



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:35 PM GMT

PDB ID : 1XSJ
Title : Structure of a Family 31 alpha glycosidase
Authors : Lovering, A.L.; Lee, S.S.; Kim, Y.W.; Withers, S.G.; Strynadka, N.C.
Deposited on : 2004-10-19
Resolution : 2.10 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

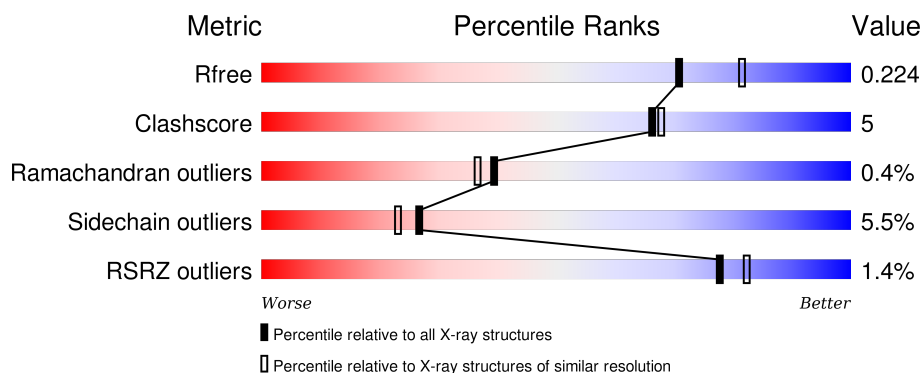
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	778	<div> <div></div> <div>84%13%..</div> </div>
1	B	778	<div> <div>2%</div> <div>83%15%..</div> </div>
1	C	778	<div> <div>%</div> <div>83%13%..</div> </div>
1	D	778	<div> <div>%</div> <div>85%13%..</div> </div>
1	E	778	<div> <div>2%</div> <div>84%12%..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	778	

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
2	TRS	A	2002	-	-	-	X
2	TRS	B	2004	-	-	-	X
2	TRS	C	2005	-	-	-	X
2	TRS	C	2006	-	-	-	X
2	TRS	D	2007	-	-	-	X
2	TRS	E	2009	-	-	-	X
2	TRS	E	2010	-	-	-	X
2	TRS	E	2012	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 38890 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 Putative family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	B	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	C	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	D	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	E	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	F	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			

There are 36 discrepancies between the modelled and reference sequences:

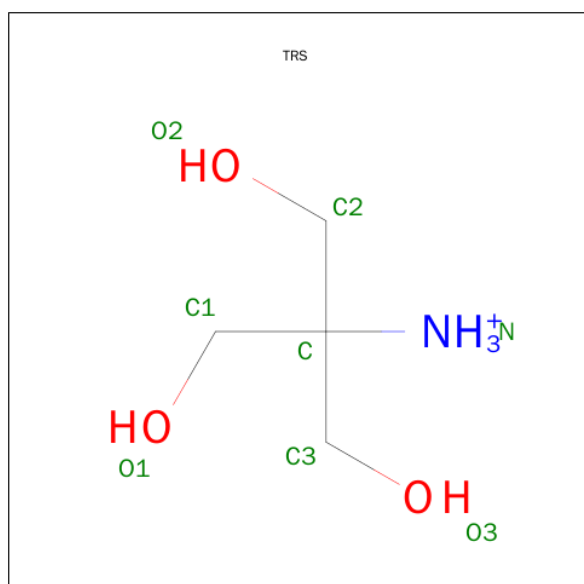
Chain	Residue	Modelled	Actual	Comment	Reference
A	773	HIS	-	EXPRESSION TAG	UNP P31434
A	774	HIS	-	EXPRESSION TAG	UNP P31434
A	775	HIS	-	EXPRESSION TAG	UNP P31434
A	776	HIS	-	EXPRESSION TAG	UNP P31434
A	777	HIS	-	EXPRESSION TAG	UNP P31434
A	778	HIS	-	EXPRESSION TAG	UNP P31434
B	773	HIS	-	EXPRESSION TAG	UNP P31434
B	774	HIS	-	EXPRESSION TAG	UNP P31434
B	775	HIS	-	EXPRESSION TAG	UNP P31434
B	776	HIS	-	EXPRESSION TAG	UNP P31434
B	777	HIS	-	EXPRESSION TAG	UNP P31434
B	778	HIS	-	EXPRESSION TAG	UNP P31434
C	773	HIS	-	EXPRESSION TAG	UNP P31434
C	774	HIS	-	EXPRESSION TAG	UNP P31434
C	775	HIS	-	EXPRESSION TAG	UNP P31434
C	776	HIS	-	EXPRESSION TAG	UNP P31434
C	777	HIS	-	EXPRESSION TAG	UNP P31434

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Chain	Residue	Modelled	Actual	Comment	Reference
C	778	HIS	-	EXPRESSION TAG	UNP P31434
D	773	HIS	-	EXPRESSION TAG	UNP P31434
D	774	HIS	-	EXPRESSION TAG	UNP P31434
D	775	HIS	-	EXPRESSION TAG	UNP P31434
D	776	HIS	-	EXPRESSION TAG	UNP P31434
D	777	HIS	-	EXPRESSION TAG	UNP P31434
D	778	HIS	-	EXPRESSION TAG	UNP P31434
E	773	HIS	-	EXPRESSION TAG	UNP P31434
E	774	HIS	-	EXPRESSION TAG	UNP P31434
E	775	HIS	-	EXPRESSION TAG	UNP P31434
E	776	HIS	-	EXPRESSION TAG	UNP P31434
E	777	HIS	-	EXPRESSION TAG	UNP P31434
E	778	HIS	-	EXPRESSION TAG	UNP P31434
F	773	HIS	-	EXPRESSION TAG	UNP P31434
F	774	HIS	-	EXPRESSION TAG	UNP P31434
F	775	HIS	-	EXPRESSION TAG	UNP P31434
F	776	HIS	-	EXPRESSION TAG	UNP P31434
F	777	HIS	-	EXPRESSION TAG	UNP P31434
F	778	HIS	-	EXPRESSION TAG	UNP P31434

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		
2	F	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		

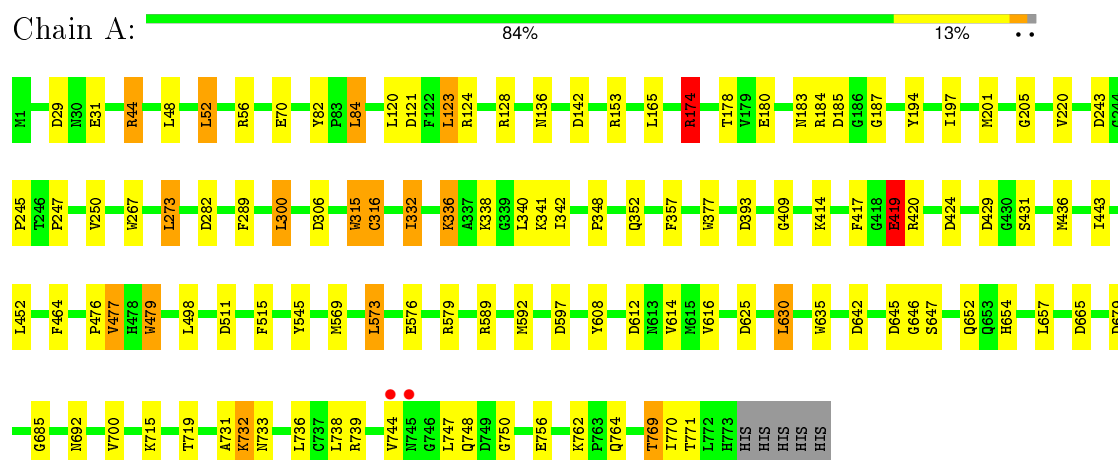
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	295	Total	O	0	0
			295	295		
3	B	208	Total	O	0	0
			208	208		
3	C	234	Total	O	0	0
			234	234		
3	D	267	Total	O	0	0
			267	267		
3	E	243	Total	O	0	0
			243	243		
3	F	191	Total	O	0	0
			191	191		

