEU
1	M	185	GLU
1	M	187	LEU
1	M	192	ARG
1	M	193	GLN
1	M	198	LYS
1	M	201	SER
1	M	213	ILE
1	M	232	LYS
1	M	234	GLN
1	M	235	SER
1	M	252	LEU
1	M	261	ILE
1	M	263	VAL
1	M	268	LYS
1	M	272	ASN
1	O	1	LEU
1	O	13	ARG
1	O	15	GLU
1	O	31	LEU

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Mol	Chain	Res	Type
1	O	36	GLU
1	O	40	LEU
1	O	56	SER
1	O	63	ILE
1	O	67	THR
1	O	70	VAL
1	O	77	ASN
1	O	102	ASP
1	O	104	SER
1	O	114	GLN
1	O	116	ARG
1	O	125	VAL
1	O	126	VAL
1	O	176	CYS
1	O	182	LEU
1	O	185	GLU
1	O	187	LEU
1	O	192	ARG
1	O	206	SER
1	O	208	GLU
1	O	216	ARG
1	O	230	GLU
1	O	234	GLN
1	O	252	LEU
1	O	261	ILE
1	O	271	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	47	HIS
1	A	78	GLN
1	A	111	GLN
1	A	143	HIS
1	A	157	ASN
1	A	160	HIS
1	A	203	HIS
1	A	272	ASN
1	C	9	ASN
1	C	78	GLN
1	C	111	GLN

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Mol	Chain	Res	Type
1	C	121	GLN
1	C	157	ASN
1	C	186	ASN
1	C	193	GLN
1	C	200	GLN
1	C	260	HIS
1	C	272	ASN
1	E	121	GLN
1	E	128	HIS
1	E	157	ASN
1	E	233	ASN
1	E	249	HIS
1	E	251	HIS
1	E	259	ASN
1	G	9	ASN
1	G	21	GLN
1	G	77	ASN
1	G	78	GLN
1	G	111	GLN
1	G	121	GLN
1	G	131	GLN
1	G	157	ASN
1	G	160	HIS
1	G	200	GLN
1	G	251	HIS
1	G	272	ASN
1	I	77	ASN
1	I	114	GLN
1	I	121	GLN
1	I	157	ASN
1	I	161	ASN
1	I	190	ASN
1	I	193	GLN
1	I	203	HIS
1	I	259	ASN
1	I	273	HIS
1	K	9	ASN
1	K	21	GLN
1	K	47	HIS
1	K	114	GLN
1	K	121	GLN
1	K	128	HIS

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Mol	Chain	Res	Type
1	K	157	ASN
1	K	160	HIS
1	K	186	ASN
1	K	190	ASN
1	K	193	GLN
1	K	221	GLN
1	K	251	HIS
1	M	9	ASN
1	M	21	GLN
1	M	80	ASN
1	M	121	GLN
1	M	128	HIS
1	M	131	GLN
1	M	157	ASN
1	M	259	ASN
1	M	272	ASN
1	O	21	GLN
1	O	77	ASN
1	O	121	GLN
1	O	157	ASN
1	O	160	HIS
1	O	189	GLN
1	O	190	ASN
1	O	203	HIS
1	O	272	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

24 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ALC	B	504	2	10,11,12	0.41	0	10,13,15	1.48	2 (20%)
2	DSN	B	506	2	4,5,6	0.66	0	2,5,7	1.25	0
2	DLY	B	507	2	7,8,9	0.47	0	6,8,10	0.90	0
2	ALC	D	504	2	10,11,12	0.52	0	10,13,15	1.70	2 (20%)
2	DSN	D	506	2	4,5,6	0.67	0	2,5,7	1.42	1 (50%)
2	DLY	D	507	2	7,8,9	0.47	0	6,8,10	0.75	0
2	ALC	F	504	2	10,11,12	0.43	0	10,13,15	1.40	2 (20%)
2	DSN	F	506	2	4,5,6	0.58	0	2,5,7	1.07	0
2	DLY	F	507	2	7,8,9	0.51	0	6,8,10	0.87	0
2	ALC	H	504	2	10,11,12	0.50	0	10,13,15	1.88	3 (30%)
2	DSN	H	506	2	4,5,6	0.64	0	2,5,7	1.43	0
2	DLY	H	507	2	7,8,9	0.59	0	6,8,10	0.69	0
2	ALC	J	504	2	10,11,12	0.49	0	10,13,15	2.27	6 (60%)
2	DSN	J	506	2	4,5,6	0.65	0	2,5,7	1.58	0
2	DLY	J	507	2	7,8,9	0.52	0	6,8,10	0.88	0
2	ALC	L	504	2	10,11,12	0.53	0	10,13,15	1.17	2 (20%)
2	DSN	L	506	2	4,5,6	0.42	0	2,5,7	1.85	0
2	DLY	L	507	2	7,8,9	0.42	0	6,8,10	1.00	1 (16%)
2	ALC	N	504	2	10,11,12	0.47	0	10,13,15	2.18	4 (40%)
2	DSN	N	506	2	4,5,6	0.60	0	2,5,7	1.51	0
2	DLY	N	507	2	7,8,9	0.39	0	6,8,10	0.70	0
2	ALC	P	504	2	10,11,12	0.52	0	10,13,15	1.02	0
2	DSN	P	506	2	4,5,6	0.43	0	2,5,7	1.62	0
2	DLY	P	507	2	7,8,9	0.48	0	6,8,10	0.90	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALC	B	504	2	-	0/4/14/16	0/1/1/1
2	DSN	B	506	2	-	0/2/4/6	0/0/0/0
2	DLY	B	507	2	-	0/5/7/9	0/0/0/0
2	ALC	D	504	2	-	0/4/14/16	0/1/1/1
2	DSN	D	506	2	-	0/2/4/6	0/0/0/0
2	DLY	D	507	2	-	0/5/7/9	0/0/0/0
2	ALC	F	504	2	-	0/4/14/16	0/1/1/1
2	DSN	F	506	2	-	0/2/4/6	0/0/0/0
2	DLY	F	507	2	-	0/5/7/9	0/0/0/0
2	ALC	H	504	2	-	0/4/14/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DSN	H	506	2	-	0/2/4/6	0/0/0/0
2	DLY	H	507	2	-	0/5/7/9	0/0/0/0
2	ALC	J	504	2	-	0/4/14/16	0/1/1/1
2	DSN	J	506	2	-	0/2/4/6	0/0/0/0
2	DLY	J	507	2	-	0/5/7/9	0/0/0/0
2	ALC	L	504	2	-	0/4/14/16	0/1/1/1
2	DSN	L	506	2	-	0/2/4/6	0/0/0/0
2	DLY	L	507	2	-	0/5/7/9	0/0/0/0
2	ALC	N	504	2	-	0/4/14/16	0/1/1/1
2	DSN	N	506	2	-	0/2/4/6	0/0/0/0
2	DLY	N	507	2	-	0/5/7/9	0/0/0/0
2	ALC	P	504	2	-	0/4/14/16	0/1/1/1
2	DSN	P	506	2	-	0/2/4/6	0/0/0/0
2	DLY	P	507	2	-	0/5/7/9	0/0/0/0