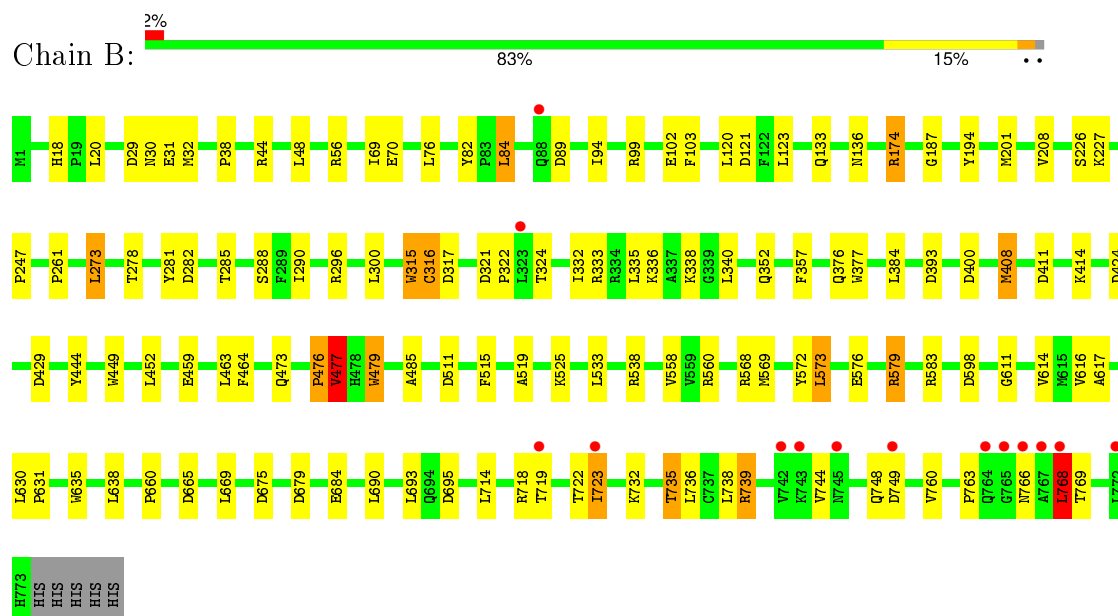
3 Residue-property plots

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.

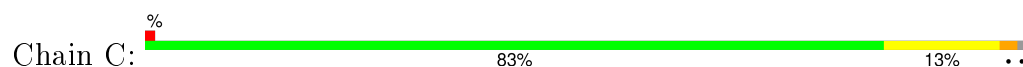
• Molecule 1: Putative family 31 glucosidase yicI

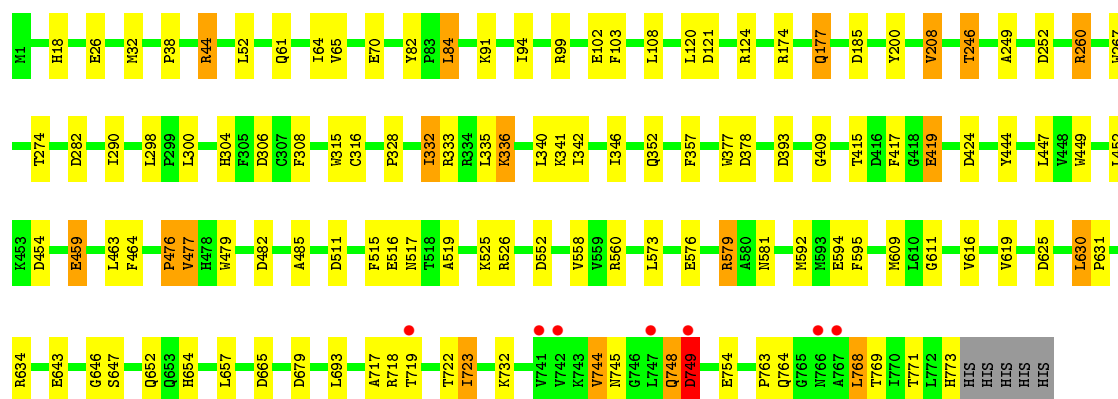


• Molecule 1: Putative family 31 glucosidase yicI

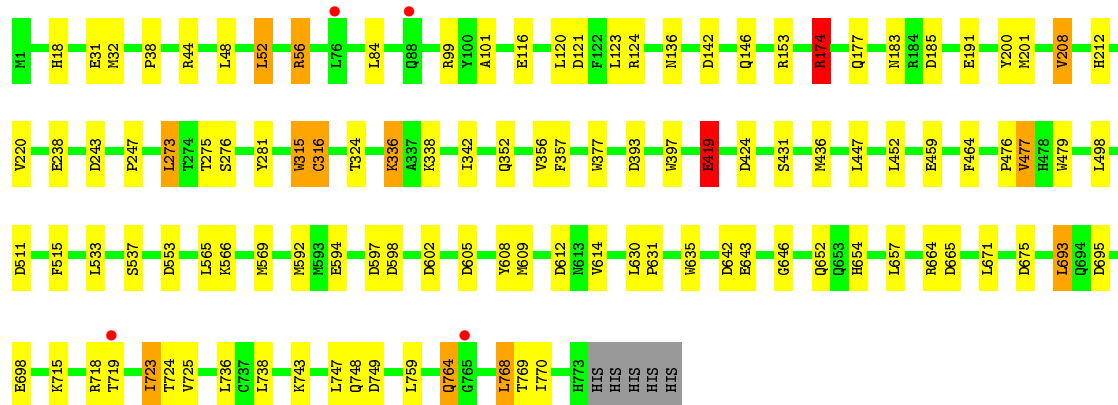
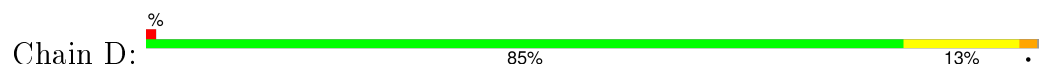


• Molecule 1: Putative family 31 glucosidase yicI

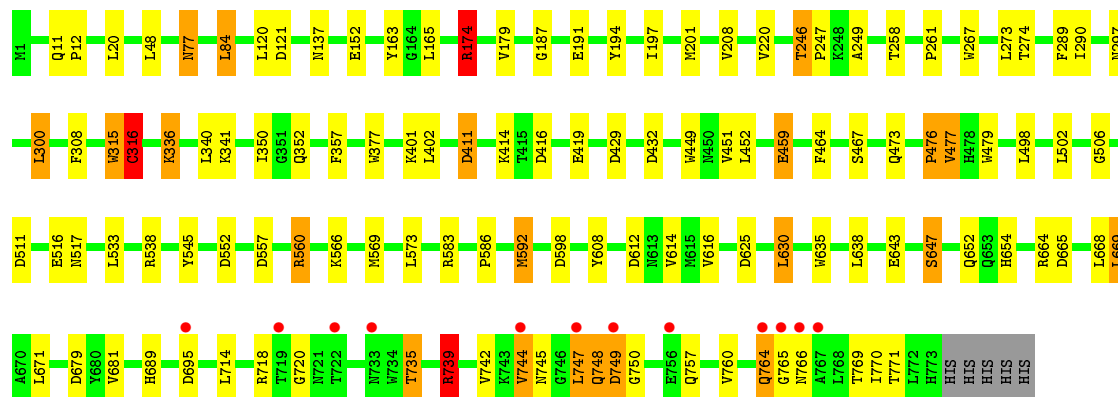
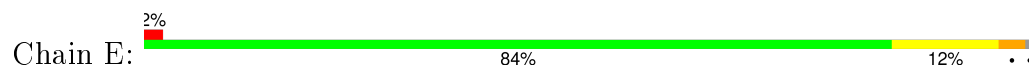




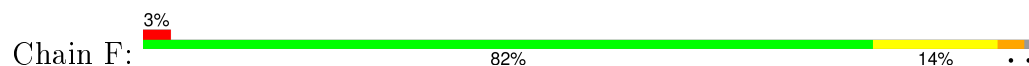
• Molecule 1: Putative family 31 glucosidase yicI



• Molecule 1: Putative family 31 glucosidase yicI



• Molecule 1: Putative family 31 glucosidase yicI





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.53Å 224.44Å 154.12Å 90.00° 101.75° 90.00°	Depositor
Resolution (Å)	29.98 – 2.10 66.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.98-2.10) 88.8 (66.09-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.220 0.187 , 0.224	Depositor DCC
R_{free} test set	15119 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 330993 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	38890	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS

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	0.80	0/6409	0.92	32/8711 (0.4%)
1	B	0.75	0/6409	0.89	24/8711 (0.3%)
1	C	0.76	0/6409	0.88	20/8711 (0.2%)
1	D	0.82	1/6409 (0.0%)	0.94	32/8711 (0.4%)
1	E	0.80	0/6409	0.93	27/8711 (0.3%)
1	F	0.75	0/6409	0.88	18/8711 (0.2%)
All	All	0.78	1/38454 (0.0%)	0.91	153/52266 (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	1
1	B	0	1
1	C	1	0
1	D	0	1
1	E	0	1
1	F	1	0
All	All	2	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	664	ARG	CB-CG	-5.12	1.38	1.52

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	739	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	D	174	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	E	476	PRO	CA-C-N	-8.36	98.80	117.20
1	C	424	ASP	CB-CG-OD2	7.90	125.41	118.30
1	C	282	ASP	CB-CG-OD2	7.89	125.40	118.30
1	D	174	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	174	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	B	282	ASP	CB-CG-OD2	7.81	125.33	118.30
1	E	476	PRO	C-N-CA	7.78	141.14	121.70
1	E	477	VAL	CB-CA-C	7.74	126.10	111.40
1	E	429	ASP	CB-CG-OD2	7.59	125.13	118.30
1	A	424	ASP	CB-CG-OD2	7.58	125.13	118.30
1	B	476	PRO	CA-C-N	-7.53	100.62	117.20
1	D	121	ASP	CB-CG-OD2	7.53	125.08	118.30
1	D	665	ASP	CB-CG-OD2	7.47	125.02	118.30
1	E	665	ASP	CB-CG-OD2	7.40	124.96	118.30
1	A	282	ASP	CB-CG-OD2	7.36	124.92	118.30
1	C	476	PRO	CA-C-N	-7.34	101.04	117.20
1	F	174	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	D	52	LEU	CA-CB-CG	7.21	131.87	115.30
1	D	476	PRO	CA-C-N	-7.18	101.39	117.20
1	A	393	ASP	CB-CG-OD2	7.10	124.69	118.30
1	D	476	PRO	C-N-CA	7.08	139.41	121.70
1	D	664	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	E	739	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	F	482	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	44	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	D	142	ASP	CB-CG-OD2	6.87	124.48	118.30
1	D	273	LEU	CA-CB-CG	6.86	131.07	115.30
1	B	316	CYS	N-CA-C	6.83	129.44	111.00
1	D	419	GLU	CA-CB-CG	6.81	128.39	113.40
1	C	121	ASP	CB-CG-OD2	6.79	124.41	118.30
1	E	598	ASP	CB-CG-OD2	6.77	124.39	118.30
1	F	174	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	174	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	665	ASP	CB-CG-OD2	6.68	124.31	118.30
1	B	89	ASP	CB-CG-OD2	6.68	124.31	118.30
1	B	665	ASP	CB-CG-OD2	6.66	124.30	118.30
1	A	476	PRO	CA-C-N	-6.66	102.56	117.20
1	A	29	ASP	CB-CG-OD2	6.64	124.28	118.30
1	E	174	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	424	ASP	CB-CG-OD2	6.56	124.20	118.30
1	F	424	ASP	CB-CG-OD2	6.55	124.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	476	PRO	CA-C-N	-6.51	102.88	117.20
1	B	393	ASP	CB-CG-OD2	6.46	124.12	118.30
1	D	598	ASP	CB-CG-OD2	6.44	124.10	118.30
1	E	560	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	F	768	LEU	CA-CB-CG	6.36	129.94	115.30
1	B	315	TRP	C-N-CA	6.34	137.56	121.70
1	A	476	PRO	C-N-CA	6.33	137.52	121.70
1	E	552	ASP	CB-CG-OD2	6.25	123.93	118.30
1	C	511	ASP	CB-CG-OD2	6.25	123.92	118.30
1	E	316	CYS	N-CA-C	6.24	127.84	111.00
1	B	429	ASP	CB-CG-OD2	6.22	123.90	118.30
1	D	315	TRP	C-N-CA	6.21	137.22	121.70
1	D	315	TRP	CA-C-N	-6.20	103.56	117.20
1	F	316	CYS	CA-CB-SG	-6.18	102.88	114.00
1	C	315	TRP	C-N-CA	6.16	137.09	121.70
1	B	679	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	477	VAL	CB-CA-C	6.13	123.06	111.40
1	F	121	ASP	CB-CG-OD2	6.13	123.81	118.30
1	B	400	ASP	CB-CG-OD2	6.12	123.81	118.30
1	D	642	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	477	VAL	CB-CA-C	6.10	122.99	111.40
1	B	476	PRO	C-N-CA	6.09	136.93	121.70
1	F	315	TRP	CA-C-N	-6.08	103.82	117.20
1	A	316	CYS	CA-CB-SG	-6.07	103.08	114.00
1	A	679	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	411	ASP	CB-CG-OD2	6.04	123.73	118.30
1	C	476	PRO	C-N-CA	6.03	136.77	121.70
1	A	597	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	598	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	477	VAL	CB-CA-C	5.99	122.77	111.40
1	C	552	ASP	CB-CG-OD2	5.98	123.68	118.30
1	C	665	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	52	LEU	CB-CG-CD2	5.94	121.11	111.00
1	A	44	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	315	TRP	CA-C-N	-5.88	104.27	117.20
1	D	393	ASP	CB-CG-OD2	5.88	123.59	118.30
1	F	142	ASP	CB-CG-OD2	5.87	123.59	118.30
1	F	315	TRP	C-N-CA	5.87	136.38	121.70
1	D	316	CYS	N-CA-C	5.86	126.82	111.00
1	C	749	ASP	CB-CG-OD2	5.85	123.56	118.30
1	C	625	ASP	CB-CG-OD2	5.83	123.55	118.30
1	D	424	ASP	CB-CG-OD2	5.82	123.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	511	ASP	CB-CG-OD2	5.81	123.53	118.30
1	E	432	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	642	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	316	CYS	CA-CB-SG	-5.79	103.58	114.00
1	B	511	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	52	LEU	CA-CB-CG	5.76	128.54	115.30
1	C	252	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	739	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	E	121	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	482	ASP	CB-CG-OD2	5.71	123.44	118.30
1	E	560	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	419	GLU	CA-CB-CG	5.67	125.88	113.40
1	C	378	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	393	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	29	ASP	CB-CG-OD2	5.64	123.37	118.30
1	D	553	ASP	CB-CG-OD2	5.58	123.32	118.30
1	E	411	ASP	CB-CG-OD2	5.57	123.32	118.30
1	F	645	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	612	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	679	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	56	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	C	454	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	121	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	429	ASP	CB-CG-OD2	5.50	123.25	118.30
1	F	511	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	20	LEU	CA-CB-CG	5.50	127.95	115.30
1	F	749	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	511	ASP	CB-CG-OD2	5.47	123.22	118.30
1	E	739	ARG	CG-CD-NE	-5.45	100.35	111.80
1	B	44	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	589	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	A	142	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	602	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	768	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	44	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	E	20	LEU	CA-CB-CG	5.37	127.66	115.30
1	E	416	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	315	TRP	C-N-CA	5.36	135.09	121.70
1	B	121	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	316	CYS	N-CA-C	5.33	125.39	111.00
1	D	273	LEU	CB-CG-CD2	5.30	120.02	111.00
1	A	645	ASP	CB-CG-OD2	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	625	ASP	CB-CG-OD2	5.29	123.06	118.30
1	F	282	ASP	CB-CG-OD2	5.29	123.06	118.30
1	F	39	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	D	597	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	317	ASP	CB-CG-OD1	5.23	123.00	118.30
1	D	612	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	612	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	316	CYS	N-CA-C	5.21	125.07	111.00
1	E	174	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	E	511	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	315	TRP	CA-C-N	-5.19	105.79	117.20
1	E	300	LEU	CB-CG-CD2	5.18	119.81	111.00
1	D	605	ASP	CB-CG-OD2	5.18	122.96	118.30
1	E	476	PRO	O-C-N	5.15	130.95	122.70
1	D	664	ARG	N-CA-CB	-5.14	101.34	110.60
1	C	44	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	F	315	TRP	O-C-N	5.10	130.86	122.70
1	B	768	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	420	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	E	679	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	315	TRP	O-C-N	5.06	130.80	122.70
1	D	675	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	625	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	476	PRO	O-C-N	5.02	130.74	122.70
1	E	664	ARG	NE-CZ-NH2	-5.01	117.79	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	316	CYS	CA
1	F	316	CYS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	315	TRP	Peptide
1	B	315	TRP	Peptide
1	D	315	TRP	Peptide
1	E	315	TRP	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	6226	0	5934	53	0
1	B	6226	0	5934	66	0
1	C	6226	0	5934	65	0
1	D	6226	0	5934	53	0
1	E	6226	0	5934	59	0
1	F	6226	0	5934	67	0
2	A	24	0	36	3	0
2	B	16	0	24	1	0
2	C	16	0	24	2	0
2	D	8	0	12	1	0
2	E	24	0	36	0	0
2	F	8	0	12	1	0
3	A	295	0	0	2	0
3	B	208	0	0	2	0
3	C	234	0	0	2	0
3	D	267	0	0	4	0
3	E	243	0	0	2	0
3	F	191	0	0	1	0
All	All	38890	0	35748	358	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 5.