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	504	ALC	CB-CG-CD1	-4.15	101.82	111.67
2	J	504	ALC	CB-CG-CD1	-3.28	103.90	111.67
2	N	504	ALC	CB-CG-CD1	-3.16	104.18	111.67
2	B	504	ALC	CB-CG-CD2	-2.76	105.13	111.67
2	D	504	ALC	CB-CG-CD1	-2.71	105.24	111.67
2	J	504	ALC	O-C-CA	-2.27	119.58	125.49
2	L	504	ALC	CB-CA-N	-2.27	104.27	109.91
2	H	504	ALC	CB-CG-CD2	-2.10	106.69	111.67
2	L	504	ALC	O-C-CA	-2.10	120.03	125.49
2	F	504	ALC	CB-CA-N	-2.10	104.70	109.91
2	B	504	ALC	O-C-CA	-2.09	120.05	125.49
2	J	504	ALC	CZ-CE2-CD2	-2.04	107.16	111.44
2	L	507	DLY	O-C-CA	-2.03	120.21	125.49
2	F	504	ALC	O-C-CA	-2.01	120.24	125.49
2	D	506	DSN	O-C-CA	-2.01	120.26	125.49
2	H	504	ALC	CE2-CD2-CG	2.01	115.46	112.22
2	J	504	ALC	CE2-CD2-CG	2.06	115.54	112.22
2	D	504	ALC	CE2-CD2-CG	3.00	117.07	112.22
2	N	504	ALC	CE1-CD1-CG	3.04	117.13	112.22
2	N	504	ALC	CD1-CG-CD2	3.07	116.99	109.26
2	J	504	ALC	CE1-CD1-CG	3.12	117.26	112.22
2	N	504	ALC	CE2-CD2-CG	3.37	117.66	112.22
2	J	504	ALC	CD1-CG-CD2	3.38	117.76	109.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	504	ALC	2	0
2	B	506	DSN	1	0
2	D	506	DSN	1	0
2	F	507	DLY	1	0
2	L	504	ALC	1	0
2	N	507	DLY	2	0
2	P	504	ALC	1	0
2	P	507	DLY	1	0

5.5 Carbohydrates [i](#)

52 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	314	1,3	14,14,15	0.54	0	15,19,21	1.32	3 (20%)
3	NAG	A	315	3	14,14,15	0.60	0	15,19,21	1.79	1 (6%)
3	FUC	A	316	3	10,10,11	0.64	0	14,14,16	1.21	1 (7%)
6	NAG	C	314	1,6	14,14,15	0.52	0	15,19,21	1.62	2 (13%)
6	FUC	C	315	6	10,10,11	0.57	0	14,14,16	1.05	2 (14%)
3	NAG	C	331	1,3	14,14,15	0.50	0	15,19,21	2.48	2 (13%)
3	NAG	C	332	3	14,14,15	0.67	0	15,19,21	1.36	2 (13%)
3	FUC	C	336	3	10,10,11	0.59	0	14,14,16	1.21	2 (14%)
3	NAG	E	314	1,3	14,14,15	0.55	0	15,19,21	1.53	2 (13%)
3	NAG	E	315	3	14,14,15	0.55	0	15,19,21	1.55	1 (6%)
3	FUC	E	316	3	10,10,11	0.66	0	14,14,16	1.65	4 (28%)
6	NAG	E	321	1,6	14,14,15	0.55	0	15,19,21	1.97	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FUC	E	326	6	10,10,11	0.88	0	14,14,16	2.04	4 (28%)
6	NAG	G	314	1,6	14,14,15	0.52	0	15,19,21	1.74	3 (20%)
6	FUC	G	315	6	10,10,11	0.53	0	14,14,16	1.38	2 (14%)
7	NAG	G	316	1,7	14,14,15	0.63	0	15,19,21	1.11	2 (13%)
7	NAG	G	317	7	14,14,15	0.57	0	15,19,21	1.51	3 (20%)
8	NDG	G	331	1,8	14,14,15	0.55	0	15,19,21	1.59	2 (13%)
8	FUC	G	336	8	10,10,11	0.67	0	14,14,16	1.59	2 (14%)
6	NAG	I	314	1,6	14,14,15	0.41	0	15,19,21	1.69	3 (20%)
6	FUC	I	315	6	10,10,11	0.72	0	14,14,16	1.92	3 (21%)
9	NDG	I	316	9,1	14,14,15	0.44	0	15,19,21	1.14	1 (6%)
9	NAG	I	317	9	14,14,15	0.59	0	15,19,21	1.04	1 (6%)
9	BMA	I	318	9	11,11,12	0.47	0	14,15,17	3.15	5 (35%)
9	MAN	I	319	9	11,11,12	0.62	0	14,15,17	2.28	3 (21%)
9	MAN	I	320	9	11,11,12	0.72	0	14,15,17	1.24	1 (7%)
6	NAG	I	331	1,6	14,14,15	0.46	0	15,19,21	1.90	2 (13%)
6	FUC	I	336	6	10,10,11	0.60	0	14,14,16	1.42	2 (14%)
3	NAG	K	314	1,3	14,14,15	0.59	0	15,19,21	1.61	3 (20%)
3	NAG	K	315	3	14,14,15	0.61	0	15,19,21	2.66	2 (13%)
3	FUC	K	316	3	10,10,11	0.60	0	14,14,16	1.09	1 (7%)
9	NDG	K	317	9,1	14,14,15	0.64	0	15,19,21	1.57	3 (20%)
9	NAG	K	318	9	14,14,15	0.66	0	15,19,21	1.20	2 (13%)
9	BMA	K	319	9	11,11,12	0.89	1 (9%)	14,15,17	2.02	3 (21%)
9	MAN	K	320	9	11,11,12	0.71	0	14,15,17	2.15	4 (28%)
9	MAN	K	321	9	11,11,12	0.68	0	14,15,17	1.34	3 (21%)
6	NAG	M	314	1,6	14,14,15	0.40	0	15,19,21	1.81	3 (20%)
6	FUC	M	315	6	10,10,11	0.67	0	14,14,16	1.48	2 (14%)
9	NDG	M	316	9,1	14,14,15	0.59	0	15,19,21	1.79	2 (13%)
9	NAG	M	317	9	14,14,15	0.58	0	15,19,21	1.22	1 (6%)
9	BMA	M	318	9	11,11,12	0.55	0	14,15,17	2.12	3 (21%)
9	MAN	M	319	9	11,11,12	0.75	0	14,15,17	2.94	5 (35%)
9	MAN	M	320	9	11,11,12	0.66	0	14,15,17	1.45	2 (14%)
7	NAG	M	321	1,7	14,14,15	0.64	0	15,19,21	1.37	1 (6%)
7	NAG	M	322	7	14,14,15	0.52	0	15,19,21	1.77	3 (20%)
6	NAG	O	314	1,6	14,14,15	0.50	0	15,19,21	1.29	2 (13%)
6	FUC	O	315	6	10,10,11	0.69	0	14,14,16	1.59	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NDG	O	316	9,1	14,14,15	0.66	0	15,19,21	1.82	3 (20%)
9	NAG	O	317	9	14,14,15	0.51	0	15,19,21	0.88	0
9	BMA	O	318	9	11,11,12	0.92	1 (9%)	14,15,17	1.78	3 (21%)
9	MAN	O	319	9	11,11,12	0.74	0	14,15,17	1.78	3 (21%)
9	MAN	O	320	9	11,11,12	0.61	0	14,15,17	1.83	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	314	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	315	3	-	0/6/23/26	0/1/1/1
3	FUC	A	316	3	2/2/4/5	0/0/17/20	0/1/1/1
6	NAG	C	314	1,6	-	0/6/23/26	0/1/1/1
6	FUC	C	315	6	2/2/4/5	0/0/17/20	0/1/1/1
3	NAG	C	331	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	332	3	-	0/6/23/26	0/1/1/1
3	FUC	C	336	3	2/2/4/5	0/0/17/20	0/1/1/1
3	NAG	E	314	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	315	3	-	0/6/23/26	0/1/1/1
3	FUC	E	316	3	2/2/4/5	0/0/17/20	0/1/1/1
6	NAG	E	321	1,6	-	0/6/23/26	0/1/1/1
6	FUC	E	326	6	2/2/4/5	0/0/17/20	0/1/1/1
6	NAG	G	314	1,6	-	0/6/23/26	0/1/1/1
6	FUC	G	315	6	2/2/4/5	0/0/17/20	0/1/1/1
7	NAG	G	316	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	317	7	-	0/6/23/26	0/1/1/1
8	NDG	G	331	1,8	-	1/6/23/26	0/1/1/1
8	FUC	G	336	8	2/2/4/5	0/0/17/20	0/1/1/1
6	NAG	I	314	1,6	-	0/6/23/26	0/1/1/1
6	FUC	I	315	6	2/2/4/5	0/0/17/20	0/1/1/1
9	NDG	I	316	9,1	-	0/6/23/26	0/1/1/1
9	NAG	I	317	9	-	0/6/23/26	0/1/1/1
9	BMA	I	318	9	-	0/2/19/22	0/1/1/1
9	MAN	I	319	9	-	0/2/19/22	0/1/1/1
9	MAN	I	320	9	-	0/2/19/22	1/1/1/1
6	NAG	I	331	1,6	-	0/6/23/26	0/1/1/1
6	FUC	I	336	6	2/2/4/5	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	314	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	315	3	-	2/6/23/26	0/1/1/1
3	FUC	K	316	3	2/2/4/5	0/0/17/20	0/1/1/1
9	NDG	K	317	9,1	-	0/6/23/26	0/1/1/1
9	NAG	K	318	9	-	0/6/23/26	0/1/1/1
9	BMA	K	319	9	-	0/2/19/22	0/1/1/1
9	MAN	K	320	9	-	0/2/19/22	0/1/1/1
9	MAN	K	321	9	-	0/2/19/22	0/1/1/1
6	NAG	M	314	1,6	-	0/6/23/26	0/1/1/1
6	FUC	M	315	6	2/2/4/5	0/0/17/20	0/1/1/1
9	NDG	M	316	9,1	-	0/6/23/26	0/1/1/1
9	NAG	M	317	9	-	0/6/23/26	0/1/1/1
9	BMA	M	318	9	-	0/2/19/22	0/1/1/1
9	MAN	M	319	9	-	0/2/19/22	1/1/1/1
9	MAN	M	320	9	-	0/2/19/22	0/1/1/1
7	NAG	M	321	1,7	-	0/6/23/26	0/1/1/1
7	NAG	M	322	7	-	0/6/23/26	0/1/1/1
6	NAG	O	314	1,6	-	0/6/23/26	0/1/1/1
6	FUC	O	315	6	2/2/4/5	0/0/17/20	0/1/1/1
9	NDG	O	316	9,1	-	0/6/23/26	0/1/1/1
9	NAG	O	317	9	-	0/6/23/26	0/1/1/1
9	BMA	O	318	9	-	0/2/19/22	0/1/1/1
9	MAN	O	319	9	-	0/2/19/22	0/1/1/1
9	MAN	O	320	9	-	0/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	318	BMA	O5-C1	-2.32	1.39	1.43
9	K	319	BMA	O5-C1	-2.17	1.40	1.43