All (358) 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:F:274:THR:HG22	1:F:276:SER:H	1.08	1.11
1:F:274:THR:HG21	1:F:540:HIS:ND1	1.67	1.06
1:E:668:LEU:HD21	1:E:714:LEU:HD12	1.33	1.06
1:F:32:MET:CE	1:F:94:ILE:HG23	1.99	0.92
1:F:32:MET:HE2	1:F:94:ILE:HG23	1.52	0.90
1:D:32:MET:HE2	1:D:101:ALA:HB1	1.57	0.86
1:E:669:LEU:HD23	1:E:671:LEU:HD11	1.56	0.86
1:D:212:HIS:HE1	1:D:238:GLU:H	1.21	0.86
1:B:579:ARG:HB2	1:B:579:ARG:HH11	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:MET:HE3	1:C:103:PHE:HB2	1.60	0.83
1:F:274:THR:CG2	1:F:276:SER:H	1.91	0.82
1:D:657:LEU:HD21	3:D:2206:HOH:O	1.79	0.81
1:B:300:LEU:HD13	1:B:340:LEU:HD21	1.62	0.81
1:A:300:LEU:HD13	1:A:340:LEU:HD21	1.62	0.81
1:D:695:ASP:OD1	1:D:719:THR:O	1.99	0.81
1:B:332:ILE:HD13	1:B:408:MET:O	1.81	0.80
1:D:723:ILE:HG23	1:D:770:ILE:HB	1.64	0.79
1:B:332:ILE:CD1	1:B:408:MET:O	2.31	0.78
1:C:246:THR:HG22	1:C:249:ALA:H	1.47	0.78
1:B:525:LYS:HG2	1:B:558:VAL:HG21	1.66	0.78
1:D:212:HIS:CE1	1:D:238:GLU:H	2.02	0.78
1:F:274:THR:HG22	1:F:276:SER:N	1.92	0.77
1:D:764:GLN:HA	1:D:764:GLN:HE21	1.49	0.77
1:D:201:MET:HE1	1:D:247:PRO:HA	1.66	0.77
1:C:525:LYS:HG2	1:C:558:VAL:HG21	1.65	0.77
1:C:332:ILE:HD11	1:C:409:GLY:HA3	1.66	0.76
1:E:638:LEU:O	1:E:739:ARG:NH2	2.18	0.76
1:F:668:LEU:HD21	1:F:714:LEU:HD22	1.67	0.75
1:F:273:LEU:HB2	1:F:300:LEU:HD21	1.69	0.75
1:B:300:LEU:CD1	1:B:340:LEU:HD21	2.16	0.74
1:A:332:ILE:HD11	1:A:409:GLY:HA3	1.69	0.73
1:F:13:GLY:O	1:F:143:THR:HB	1.88	0.72
1:D:566:LYS:HA	1:D:569:MET:HE2	1.71	0.72
1:D:32:MET:CE	1:D:101:ALA:HB1	2.20	0.71
1:B:695:ASP:HA	1:B:718:ARG:HG2	1.72	0.71
1:F:290:ILE:HD13	1:F:340:LEU:HD11	1.71	0.71
1:B:32:MET:HE3	1:B:103:PHE:HB2	1.71	0.70
1:C:764:GLN:HE21	1:C:764:GLN:HA	1.56	0.69
1:F:548:PRO:HG3	1:F:559:VAL:HG21	1.73	0.69
1:F:668:LEU:CD2	1:F:714:LEU:HD22	2.21	0.69
1:B:32:MET:HE2	1:B:94:ILE:HG23	1.75	0.69
1:D:723:ILE:C	1:D:723:ILE:HD13	2.13	0.68
1:B:290:ILE:CD1	1:B:335:LEU:HD22	2.22	0.68
1:B:32:MET:CE	1:B:94:ILE:HG23	2.24	0.68
1:A:744:VAL:HG21	1:A:770:ILE:HG23	1.76	0.67
1:C:174:ARG:O	1:C:177:GLN:HG3	1.95	0.66
1:B:30:ASN:ND2	3:B:2201:HOH:O	2.19	0.65
1:F:124:ARG:NH2	1:F:243:ASP:OD1	2.29	0.65
1:E:750:GLY:HA2	1:E:764:GLN:HG2	1.78	0.65
1:D:657:LEU:N	1:D:657:LEU:HD22	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:MET:HE1	1:F:94:ILE:HG23	1.75	0.64
1:A:744:VAL:HG22	1:A:771:THR:O	1.97	0.64
1:E:744:VAL:HG22	1:E:771:THR:O	1.98	0.64
1:F:560:ARG:HG3	1:F:560:ARG:HH11	1.63	0.64
1:C:185:ASP:OD2	2:C:2006:TRS:H31	1.98	0.64
1:D:723:ILE:CG2	1:D:770:ILE:HB	2.29	0.63
1:D:124:ARG:NH2	1:D:243:ASP:OD1	2.28	0.63
1:E:668:LEU:HD21	1:E:714:LEU:CD1	2.19	0.63
1:D:764:GLN:HA	1:D:764:GLN:NE2	2.12	0.63
1:F:290:ILE:HD13	1:F:340:LEU:CD1	2.27	0.63
1:B:579:ARG:HB2	1:B:579:ARG:NH1	2.14	0.62
1:E:174:ARG:HB3	1:E:220:VAL:HG11	1.80	0.62
1:B:463:LEU:O	1:B:477:VAL:HB	2.00	0.60
1:D:693:LEU:HD13	1:D:718:ARG:HB2	1.82	0.60
1:C:459:GLU:H	1:C:459:GLU:CD	2.03	0.59
1:E:630:LEU:O	1:E:647:SER:N	2.35	0.59
1:A:201:MET:HE1	1:A:250:VAL:HB	1.83	0.59
1:E:566:LYS:HA	1:E:569:MET:HE2	1.84	0.59
1:C:70:GLU:HG3	3:C:2154:HOH:O	2.02	0.59
1:B:638:LEU:O	1:B:739:ARG:NH2	2.36	0.58
1:D:352:GLN:HA	1:D:357:PHE:CD2	2.38	0.58
1:A:576:GLU:OE2	1:A:579:ARG:NH1	2.36	0.58
1:B:459:GLU:CD	1:B:459:GLU:H	2.07	0.58
1:E:735:THR:HG23	1:E:760:VAL:HG13	1.86	0.58
1:E:246:THR:HG22	1:E:249:ALA:H	1.69	0.58
1:F:744:VAL:HG22	1:F:771:THR:O	2.04	0.57
1:C:763:PRO:CB	1:C:768:LEU:HD21	2.35	0.57
1:E:459:GLU:CD	1:E:459:GLU:H	2.07	0.57
1:E:671:LEU:HD12	1:E:671:LEU:N	2.20	0.56
1:F:417:PHE:HA	1:F:419:GLU:OE2	2.06	0.56
1:B:31:GLU:OE1	1:B:56:ARG:HD3	2.05	0.56
1:A:124:ARG:HD3	1:A:243:ASP:OD1	2.05	0.56
1:E:289:PHE:HZ	1:E:545:TYR:CD1	2.24	0.56
1:F:744:VAL:HG21	1:F:770:ILE:HG23	1.88	0.56
1:B:579:ARG:CB	1:B:579:ARG:HH11	2.18	0.56
1:A:174:ARG:HB3	1:A:220:VAL:HG11	1.88	0.56
1:A:201:MET:HE2	1:A:247:PRO:HA	1.87	0.56
1:C:417:PHE:HA	1:C:419:GLU:OE2	2.06	0.55
1:F:220:VAL:HG13	1:F:228:VAL:HG22	1.88	0.55
1:A:652:GLN:NE2	1:A:654:HIS:NE2	2.55	0.55
1:C:341:LYS:C	1:C:342:ILE:HD12	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ILE:N	1:C:342:ILE:HD12	2.22	0.55
1:A:352:GLN:HA	1:A:357:PHE:CD2	2.42	0.55
1:A:123:LEU:HD12	1:A:128:ARG:HA	1.87	0.54
1:C:336:LYS:HE2	1:C:342:ILE:HD13	1.89	0.54
1:B:763:PRO:HB3	1:B:768:LEU:HD21	1.89	0.54
2:A:2008:TRS:H32	1:D:185:ASP:OD2	2.07	0.54
1:A:750:GLY:HA2	1:A:764:GLN:HG2	1.89	0.54
1:D:336:LYS:HD2	1:D:342:ILE:HD13	1.90	0.53
1:C:576:GLU:HG3	1:C:611:GLY:HA3	1.91	0.53
1:C:764:GLN:NE2	1:C:764:GLN:HA	2.22	0.53
1:E:201:MET:CE	1:E:247:PRO:HB3	2.38	0.53
1:A:515:PHE:CZ	2:A:2001:TRS:H22	2.44	0.53
1:E:583:ARG:NH1	3:E:2111:HOH:O	2.42	0.53
1:B:485:ALA:HB1	1:B:519:ALA:HB2	1.91	0.53
1:D:324:THR:HG21	3:D:2074:HOH:O	2.08	0.53
1:E:748:GLN:O	1:E:749:ASP:HB2	2.09	0.53
1:A:165:LEU:HA	1:A:197:ILE:O	2.09	0.53
1:B:560:ARG:HH11	1:B:560:ARG:HG3	1.74	0.53
1:A:336:LYS:HD2	1:A:342:ILE:HD13	1.90	0.52
1:C:260:ARG:HG3	1:C:581:ASN:O	2.09	0.52
1:C:65:VAL:HG12	1:C:108:LEU:HD21	1.90	0.52
1:C:65:VAL:HG12	1:C:108:LEU:CD2	2.40	0.52
1:D:201:MET:HE1	1:D:247:PRO:CA	2.39	0.52
1:A:183:ASN:HB3	1:A:419:GLU:HB3	1.92	0.52
1:C:308:PHE:CZ	1:D:44:ARG:HB3	2.44	0.52
1:F:248:LYS:NZ	1:F:594:GLU:OE1	2.34	0.52
1:E:273:LEU:HD13	1:E:274:THR:N	2.24	0.52
1:D:723:ILE:HD13	1:D:724:THR:N	2.25	0.52
1:C:634:ARG:HD3	1:C:643:GLU:OE2	2.10	0.52
1:F:300:LEU:HD12	1:F:340:LEU:HD21	1.92	0.51