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	319	MAN	C1-C2-C3	-7.88	100.22	109.54
9	I	319	MAN	C1-C2-C3	-6.74	101.56	109.54
9	K	320	MAN	C1-C2-C3	-6.02	102.42	109.54
9	O	319	MAN	C1-C2-C3	-4.58	104.12	109.54
9	M	319	MAN	C1-O5-C5	-4.12	107.02	112.25
6	I	314	NAG	C4-C3-C2	-3.66	105.54	111.23
9	O	316	NDG	C2-N2-C7	-3.61	118.41	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	318	BMA	O3-C3-C2	-3.59	103.51	110.00
9	K	319	BMA	O3-C3-C2	-3.58	103.54	110.00
6	M	314	NAG	C2-N2-C7	-3.50	118.55	123.04
9	M	318	BMA	O3-C3-C2	-3.36	103.94	110.00
8	G	336	FUC	C1-C2-C3	-3.19	105.77	109.54
6	M	314	NAG	C4-C3-C2	-3.10	106.41	111.23
6	G	315	FUC	C1-C2-C3	-2.62	106.44	109.54
6	O	314	NAG	C2-N2-C7	-2.59	119.72	123.04
8	G	336	FUC	O5-C1-C2	-2.57	106.69	110.86
9	O	319	MAN	O5-C1-C2	-2.55	106.72	110.86
9	M	319	MAN	C2-C3-C4	-2.53	106.74	111.04
6	G	314	NAG	C6-C5-C4	-2.50	106.84	113.02
6	C	314	NAG	C2-N2-C7	-2.46	119.88	123.04
9	O	318	BMA	O5-C1-C2	-2.46	106.87	110.86
6	E	326	FUC	O5-C1-C2	-2.45	106.88	110.86
9	K	321	MAN	O3-C3-C4	-2.41	104.91	110.34
9	K	321	MAN	O6-C6-C5	-2.32	103.67	111.33
9	K	318	NAG	O4-C4-C3	-2.26	105.26	110.34
9	M	316	NDG	C2-N2-C7	-2.16	120.27	123.04
9	K	317	NDG	O7-C7-C8	-2.12	118.17	122.06
9	O	318	BMA	O3-C3-C4	-2.08	105.65	110.34
6	I	314	NAG	C2-N2-C7	-2.08	120.37	123.04
3	E	316	FUC	O3-C3-C2	-2.06	106.28	110.00
6	O	315	FUC	C1-C2-C3	-2.04	107.12	109.54
6	O	314	NAG	C3-C4-C5	-2.03	106.65	110.20
9	I	317	NAG	C3-C4-C5	-2.02	106.68	110.20
3	A	314	NAG	O3-C3-C4	-2.01	105.81	110.34
7	G	316	NAG	O7-C7-C8	-2.01	118.38	122.06
6	O	315	FUC	O5-C5-C4	2.01	113.02	109.53
9	O	320	MAN	C3-C4-C5	2.06	113.79	110.20
6	I	331	NAG	C2-N2-C7	2.09	125.73	123.04
3	C	336	FUC	C1-C2-C3	2.12	112.05	109.54
9	K	321	MAN	O5-C5-C6	2.13	111.95	107.35
3	K	314	NAG	O4-C4-C3	2.14	115.16	110.34
8	G	331	NDG	O-C5-C6	2.16	112.03	107.35
6	E	321	NAG	C4-C3-C2	2.18	114.61	111.23
6	C	315	FUC	C1-O5-C5	2.19	115.76	112.38
9	K	320	MAN	O5-C5-C6	2.20	112.11	107.35
6	I	336	FUC	C1-O5-C5	2.22	115.80	112.38
3	A	314	NAG	C4-C3-C2	2.23	114.69	111.23
3	K	316	FUC	O5-C5-C6	2.24	109.83	106.13
6	C	315	FUC	O5-C5-C6	2.25	109.84	106.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	316	FUC	C2-C3-C4	2.25	114.86	111.04
9	I	318	BMA	O5-C1-C2	2.28	114.56	110.86
9	I	319	MAN	C3-C4-C5	2.28	114.18	110.20
7	G	317	NAG	C3-C2-N2	2.29	116.05	110.56
9	M	319	MAN	O5-C5-C6	2.29	112.32	107.35
7	G	316	NAG	C1-O5-C5	2.31	115.18	112.25
3	A	314	NAG	C1-O5-C5	2.34	115.22	112.25
9	M	320	MAN	C1-C2-C3	2.36	112.33	109.54
3	E	316	FUC	O5-C5-C6	2.36	110.04	106.13
9	K	320	MAN	O2-C2-C1	2.43	114.07	109.21
9	K	318	NAG	O5-C5-C6	2.44	112.62	107.35
9	I	320	MAN	O2-C2-C1	2.46	114.13	109.21
3	A	316	FUC	C3-C4-C5	2.46	113.87	109.72
6	E	326	FUC	C1-O5-C5	2.49	116.23	112.38
7	M	322	NAG	C3-C4-C5	2.51	114.57	110.20
9	K	320	MAN	C3-C4-C5	2.53	114.60	110.20
7	M	322	NAG	C4-C3-C2	2.56	115.20	111.23
9	K	319	BMA	C3-C4-C5	2.60	114.73	110.20
9	K	317	NDG	O-C5-C6	2.66	113.11	107.35
6	I	315	FUC	O5-C5-C6	2.71	110.60	106.13
6	E	321	NAG	O5-C5-C6	2.71	113.21	107.35
3	E	314	NAG	C1-O5-C5	2.74	115.72	112.25
6	I	315	FUC	C2-C3-C4	2.77	115.75	111.04
6	G	315	FUC	C1-O5-C5	2.80	116.70	112.38
3	K	314	NAG	C1-O5-C5	2.80	115.80	112.25
6	O	315	FUC	C3-C4-C5	2.89	114.58	109.72
3	C	336	FUC	C1-O5-C5	2.98	116.98	112.38
9	O	316	NDG	C4-C3-C2	3.03	115.94	111.23
3	K	315	NAG	C3-C4-C5	3.06	115.53	110.20
9	O	319	MAN	C3-C4-C5	3.08	115.57	110.20
6	M	315	FUC	O5-C5-C6	3.09	111.23	106.13
3	E	314	NAG	C4-C3-C2	3.11	116.06	111.23
7	G	317	NAG	C1-O5-C5	3.21	116.32	112.25
3	C	332	NAG	C1-O5-C5	3.25	116.37	112.25
6	G	314	NAG	O5-C5-C6	3.30	114.48	107.35
9	I	318	BMA	C3-C4-C5	3.34	116.02	110.20
3	C	332	NAG	C4-C3-C2	3.34	116.43	111.23
6	I	336	FUC	O5-C5-C6	3.39	111.73	106.13
9	M	320	MAN	C1-O5-C5	3.43	116.61	112.25
7	M	321	NAG	C1-O5-C5	3.47	116.65	112.25
9	K	317	NDG	C1-O-C5	3.48	116.67	112.25
3	K	314	NAG	O4-C4-C5	3.49	118.48	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	315	FUC	O5-C5-C6	3.50	111.92	106.13
9	I	316	NDG	C1-O-C5	3.51	116.70	112.25
9	M	317	NAG	C1-O5-C5	3.53	116.72	112.25
7	G	317	NAG	C2-N2-C7	3.56	127.61	123.04
9	I	319	MAN	O2-C2-C1	3.59	116.40	109.21
9	O	316	NDG	C1-O-C5	3.59	116.81	112.25
6	E	326	FUC	C3-C4-C5	3.64	115.85	109.72
6	E	321	NAG	C3-C4-C5	3.66	116.57	110.20
9	I	318	BMA	C1-C2-C3	3.71	113.93	109.54
9	O	320	MAN	O5-C5-C6	3.73	115.41	107.35
9	M	318	BMA	C1-O5-C5	3.86	117.14	112.25
6	G	314	NAG	C1-O5-C5	3.98	117.31	112.25
6	I	314	NAG	C1-O5-C5	4.01	117.34	112.25
6	M	315	FUC	C1-O5-C5	4.15	118.78	112.38
6	M	314	NAG	C1-O5-C5	4.21	117.59	112.25
9	O	320	MAN	C1-O5-C5	4.25	117.65	112.25
3	E	316	FUC	C1-C2-C3	4.29	114.62	109.54
6	E	326	FUC	O5-C5-C4	4.31	117.00	109.53
3	C	331	NAG	C4-C3-C2	4.35	117.99	111.23
8	G	331	NDG	C1-O-C5	4.56	118.04	112.25
9	O	318	BMA	C1-C2-C3	4.65	115.04	109.54
9	M	319	MAN	O2-C2-C1	4.72	118.67	109.21
6	E	321	NAG	C1-O5-C5	4.75	118.28	112.25
6	C	314	NAG	C1-O5-C5	4.84	118.39	112.25
9	M	318	BMA	C1-C2-C3	4.94	115.39	109.54
6	I	315	FUC	C1-C2-C3	5.15	115.64	109.54
7	M	322	NAG	C1-O5-C5	5.32	119.00	112.25
3	E	315	NAG	C1-O5-C5	5.32	119.00	112.25
9	K	319	BMA	C1-C2-C3	5.35	115.87	109.54
6	I	331	NAG	C1-O5-C5	5.90	119.74	112.25
3	A	315	NAG	C1-O5-C5	6.00	119.86	112.25
9	M	316	NDG	C1-O-C5	6.06	119.94	112.25
3	C	331	NAG	C1-O5-C5	8.09	122.51	112.25
3	K	315	NAG	C1-O5-C5	9.03	123.71	112.25
9	I	318	BMA	C1-O5-C5	9.42	124.20	112.25