1:D:183:ASN:HB3	1:D:419:GLU:HB3	1.91	0.51
1:B:572:TYR:CD1	1:B:669:LEU:HD11	2.45	0.51
1:A:185:ASP:OD2	2:A:2002:TRS:H32	2.11	0.51
1:C:328:PRO:O	1:C:332:ILE:HG23	2.11	0.51
1:F:652:GLN:NE2	1:F:654:HIS:NE2	2.58	0.51
1:C:298:LEU:CD2	1:C:560:ARG:HB2	2.41	0.51
1:E:695:ASP:HA	1:E:718:ARG:HG2	1.91	0.51
1:C:352:GLN:HA	1:C:357:PHE:CD2	2.45	0.51
1:F:429:ASP:OD1	1:F:431:SER:OG	2.23	0.51
1:A:31:GLU:OE1	1:A:56:ARG:HD3	2.11	0.51
1:F:668:LEU:O	1:F:701:CYS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLY:HA2	1:B:194:TYR:OH	2.11	0.50
1:E:163:TYR:HB3	1:E:502:LEU:HD13	1.92	0.50
1:D:725:VAL:HB	1:D:768:LEU:HB2	1.92	0.50
1:E:289:PHE:CZ	1:E:545:TYR:CD1	3.00	0.50
1:F:515:PHE:CZ	2:F:2011:TRS:H22	2.47	0.50
1:E:592:MET:HE2	1:E:592:MET:O	2.11	0.50
1:F:630:LEU:O	1:F:647:SER:N	2.43	0.50
1:E:137:ASN:HB3	1:E:152:GLU:OE1	2.11	0.50
1:C:32:MET:HE1	1:C:94:ILE:HG23	1.94	0.50
1:B:352:GLN:HA	1:B:357:PHE:CD2	2.47	0.49
1:E:557:ASP:OD1	1:E:560:ARG:NH2	2.45	0.49
1:B:70:GLU:HG3	3:B:2120:HOH:O	2.12	0.49
1:B:749:ASP:HB2	1:B:768:LEU:HA	1.94	0.49
1:F:690:LEU:HD21	1:F:693:LEU:HD12	1.94	0.49
1:C:447:LEU:HD23	1:C:447:LEU:C	2.32	0.49
1:E:506:GLY:HA2	1:E:586:PRO:HA	1.94	0.49
1:B:226:SER:O	1:B:227:LYS:HG3	2.13	0.49
1:E:449:TRP:CH2	1:E:476:PRO:HD2	2.48	0.49
1:A:273:LEU:HB2	1:A:300:LEU:HD21	1.95	0.49
1:B:768:LEU:N	1:B:768:LEU:CD1	2.76	0.49
1:D:736:LEU:HD11	1:D:738:LEU:HD23	1.95	0.49
1:B:32:MET:HE1	1:B:102:GLU:O	2.14	0.48
1:B:735:THR:HG23	1:B:760:VAL:HG13	1.95	0.48
1:E:201:MET:HE3	1:E:247:PRO:HB3	1.96	0.48
1:F:463:LEU:O	1:F:477:VAL:HB	2.13	0.48
1:D:565:LEU:HG	1:D:569:MET:HE1	1.96	0.48
1:C:516:GLU:O	1:C:517:ASN:HB2	2.13	0.48
1:C:718:ARG:HA	1:C:723:ILE:HG22	1.96	0.48
1:B:332:ILE:HD11	1:B:408:MET:O	2.12	0.48
1:A:744:VAL:HG21	1:A:770:ILE:CG2	2.44	0.48
1:B:572:TYR:CD1	1:B:669:LEU:CD1	2.97	0.48
1:D:631:PRO:O	1:D:646:GLY:HA3	2.14	0.48
1:F:763:PRO:HB2	1:F:765:GLY:O	2.14	0.48
1:B:736:LEU:CD1	1:B:738:LEU:HD21	2.44	0.48
1:C:579:ARG:NH1	1:C:579:ARG:HG3	2.28	0.48
1:C:745:ASN:HB2	1:C:773:HIS:HA	1.96	0.48
1:A:336:LYS:HD2	1:A:342:ILE:CD1	2.43	0.48
1:C:652:GLN:NE2	1:C:654:HIS:NE2	2.61	0.48
1:E:747:LEU:HD22	1:E:750:GLY:O	2.14	0.47
1:F:560:ARG:NH1	1:F:560:ARG:HG3	2.29	0.47
1:F:300:LEU:HD12	1:F:340:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:668:LEU:HD23	1:F:701:CYS:HB3	1.96	0.47
1:E:401:LYS:HE3	3:E:2183:HOH:O	2.14	0.47
1:D:698:GLU:OE1	1:D:715:LYS:HD3	2.14	0.47
1:A:736:LEU:CD1	1:A:738:LEU:CD2	2.93	0.47
1:D:431:SER:HB3	1:D:436:MET:HG2	1.95	0.47
1:A:443:ILE:HD11	3:A:2165:HOH:O	2.14	0.47
1:C:346:ILE:HD11	1:C:415:THR:HG22	1.96	0.47
1:A:569:MET:HB3	1:A:573:LEU:HD22	1.97	0.47
1:F:447:LEU:C	1:F:447:LEU:HD23	2.35	0.47
1:B:261:PRO:HA	1:B:473:GLN:O	2.15	0.47
1:F:526:ARG:HD2	1:F:619:VAL:HB	1.97	0.47
1:C:32:MET:HE3	1:C:103:PHE:CB	2.40	0.47
1:C:748:GLN:O	1:C:749:ASP:HB2	2.15	0.47
1:D:174:ARG:O	1:D:177:GLN:HG2	2.14	0.47
1:A:136:ASN:HB3	1:A:153:ARG:HB2	1.97	0.47
1:C:763:PRO:HB3	1:C:768:LEU:HD21	1.97	0.46
1:A:736:LEU:HD11	1:A:738:LEU:CD2	2.45	0.46
1:E:498:LEU:HD21	1:E:608:TYR:HB3	1.97	0.46
1:B:414:LYS:HE3	1:B:479:TRP:CH2	2.50	0.46
1:D:356:VAL:HG11	1:D:397:TRP:CZ2	2.50	0.46
1:E:165:LEU:HA	1:E:197:ILE:O	2.15	0.46
1:D:657:LEU:CD2	3:D:2206:HOH:O	2.53	0.46
1:E:246:THR:CG2	1:E:249:ALA:H	2.28	0.46
1:B:719:THR:HG22	1:B:722:THR:HB	1.97	0.46
1:F:200:TYR:CZ	1:F:208:VAL:HG13	2.50	0.46
1:F:246:THR:HG22	1:F:249:ALA:H	1.81	0.46
1:A:736:LEU:CD1	1:A:738:LEU:HD23	2.46	0.46
1:E:11:GLN:HA	1:E:12:PRO:HD3	1.81	0.46
1:F:165:LEU:HA	1:F:197:ILE:O	2.16	0.46
1:C:463:LEU:O	1:C:477:VAL:HB	2.16	0.46
1:B:273:LEU:HB2	1:B:300:LEU:HD21	1.98	0.46
1:E:336:LYS:HE3	1:E:411:ASP:OD2	2.16	0.46
1:C:631:PRO:O	1:C:646:GLY:HA3	2.16	0.46
1:A:332:ILE:HD12	1:A:336:LYS:HD3	1.97	0.46
1:B:568:ARG:CG	1:B:675:ASP:HB3	2.46	0.46
1:C:515:PHE:CZ	2:C:2005:TRS:H22	2.51	0.46
1:D:174:ARG:HB3	1:D:220:VAL:HG11	1.98	0.45
1:C:246:THR:HG23	3:C:2209:HOH:O	2.16	0.45
1:A:498:LEU:HD21	1:A:608:TYR:HB3	1.97	0.45
1:D:537:SER:HA	3:D:2245:HOH:O	2.16	0.45
1:A:201:MET:CE	1:A:250:VAL:HB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:TYR:HB3	1:B:84:LEU:HD13	1.98	0.45
1:C:32:MET:CE	1:C:103:PHE:HB2	2.39	0.45
1:B:631:PRO:HD2	1:B:635:TRP:CZ2	2.52	0.45
1:F:290:ILE:HD12	1:F:335:LEU:HD22	1.99	0.45
1:C:44:ARG:HB3	1:E:308:PHE:CZ	2.51	0.45
1:E:652:GLN:NE2	1:E:654:HIS:NE2	2.64	0.45
1:B:414:LYS:NZ	1:B:538:ARG:HH12	2.15	0.45
1:F:735:THR:HG23	1:F:760:VAL:HG13	1.98	0.45
1:A:44:ARG:HB3	1:F:308:PHE:CZ	2.52	0.45
1:F:18:HIS:O	1:F:38:PRO:HA	2.17	0.45
1:A:736:LEU:HD11	1:A:738:LEU:HD23	1.99	0.44
1:F:134:VAL:O	1:F:135:LYS:HB2	2.17	0.44
1:B:376:GLN:HA	1:B:384:LEU:O	2.18	0.44
1:D:447:LEU:C	1:D:447:LEU:HD23	2.37	0.44
1:D:723:ILE:C	1:D:723:ILE:CD1	2.84	0.44
1:C:290:ILE:CD1	1:C:335:LEU:HD22	2.48	0.44
1:D:736:LEU:CD1	1:D:738:LEU:HD23	2.47	0.44
1:B:576:GLU:HG3	1:B:611:GLY:HA3	1.99	0.44
1:D:515:PHE:CZ	2:D:2007:TRS:H22	2.52	0.44
1:F:588:MET:HG3	1:F:608:TYR:CD1	2.51	0.44
1:E:273:LEU:HD13	1:E:273:LEU:C	2.38	0.44
1:F:414:LYS:HE3	1:F:479:TRP:CH2	2.53	0.44
1:D:18:HIS:O	1:D:38:PRO:HA	2.16	0.44
1:C:32:MET:CE	1:C:94:ILE:HG23	2.48	0.44
1:D:764:GLN:CA	1:D:764:GLN:NE2	2.80	0.44
1:A:187:GLY:HA2	1:A:194:TYR:OH	2.18	0.44
1:B:768:LEU:HD12	1:B:768:LEU:N	2.33	0.44
1:C:526:ARG:HD2	1:C:619:VAL:HB	1.99	0.44
1:E:516:GLU:O	1:E:517:ASN:HB2	2.18	0.44
1:F:459:GLU:CD	1:F:459:GLU:H	2.21	0.44
1:F:444:TYR:O	1:F:448:VAL:HG23	2.18	0.44
1:F:598:ASP:HA	1:F:599:PRO:HD2	1.91	0.43
1:F:84:LEU:HB3	1:F:86:ILE:HD11	2.00	0.43
1:C:61:GLN:HB2	1:C:64:ILE:HD12	1.99	0.43
1:C:200:TYR:CZ	1:C:208:VAL:HG13	2.53	0.43
1:F:352:GLN:HA	1:F:357:PHE:CD2	2.53	0.43
1:A:431:SER:HB3	1:A:436:MET:HG2	2.00	0.43
1:B:690:LEU:O	1:B:739:ARG:HB2	2.17	0.43
1:D:498:LEU:HD21	1:D:608:TYR:HB3	2.01	0.43
1:B:285:THR:O	1:B:288:SER:HB3	2.19	0.43
1:A:205:GLY:HA3	1:A:245:PRO:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:HIS:O	1:C:38:PRO:HA	2.18	0.43
1:A:414:LYS:HE3	1:A:479:TRP:CH2	2.53	0.43
1:F:576:GLU:HG3	1:F:611:GLY:HA3	2.00	0.43
1:E:635:TRP:O	1:E:643:GLU:HA	2.19	0.43
1:F:273:LEU:HD22	1:F:274:THR:H	1.81	0.43
1:C:82:TYR:HB3	1:C:84:LEU:HD13	2.00	0.43
1:A:201:MET:HE3	1:A:201:MET:HB2	1.82	0.43
1:C:595:PHE:CE1	1:C:631:PRO:HG2	2.52	0.43
1:B:133:GLN:O	1:B:136:ASN:HB2	2.19	0.43
1:E:419:GLU:HG3	1:E:467:SER:HB3	2.00	0.43
1:B:32:MET:HB2	1:B:32:MET:HE2	1.67	0.43
1:B:296:ARG:O	1:B:560:ARG:NH1	2.37	0.43
1:A:646:GLY:O	1:A:647:SER:HB2	2.19	0.43
1:E:261:PRO:HA	1:E:473:GLN:O	2.18	0.43
1:C:267:TRP:CE3	1:C:341:LYS:HG3	2.54	0.43
1:B:768:LEU:H	1:B:768:LEU:CD1	2.31	0.43
1:F:635:TRP:CH2	1:F:664:ARG:HB3	2.54	0.43
1:B:18:HIS:O	1:B:38:PRO:HA	2.19	0.43
1:C:630:LEU:O	1:C:647:SER:N	2.51	0.43
1:C:274:THR:HG22	1:C:304:HIS:HB3	2.01	0.43
1:B:321:ASP:HA	1:B:322:PRO:HD3	1.91	0.43
1:D:565:LEU:HG	1:D:569:MET:CE	2.49	0.43
1:F:498:LEU:HD21	1:F:608:TYR:HB3	2.01	0.42
1:A:731:ALA:O	1:A:732:LYS:HD2	2.18	0.42
1:F:80:PRO:HD3	1:F:431:SER:HB3	2.01	0.42
1:C:579:ARG:HH11	1:C:579:ARG:HG3	1.83	0.42
1:E:290:ILE:HD13	1:E:340:LEU:CD1	2.48	0.42
1:E:187:GLY:HA2	1:E:194:TYR:OH	2.19	0.42
1:A:267:TRP:CE3	1:A:341:LYS:HG3	2.54	0.42
1:C:449:TRP:CH2	1:C:476:PRO:HD2	2.54	0.42
1:D:31:GLU:OE1	1:D:56:ARG:HD3	2.19	0.42
1:F:500:ILE:HG12	1:F:505:PHE:HB2	2.00	0.42
1:E:671:LEU:N	1:E:671:LEU:CD1	2.82	0.42
1:B:32:MET:HE1	1:B:94:ILE:HG23	1.99	0.42
1:E:246:THR:HG22	1:E:249:ALA:CB	2.50	0.42
1:E:267:TRP:CE3	1:E:341:LYS:HG3	2.54	0.42
1:C:744:VAL:HG22	1:C:771:THR:O	2.18	0.42
1:D:275:THR:O	1:D:276:SER:HB2	2.20	0.42
1:C:32:MET:HE1	1:C:102:GLU:O	2.18	0.42
1:D:657:LEU:N	1:D:657:LEU:CD2	2.81	0.42
1:A:300:LEU:CD1	1:A:340:LEU:HD21	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:PHE:CZ	2:B:2003:TRS:H22	2.55	0.42
1:E:669:LEU:HD23	1:E:671:LEU:CD1	2.40	0.42
1:E:297:ASN:O	1:E:560:ARG:CD	2.68	0.42
1:A:289:PHE:HZ	1:A:545:TYR:CD1	2.37	0.42
1:D:635:TRP:O	1:D:643:GLU:HA	2.20	0.42
1:B:332:ILE:HD12	1:B:333:ARG:N	2.35	0.42
1:E:744:VAL:HG21	1:E:770:ILE:CG2	2.49	0.42
1:B:32:MET:HE3	1:B:103:PHE:CB	2.46	0.42
1:B:572:TYR:CG	1:B:669:LEU:HD11	2.55	0.42
1:F:179:VAL:HG22	1:F:218:PHE:HB2	2.00	0.42
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.84	0.42
1:B:278:THR:HG21	1:F:45:THR:HA	2.01	0.41
1:E:77:ASN:O	1:E:77:ASN:ND2	2.50	0.41
1:B:525:LYS:CG	1:B:558:VAL:HG21	2.45	0.41
1:F:246:THR:CG2	1:F:249:ALA:H	2.33	0.41
1:A:685:GLY:HA2	1:A:733:ASN:O	2.21	0.41
1:C:485:ALA:HB1	1:C:519:ALA:HB2	2.02	0.41
1:F:274:THR:HB	1:F:539:LEU:O	2.20	0.41
1:C:447:LEU:HD23	1:C:447:LEU:O	2.21	0.41
1:B:449:TRP:CH2	1:B:476:PRO:HD2	2.55	0.41
1:E:315:TRP:O	1:E:350:ILE:HA	2.20	0.41
1:F:277:PHE:CD2	1:F:278:THR:HG23	2.55	0.41
1:A:300:LEU:HD13	1:A:340:LEU:CD2	2.42	0.41
1:A:336:LYS:CD	1:A:342:ILE:HD13	2.49	0.41
1:A:184:ARG:HD2	3:A:2032:HOH:O	2.19	0.41
1:E:191:GLU:HB3	1:F:222:SER:O	2.20	0.41
1:C:32:MET:HB2	1:C:32:MET:HE2	1.63	0.41
1:E:689:HIS:ND1	1:E:739:ARG:NH1	2.64	0.41
1:C:267:TRP:CD2	1:C:341:LYS:HG3	2.55	0.41
1:E:273:LEU:HD13	1:E:274:THR:O	2.21	0.41
1:D:136:ASN:HB3	1:D:153:ARG:HB2	2.02	0.41
1:C:719:THR:CG2	1:C:722:THR:HB	2.50	0.41
1:D:200:TYR:CZ	1:D:208:VAL:HG13	2.55	0.41
1:C:298:LEU:HD23	1:C:560:ARG:HB2	2.01	0.41
1:C:300:LEU:HG	1:C:340:LEU:HD21	2.02	0.41
1:C:594:GLU:HG2	1:C:609:MET:HG3	2.02	0.41
1:E:201:MET:HE1	1:E:247:PRO:HB3	2.03	0.41
1:F:208:VAL:HA	1:F:240:PHE:O	2.21	0.41
1:E:414:LYS:NZ	1:E:538:ARG:HH12	2.19	0.41
1:D:191:GLU:N	1:D:191:GLU:OE1	2.50	0.41
1:D:652:GLN:NE2	1:D:654:HIS:NE2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:TRP:O	1:F:350:ILE:HA	2.21	0.41
1:A:82:TYR:HB3	1:A:84:LEU:HD13	2.02	0.41
1:F:174:ARG:NH2	3:F:2078:HOH:O	2.33	0.41
1:F:163:TYR:HB3	1:F:502:LEU:HD13	2.03	0.41
1:A:736:LEU:HD13	1:A:736:LEU:C	2.41	0.40
1:B:569:MET:HB3	1:B:573:LEU:HD22	2.02	0.40
1:D:594:GLU:HG2	1:D:609:MET:HG3	2.02	0.40
1:A:748:GLN:HB3	1:A:769:THR:HG23	2.02	0.40
1:B:201:MET:HE1	1:B:247:PRO:HA	2.02	0.40
1:A:700:VAL:HG22	1:A:715:LYS:HG2	2.04	0.40
1:A:630:LEU:HG	1:A:635:TRP:CD1	2.57	0.40
1:E:402:LEU:HD12	1:E:451:VAL:HG21	2.03	0.40
1:B:718:ARG:HA	1:B:723:ILE:HG22	2.03	0.40
1:D:736:LEU:C	1:D:736:LEU:HD13	2.42	0.40
1:C:717:ALA:O	1:C:723:ILE:HA	2.21	0.40
1:B:617:ALA:O	1:B:660:PRO:HD2	2.22	0.40
1:A:417:PHE:HA	1:A:419:GLU:OE2	2.22	0.40
1:F:635:TRP:O	1:F:643:GLU:HA	2.21	0.40
1:B:684:GLU:HG2	1:B:732:LYS:HB2	2.03	0.40
1:E:84:LEU:HD12	1:E:258:THR:HG22	2.03	0.40
1:E:352:GLN:HA	1:E:357:PHE:CD2	2.55	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	771/778 (99%)	742 (96%)	25 (3%)	4 (0%)	34	30
1	B	771/778 (99%)	746 (97%)	24 (3%)	1 (0%)	56	58
1	C	771/778 (99%)	745 (97%)	24 (3%)	2 (0%)	46	45
1	D	771/778 (99%)	741 (96%)	28 (4%)	2 (0%)	46	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	771/778 (99%)	738 (96%)	27 (4%)	6 (1%)	24	17
1	F	771/778 (99%)	737 (96%)	29 (4%)	5 (1%)	30	24
All	All	4626/4668 (99%)	4449 (96%)	157 (3%)	20 (0%)	39	37