All (25) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	315	FUC	C5
6	C	315	FUC	C1
3	K	316	FUC	C5

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Mol	Chain	Res	Type	Atom
3	K	316	FUC	C1
6	M	315	FUC	C5
6	M	315	FUC	C1
8	G	336	FUC	C5
8	G	336	FUC	C1
6	G	315	FUC	C5
6	G	315	FUC	C1
3	C	336	FUC	C5
3	C	336	FUC	C1
6	O	315	FUC	C5
6	O	315	FUC	C1
3	E	316	FUC	C5
3	E	316	FUC	C1
6	E	326	FUC	C5
6	E	326	FUC	C1
3	A	316	FUC	C5
3	A	316	FUC	C1
6	I	315	FUC	C5
6	I	315	FUC	C1
6	I	336	FUC	C5
6	I	336	FUC	C1
3	C	331	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	315	NAG	C8-C7-N2-C2
8	G	331	NDG	O7-C7-N2-C2
3	K	315	NAG	O7-C7-N2-C2

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	O	320	MAN	C1-C2-C3-C4-C5-O5
9	M	319	MAN	C1-C2-C3-C4-C5-O5
9	I	320	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	321	NAG	1	0
7	G	316	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	317	NAG	1	0
6	I	314	NAG	1	0
9	I	316	NDG	1	0
9	K	317	NDG	1	0
6	M	314	NAG	1	0
9	M	316	NDG	1	0
9	O	319	MAN	1	0

5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NDG	A	317	1	14,14,15	0.45	0	15,19,21	1.79	2 (13%)
5	NAG	A	321	1	14,14,15	0.66	0	15,19,21	2.19	4 (26%)
10	SO4	A	801	-	4,4,4	0.23	0	6,6,6	0.36	0
10	SO4	A	805	-	4,4,4	0.22	0	6,6,6	0.13	0
10	SO4	A	813	-	4,4,4	0.21	0	6,6,6	0.34	0
5	NAG	C	316	1	14,14,15	0.42	0	15,19,21	1.09	1 (6%)
5	NAG	C	321	1	14,14,15	0.62	0	15,19,21	0.96	1 (6%)
10	SO4	C	806	-	4,4,4	0.11	0	6,6,6	0.19	0
10	SO4	C	814	-	4,4,4	0.14	0	6,6,6	0.31	0
10	SO4	C	818	-	4,4,4	0.20	0	6,6,6	0.25	0
5	NAG	E	317	1	14,14,15	0.55	0	15,19,21	1.45	1 (6%)
10	SO4	E	807	-	4,4,4	0.24	0	6,6,6	0.15	0
10	SO4	E	815	-	4,4,4	0.25	0	6,6,6	0.51	0
10	SO4	E	820	-	4,4,4	0.11	0	6,6,6	0.13	0
5	NAG	G	321	1	14,14,15	0.66	0	15,19,21	1.30	2 (13%)
10	SO4	G	802	-	4,4,4	0.20	0	6,6,6	0.22	0
10	SO4	G	808	-	4,4,4	0.15	0	6,6,6	0.35	0
10	SO4	G	816	-	4,4,4	0.26	0	6,6,6	0.42	0
10	SO4	G	817	-	4,4,4	0.25	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	I	321	1	14,14,15	0.68	1 (7%)	15,19,21	1.07	0
10	SO4	I	804	-	4,4,4	0.21	0	6,6,6	0.17	0
10	SO4	I	809	-	4,4,4	0.20	0	6,6,6	0.07	0
10	SO4	I	821	-	4,4,4	0.15	0	6,6,6	0.09	0
5	NAG	K	322	1	14,14,15	0.80	0	15,19,21	1.38	2 (13%)
4	NDG	K	331	1	14,14,15	0.51	0	15,19,21	1.68	3 (20%)
10	SO4	K	803	-	4,4,4	0.16	0	6,6,6	0.15	0
10	SO4	K	810	-	4,4,4	0.21	0	6,6,6	0.14	0
5	NAG	M	331	1	14,14,15	0.39	0	15,19,21	1.70	1 (6%)
10	SO4	M	811	-	4,4,4	0.10	0	6,6,6	0.28	0
10	SO4	M	819	-	4,4,4	0.15	0	6,6,6	0.06	0
4	NDG	O	321	1	14,14,15	0.69	0	15,19,21	0.83	1 (6%)
10	SO4	O	812	-	4,4,4	0.10	0	6,6,6	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDG	A	317	1	-	0/6/23/26	0/1/1/1
5	NAG	A	321	1	1/1/5/7	0/6/23/26	0/1/1/1
10	SO4	A	801	-	-	0/0/0/0	0/0/0/0
10	SO4	A	805	-	-	0/0/0/0	0/0/0/0
10	SO4	A	813	-	-	0/0/0/0	0/0/0/0
5	NAG	C	316	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	C	321	1	1/1/5/7	0/6/23/26	0/1/1/1
10	SO4	C	806	-	-	0/0/0/0	0/0/0/0
10	SO4	C	814	-	-	0/0/0/0	0/0/0/0
10	SO4	C	818	-	-	0/0/0/0	0/0/0/0
5	NAG	E	317	1	-	0/6/23/26	0/1/1/1
10	SO4	E	807	-	-	0/0/0/0	0/0/0/0
10	SO4	E	815	-	-	0/0/0/0	0/0/0/0
10	SO4	E	820	-	-	0/0/0/0	0/0/0/0
5	NAG	G	321	1	-	0/6/23/26	0/1/1/1
10	SO4	G	802	-	-	0/0/0/0	0/0/0/0
10	SO4	G	808	-	-	0/0/0/0	0/0/0/0
10	SO4	G	816	-	-	0/0/0/0	0/0/0/0
10	SO4	G	817	-	-	0/0/0/0	0/0/0/0
5	NAG	I	321	1	-	0/6/23/26	0/1/1/1
10	SO4	I	804	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SO4	I	809	-	-	0/0/0/0	0/0/0/0
10	SO4	I	821	-	-	0/0/0/0	0/0/0/0
5	NAG	K	322	1	-	1/6/23/26	0/1/1/1
4	NDG	K	331	1	-	0/6/23/26	0/1/1/1
10	SO4	K	803	-	-	0/0/0/0	0/0/0/0
10	SO4	K	810	-	-	0/0/0/0	0/0/0/0
5	NAG	M	331	1	-	0/6/23/26	0/1/1/1
10	SO4	M	811	-	-	0/0/0/0	0/0/0/0
10	SO4	M	819	-	-	0/0/0/0	0/0/0/0
4	NDG	O	321	1	-	0/6/23/26	0/1/1/1
10	SO4	O	812	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	321	NAG	C1-C2	2.05	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	321	NAG	C4-C3-C2	-2.32	107.63	111.23
5	A	321	NAG	C2-N2-C7	2.04	125.66	123.04
5	G	321	NAG	C4-C3-C2	2.05	114.42	111.23
5	A	321	NAG	C8-C7-N2	2.10	120.12	116.11
4	O	321	NDG	C4-C3-C2	2.19	114.63	111.23
5	C	321	NAG	C2-N2-C7	2.37	126.09	123.04
5	K	322	NAG	C4-C3-C2	2.48	115.09	111.23
4	K	331	NDG	C4-C3-C2	2.69	115.40	111.23
5	C	316	NAG	C1-O5-C5	2.71	115.69	112.25
4	K	331	NDG	C3-C4-C5	2.78	115.05	110.20
4	A	317	NDG	C3-C4-C5	2.86	115.19	110.20
5	G	321	NAG	C3-C4-C5	3.13	115.66	110.20
5	K	322	NAG	C2-N2-C7	3.46	127.48	123.04
4	K	331	NDG	C1-O-C5	3.92	117.23	112.25
5	E	317	NAG	C1-O5-C5	3.98	117.30	112.25
4	A	317	NDG	C1-O-C5	5.57	119.32	112.25
5	M	331	NAG	C1-O5-C5	6.13	120.02	112.25
5	A	321	NAG	C1-O5-C5	6.92	121.03	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	321	NAG	C1
5	C	316	NAG	C1
5	A	321	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	322	NAG	O7-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	801	SO4	1	0
10	C	818	SO4	1	0
10	G	817	SO4	1	0
10	I	804	SO4	1	0
10	K	803	SO4	1	0
10	K	810	SO4	2	0
10	M	811	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	268/313 (85%)	1.00	36 (13%) 4 3	45, 57, 69, 98	0
1	C	259/313 (82%)	0.89	37 (14%) 4 3	48, 58, 66, 76	0
1	E	262/313 (83%)	0.84	32 (12%) 5 4	46, 56, 64, 72	0
1	G	258/313 (82%)	0.78	28 (10%) 7 5	46, 57, 67, 69	0
1	I	264/313 (84%)	0.98	46 (17%) 2 1	44, 58, 69, 89	0
1	K	257/313 (82%)	0.93	34 (13%) 4 4	45, 58, 67, 78	0
1	M	263/313 (84%)	0.89	35 (13%) 4 3	43, 57, 66, 83	0
1	O	258/313 (82%)	0.97	34 (13%) 4 4	47, 58, 68, 87	0
2	B	10/13 (76%)	0.91	1 (10%) 9 7	53, 60, 69, 71	0
2	D	10/13 (76%)	1.12	1 (10%) 9 7	50, 57, 64, 66	0
2	F	10/13 (76%)	1.24	2 (20%) 1 1	51, 63, 71, 71	0
2	H	10/13 (76%)	1.02	1 (10%) 9 7	52, 56, 65, 69	0
2	J	10/13 (76%)	1.33	2 (20%) 1 1	47, 54, 64, 70	0
2	L	10/13 (76%)	1.11	2 (20%) 1 1	50, 56, 72, 75	0
2	N	10/13 (76%)	1.17	1 (10%) 9 7	49, 55, 66, 71	0
2	P	10/13 (76%)	1.10	2 (20%) 1 1	52, 58, 72, 74	0
All	All	2169/2608 (83%)	0.92	294 (13%) 4 3	43, 57, 67, 98	0

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	VAL	10.0
1	E	231	PRO	8.8
1	A	138	PRO	8.3
1	I	275	ASP	8.1
1	A	279	GLN	8.0

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Mol	Chain	Res	Type	RSRZ
1	I	274	PRO	7.5
1	O	233	ASN	7.3
1	A	277	ASP	6.7
1	O	231	PRO	6.6
1	K	231	PRO	6.2
1	K	208	GLU	5.9
1	C	80	ASN	5.8
1	A	231	PRO	5.8
1	O	208	GLU	5.8
1	I	138	PRO	5.7
1	C	139	LYS	5.7
1	M	90	SER	5.6
1	G	107	ARG	5.6
1	I	82	GLY	5.5
1	G	202	THR	5.4
1	C	202	THR	5.3
1	A	131	GLN	5.3
1	I	19	LEU	5.3
1	O	202	THR	5.2
1	A	232	LYS	5.2
1	A	276	LEU	5.2
1	E	89	ARG	5.2
1	M	107	ARG	5.1
1	G	132	GLU	5.0
1	O	267	THR	5.0
1	O	92	TYR	5.0
1	K	102	ASP	5.0
1	K	233	ASN	5.0
1	I	33	GLU	5.0
1	C	102	ASP	4.9
1	M	277	ASP	4.9
1	M	106	GLU	4.8
1	I	107	ARG	4.8
1	M	19	LEU	4.8
1	K	230	GLU	4.7
1	A	102	ASP	4.7
1	M	89	ARG	4.7
1	C	203	HIS	4.7
1	A	137	ARG	4.7
1	K	203	HIS	4.6
1	I	110	HIS	4.6
1	A	107	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	131	GLN	4.6
1	A	202	THR	4.6
1	I	118	PRO	4.5
1	M	109	ARG	4.4
1	I	84	ALA	4.4
1	C	138	PRO	4.4
1	O	204	GLY	4.3
1	K	207	SER	4.3
1	M	92	TYR	4.3
1	C	107	ARG	4.2
1	C	231	PRO	4.2
1	O	232	LYS	4.2
1	C	91	ARG	4.1
1	K	202	THR	4.1
1	K	90	SER	4.1
1	K	229	HIS	4.1
1	A	259	ASN	4.1
1	E	232	LYS	4.1
1	O	276	LEU	4.1
1	C	274	PRO	4.1
1	G	110	HIS	4.0
1	C	230	GLU	4.0
1	A	90	SER	4.0
1	I	103	MET	3.9
1	K	232	LYS	3.9
1	I	273	HIS	3.9
1	I	92	TYR	3.9
1	M	102	ASP	3.9
1	A	234	GLN	3.8
1	O	107	ARG	3.8
1	O	106	GLU	3.8
1	E	107	ARG	3.8
1	I	83	ARG	3.8
1	M	91	ARG	3.7
1	I	85	VAL	3.7
1	I	137	ARG	3.7
1	I	81	SER	3.7
1	A	208	GLU	3.7
1	O	275	ASP	3.7
1	M	35	GLY	3.7
1	K	92	TYR	3.7
1	E	233	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	260	HIS	3.7
1	K	234	GLN	3.7
1	C	207	SER	3.7
1	M	232	LYS	3.7
2	D	501	LYS	3.7
1	C	106	GLU	3.6
1	E	123	LEU	3.6
1	E	106	GLU	3.6
1	K	110	HIS	3.6
1	G	102	ASP	3.6
1	O	260	HIS	3.6
1	K	139	LYS	3.6
1	E	102	ASP	3.6
1	E	90	SER	3.5
1	E	49	GLU	3.5
1	A	236	TYR	3.5
1	G	208	GLU	3.5
1	E	158	GLY	3.4
1	O	49	GLU	3.4
1	C	275	ASP	3.4
2	H	501	LYS	3.4
1	K	107	ARG	3.4
1	I	108	GLY	3.3
1	O	102	ASP	3.3
1	G	19	LEU	3.3
1	A	233	ASN	3.3
1	E	48	SER	3.3
1	C	130	ILE	3.3
1	O	234	GLN	3.3
1	C	211	PHE	3.3
1	K	235	SER	3.3
1	G	203	HIS	3.2
1	I	209	GLU	3.2
1	K	146	GLY	3.2
1	G	106	GLU	3.2
1	C	209	GLU	3.2
1	C	206	SER	3.2
1	E	242	ALA	3.2
1	I	146	GLY	3.1
1	E	168	LEU	3.1
1	A	81	SER	3.1
1	E	92	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	233	ASN	3.1
1	M	276	LEU	3.1
1	I	139	LYS	3.1
1	M	61	LEU	3.0
1	A	229	HIS	3.0
1	C	61	LEU	3.0
1	C	101	SER	3.0
1	G	131	GLN	3.0
1	I	102	ASP	3.0
1	C	208	GLU	3.0
1	K	118	PRO	3.0
1	A	103	MET	2.9
1	C	131	GLN	2.9
1	M	146	GLY	2.9
1	G	229	HIS	2.9
1	E	34	GLU	2.9
1	M	108	GLY	2.9
1	O	235	SER	2.9
1	C	109	ARG	2.9
1	C	110	HIS	2.9
1	I	232	LYS	2.9
1	A	130	ILE	2.9
1	I	61	LEU	2.9
1	K	262	ASP	2.9
1	C	146	GLY	2.9
1	M	148	GLY	2.9
1	C	193	GLN	2.8
1	M	88	SER	2.8
1	I	34	GLU	2.8
1	I	106	GLU	2.8
1	C	103	MET	2.8
1	A	260	HIS	2.8
1	E	146	GLY	2.8
1	A	79	GLY	2.8
1	C	108	GLY	2.8
1	G	146	GLY	2.8
1	E	208	GLU	2.7
1	E	229	HIS	2.7
1	K	259	ASN	2.7
1	O	230	GLU	2.7
1	G	234	GLN	2.7
1	G	148	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	48	SER	2.7