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	477	VAL
1	E	766	ASN
1	F	749	ASP
1	C	749	ASP
1	A	338	LYS
1	E	316	CYS
1	E	477	VAL
1	F	77	ASN
1	A	477	VAL
1	A	692	ASN
1	B	477	VAL
1	D	338	LYS
1	E	720	GLY
1	F	477	VAL
1	F	692	ASN
1	C	477	VAL
1	A	348	PRO
1	E	765	GLY
1	E	681	VAL
1	F	348	PRO

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	659/665 (99%)	627 (95%)	32 (5%)	31	28
1	B	659/665 (99%)	622 (94%)	37 (6%)	26	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	659/665 (99%)	622 (94%)	37 (6%)	26	22
1	D	659/665 (99%)	625 (95%)	34 (5%)	29	25
1	E	659/665 (99%)	624 (95%)	35 (5%)	28	25
1	F	659/665 (99%)	617 (94%)	42 (6%)	22	18
All	All	3954/3990 (99%)	3737 (94%)	217 (6%)	27	23

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	52	LEU
1	A	70	GLU
1	A	84	LEU
1	A	120	LEU
1	A	123	LEU
1	A	174	ARG
1	A	178	THR
1	A	180	GLU
1	A	273	LEU
1	A	300	LEU
1	A	306	ASP
1	A	316	CYS
1	A	332	ILE
1	A	336	LYS
1	A	377	TRP
1	A	419	GLU
1	A	452	LEU
1	A	464	PHE
1	A	479	TRP
1	A	573	LEU
1	A	592	MET
1	A	614	VAL
1	A	616	VAL
1	A	630	LEU
1	A	657	LEU
1	A	719	THR
1	A	732	LYS
1	A	747	LEU
1	A	756	GLU
1	A	762	LYS
1	A	769	THR