1	O	48	SER	2.7
2	J	501	LYS	2.7
1	O	271	CYS	2.7
1	E	230	GLU	2.7
1	K	106	GLU	2.7
1	G	139	LYS	2.7
1	M	47	HIS	2.6
1	E	140	ASP	2.6
1	G	230	GLU	2.6
1	M	202	THR	2.6
1	C	262	ASP	2.6
1	A	230	GLU	2.6
1	M	34	GLU	2.6
1	K	240	GLY	2.6
2	P	501	LYS	2.6
1	A	106	GLU	2.6
1	E	203	HIS	2.6
1	A	147	CYS	2.6
1	K	49	GLU	2.6
1	G	147	CYS	2.6
1	C	19	LEU	2.5
1	A	140	ASP	2.5
1	M	81	SER	2.5
1	G	231	PRO	2.5
1	C	140	ASP	2.5
1	G	232	LYS	2.5
1	I	207	SER	2.5
1	G	109	ARG	2.5
2	N	509	LEU	2.5
1	A	92	TYR	2.5
1	A	235	SER	2.5
1	O	207	SER	2.5
2	B	501	LYS	2.4
1	O	229	HIS	2.4
1	E	157	ASN	2.4
1	I	172	ASN	2.4
1	M	147	CYS	2.4
1	I	131	GLN	2.4
1	I	148	GLY	2.4
1	G	140	ASP	2.4
1	A	274	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	118	PRO	2.4
1	G	240	GLY	2.4
1	K	204	GLY	2.4
1	M	125	VAL	2.4
2	L	502	SER	2.4
1	O	146	GLY	2.4
2	P	502	SER	2.4
1	O	266	CYS	2.4
1	I	55	LEU	2.3
1	I	36	GLU	2.3
1	O	268	LYS	2.3
1	G	101	SER	2.3
1	E	159	PHE	2.3
1	O	79	GLY	2.3
1	K	108	GLY	2.3
1	O	168	LEU	2.3
1	I	267	THR	2.3
1	I	18	ALA	2.3
1	K	111	GLN	2.3
1	A	211	PHE	2.3
1	E	278	VAL	2.3
1	E	234	GLN	2.3
1	M	208	GLU	2.2
2	F	501	LYS	2.2
2	L	501	LYS	2.2
1	O	56	SER	2.2
1	E	139	LYS	2.2
1	K	266	CYS	2.2
2	J	509	LEU	2.2
1	G	211	PHE	2.2
1	K	56	SER	2.2
1	C	233	ASN	2.2
1	I	80	ASN	2.2
1	M	158	GLY	2.2
1	G	204	GLY	2.2
1	I	208	GLU	2.2
1	M	110	HIS	2.2
1	E	125	VAL	2.2
1	O	203	HIS	2.2
1	M	55	LEU	2.2
2	F	512	SER	2.2
1	C	118	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	158	GLY	2.2
1	I	125	VAL	2.2
1	K	103	MET	2.2
1	C	180	PRO	2.2
1	I	240	GLY	2.2
1	I	112	SER	2.1
1	A	82	GLY	2.1
1	O	118	PRO	2.1
1	O	259	ASN	2.1
1	A	109	ARG	2.1
1	A	146	GLY	2.1
1	I	67	THR	2.1
1	I	54	THR	2.1
1	M	233	ASN	2.1
1	I	268	LYS	2.1
1	C	204	GLY	2.1
1	E	108	GLY	2.1
1	E	222	CYS	2.1
1	G	92	TYR	2.1
1	G	122	CYS	2.1
1	O	131	GLN	2.0
1	M	67	THR	2.0
1	C	159	PHE	2.0
1	O	34	GLU	2.0
1	E	61	LEU	2.0
1	K	172	ASN	2.0
1	I	181	ILE	2.0
1	O	35	GLY	2.0
1	G	56	SER	2.0
1	M	168	LEU	2.0
1	A	199	GLY	2.0
1	I	35	GLY	2.0
1	M	203	HIS	2.0
1	C	65	SER	2.0
1	K	236	TYR	2.0
1	M	123	LEU	2.0
1	M	54	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	DSN	P	506	6/7	0.94	0.17	-	56,56,56,57	0
2	DLY	H	507	9/10	0.97	0.22	-	50,50,51,51	0
2	DLY	L	507	9/10	0.94	0.23	-	51,52,59,61	0
2	DLY	N	507	9/10	0.95	0.32	-	47,50,50,51	0
2	DSN	B	506	6/7	0.97	0.16	-	52,54,54,54	0
2	DLY	D	507	9/10	0.94	0.29	-	51,52,53,53	0
2	DSN	N	506	6/7	0.96	0.28	-	51,51,52,53	0
2	DSN	L	506	6/7	0.98	0.16	-	53,54,54,55	0
2	ALC	P	504	11/12	0.96	0.26	-	59,60,61,63	0
2	ALC	H	504	11/12	0.93	0.27	-	54,56,61,61	0
2	ALC	J	504	11/12	0.94	0.28	-	55,56,57,57	0
2	ALC	L	504	11/12	0.96	0.23	-	60,61,63,63	0
2	DSN	H	506	6/7	0.97	0.24	-	48,50,50,50	0
2	ALC	F	504	11/12	0.96	0.25	-	54,54,56,58	0
2	DLY	P	507	9/10	0.87	0.27	-	54,55,61,63	0
2	ALC	D	504	11/12	0.94	0.27	-	53,54,55,56	0
2	DLY	J	507	9/10	0.96	0.30	-	49,50,50,51	0
2	DLY	B	507	9/10	0.89	0.26	-	53,54,58,58	0
2	ALC	N	504	11/12	0.93	0.28	-	55,56,57,58	0
2	DSN	F	506	6/7	0.97	0.22	-	49,50,50,50	0
2	DLY	F	507	9/10	0.93	0.22	-	51,52,57,57	0
2	DSN	D	506	6/7	0.96	0.23	-	51,52,52,52	0
2	DSN	J	506	6/7	0.97	0.27	-	52,52,52,54	0
2	ALC	B	504	11/12	0.96	0.25	-	56,57,58,60	0

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	FUC	E	326	10/11	0.67	0.42	3.25	84,85,86,86	0
6	FUC	G	315	10/11	0.87	0.35	2.31	71,73,74,75	0
6	FUC	O	315	10/11	0.90	0.35	2.18	71,72,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	FUC	C	315	10/11	0.82	0.34	1.56	71,72,73,73	0
3	FUC	E	316	10/11	0.72	0.30	1.26	84,85,85,85	0
3	FUC	A	316	10/11	0.94	0.28	0.40	81,82,82,83	0
9	NDG	O	316	14/15	0.88	0.21	-0.00	61,65,67,67	0
9	NAG	I	317	14/15	0.92	0.18	-0.09	60,61,63,64	0
9	NDG	M	316	14/15	0.93	0.15	-0.42	44,47,48,49	0
3	FUC	K	316	10/11	0.90	0.23	-0.44	76,77,77,78	0
9	NDG	K	317	14/15	0.94	0.16	-0.52	45,51,53,53	0
9	MAN	K	321	11/12	0.91	0.18	-0.70	45,47,48,49	0
9	NDG	I	316	14/15	0.93	0.16	-0.79	57,58,61,63	0
9	MAN	M	320	11/12	0.93	0.17	-0.89	43,45,46,48	0
6	FUC	I	315	10/11	0.85	0.23	-1.35	73,75,76,76	0
3	NAG	A	314	14/15	0.92	0.17	-1.54	68,73,79,80	0
6	NAG	I	314	14/15	0.90	0.19	-	58,61,67,71	0
3	NAG	C	332	14/15	0.68	0.46	-	99,101,101,102	0
7	NAG	M	321	14/15	0.57	0.48	-	82,86,88,92	0
8	NDG	G	331	14/15	0.73	0.45	-	80,84,89,92	0
3	FUC	C	336	10/11	0.84	0.47	-	96,97,97,98	0
6	NAG	M	314	14/15	0.87	0.26	-	57,59,61,64	0
9	MAN	K	320	11/12	0.75	0.21	-	55,57,59,59	0
6	NAG	I	331	14/15	0.78	0.28	-	76,79,81,82	0
9	NAG	M	317	14/15	0.96	0.17	-	47,48,48,50	0
3	NAG	E	315	14/15	0.75	0.40	-	89,91,92,93	0
6	NAG	C	314	14/15	0.93	0.21	-	62,65,66,68	0
6	FUC	M	315	10/11	0.83	0.33	-	66,68,69,69	0
9	MAN	O	319	11/12	0.74	0.39	-	74,76,77,77	0
9	BMA	M	318	11/12	0.92	0.16	-	47,49,51,54	0
3	NAG	K	314	14/15	0.88	0.17	-	68,72,74,78	0
9	BMA	I	318	11/12	0.83	0.16	-	64,66,68,71	0
6	NAG	O	314	14/15	0.86	0.21	-	63,65,67,70	0
7	NAG	M	322	14/15	0.69	0.48	-	95,96,98,99	0
6	NAG	E	321	14/15	0.67	0.51	-	76,79,82,83	0
7	NAG	G	317	14/15	0.72	0.41	-	91,92,93,93	0
9	MAN	O	320	11/12	0.81	0.20	-	65,69,71,72	0
3	NAG	A	315	14/15	0.74	0.35	-	83,84,86,86	0
9	NAG	K	318	14/15	0.93	0.19	-	50,52,54,54	0
9	MAN	I	320	11/12	0.84	0.17	-	67,68,71,72	0
9	BMA	K	319	11/12	0.90	0.18	-	48,50,52,52	0
9	MAN	I	319	11/12	0.74	0.31	-	73,75,77,77	0
6	FUC	I	336	10/11	0.71	0.41	-	83,84,84,84	0
6	NAG	G	314	14/15	0.96	0.16	-	57,60,63,67	0
3	NAG	K	315	14/15	0.76	0.45	-	81,83,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	FUC	G	336	10/11	0.55	0.54	-	94,95,96,96	0
3	NAG	C	331	14/15	0.79	0.33	-	85,91,95,96	0
9	BMA	O	318	11/12	0.89	0.28	-	70,71,72,73	0
9	NAG	O	317	14/15	0.87	0.24	-	66,69,71,71	0
9	MAN	M	319	11/12	0.83	0.29	-	54,58,62,63	0
7	NAG	G	316	14/15	0.79	0.46	-	80,86,87,90	0
3	NAG	E	314	14/15	0.77	0.19	-	74,77,83,86	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	SO4	A	805	5/5	0.82	0.28	0.98	132,132,133,133	0
10	SO4	E	807	5/5	0.87	0.34	0.91	125,125,125,125	0
10	SO4	O	812	5/5	0.92	0.26	0.31	79,79,80,80	0
10	SO4	K	810	5/5	0.90	0.21	-0.15	84,85,86,86	0
10	SO4	E	820	5/5	0.93	0.21	-0.49	86,87,87,87	0
10	SO4	I	809	5/5	0.98	0.16	-0.77	64,65,65,65	0
10	SO4	G	816	5/5	0.92	0.20	-0.80	61,62,63,63	0
10	SO4	C	806	5/5	0.92	0.17	-0.83	79,80,81,81	0
10	SO4	I	821	5/5	0.97	0.18	-1.37	71,72,72,73	0
10	SO4	G	808	5/5	0.97	0.16	-1.56	58,58,60,60	0
10	SO4	A	813	5/5	0.96	0.12	-1.68	64,66,66,67	0
10	SO4	M	811	5/5	0.97	0.10	-1.81	63,63,63,64	0
10	SO4	C	814	5/5	0.93	0.16	-1.91	65,67,68,69	0
10	SO4	C	818	5/5	0.95	0.13	-1.96	75,75,76,77	0
10	SO4	M	819	5/5	0.94	0.16	-2.30	79,79,80,80	0
10	SO4	G	817	5/5	0.97	0.12	-2.78	67,69,69,70	0
10	SO4	E	815	5/5	0.96	0.11	-3.04	56,57,58,58	0
10	SO4	G	802	5/5	0.92	0.16	-	56,57,58,58	0
5	NAG	I	321	14/15	0.77	0.49	-	76,79,80,80	0
5	NAG	C	316	14/15	0.86	0.52	-	77,80,84,84	0
5	NAG	E	317	14/15	0.83	0.38	-	72,75,80,80	0
10	SO4	I	804	5/5	0.94	0.20	-	58,58,59,60	0
10	SO4	K	803	5/5	0.96	0.12	-	61,61,61,62	0
5	NAG	A	321	14/15	0.52	0.50	-	75,78,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NDG	O	321	14/15	0.74	0.37	-	78,82,82,83	0
4	NDG	A	317	14/15	0.79	0.36	-	78,82,85,85	0
4	NDG	K	331	14/15	0.39	0.51	-	84,86,88,88	0
5	NAG	K	322	14/15	0.68	0.41	-	76,79,80,81	0
5	NAG	G	321	14/15	0.67	0.52	-	76,80,82,83	0
5	NAG	M	331	14/15	0.77	0.33	-	72,75,76,76	0
10	SO4	A	801	5/5	0.94	0.13	-	70,70,72,72	0
5	NAG	C	321	14/15	0.85	0.49	-	78,82,83,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.