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Mol	Chain	Res	Type
1	B	48	LEU
1	B	69	ILE
1	B	84	LEU
1	B	99	ARG
1	B	120	LEU
1	B	123	LEU
1	B	174	ARG
1	B	208	VAL
1	B	273	LEU
1	B	281	TYR
1	B	316	CYS
1	B	324	THR
1	B	336	LYS
1	B	338	LYS
1	B	377	TRP
1	B	408	MET
1	B	444	TYR
1	B	452	LEU
1	B	464	PHE
1	B	479	TRP
1	B	533	LEU
1	B	573	LEU
1	B	579	ARG
1	B	583	ARG
1	B	614	VAL
1	B	616	VAL
1	B	630	LEU
1	B	693	LEU
1	B	714	LEU
1	B	723	ILE
1	B	735	THR
1	B	739	ARG
1	B	744	VAL
1	B	748	GLN
1	B	766	ASN
1	B	768	LEU
1	B	769	THR
1	C	26	GLU
1	C	52	LEU
1	C	84	LEU
1	C	91	LYS
1	C	99	ARG

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Mol	Chain	Res	Type
1	C	120	LEU
1	C	124	ARG
1	C	177	GLN
1	C	208	VAL
1	C	246	THR
1	C	260	ARG
1	C	306	ASP
1	C	316	CYS
1	C	332	ILE
1	C	333	ARG
1	C	336	LYS
1	C	377	TRP
1	C	419	GLU
1	C	444	TYR
1	C	452	LEU
1	C	459	GLU
1	C	464	PHE
1	C	479	TRP
1	C	573	LEU
1	C	579	ARG
1	C	592	MET
1	C	616	VAL
1	C	630	LEU
1	C	657	LEU
1	C	693	LEU
1	C	723	ILE
1	C	732	LYS
1	C	744	VAL
1	C	748	GLN
1	C	754	GLU
1	C	768	LEU
1	C	769	THR
1	D	48	LEU
1	D	52	LEU
1	D	84	LEU
1	D	99	ARG
1	D	116	GLU
1	D	120	LEU
1	D	123	LEU
1	D	146	GLN
1	D	174	ARG
1	D	208	VAL

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Mol	Chain	Res	Type
1	D	273	LEU
1	D	281	TYR
1	D	316	CYS
1	D	336	LYS
1	D	377	TRP
1	D	419	GLU
1	D	452	LEU
1	D	459	GLU
1	D	464	PHE
1	D	479	TRP
1	D	533	LEU
1	D	592	MET
1	D	614	VAL
1	D	630	LEU
1	D	671	LEU
1	D	693	LEU
1	D	723	ILE
1	D	743	LYS
1	D	747	LEU
1	D	748	GLN
1	D	749	ASP
1	D	759	LEU
1	D	764	GLN
1	D	769	THR
1	E	48	LEU
1	E	77	ASN
1	E	84	LEU
1	E	120	LEU
1	E	174	ARG
1	E	179	VAL
1	E	208	VAL
1	E	246	THR
1	E	300	LEU
1	E	316	CYS
1	E	336	LYS
1	E	377	TRP
1	E	452	LEU
1	E	459	GLU
1	E	464	PHE
1	E	479	TRP
1	E	533	LEU
1	E	573	LEU

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Mol	Chain	Res	Type
1	E	592	MET
1	E	614	VAL
1	E	616	VAL
1	E	630	LEU
1	E	647	SER
1	E	669	LEU
1	E	735	THR
1	E	739	ARG
1	E	742	VAL
1	E	744	VAL
1	E	745	ASN
1	E	747	LEU
1	E	748	GLN
1	E	749	ASP
1	E	757	GLN
1	E	764	GLN
1	E	769	THR
1	F	48	LEU
1	F	52	LEU
1	F	84	LEU
1	F	91	LYS
1	F	95	GLU
1	F	99	ARG
1	F	120	LEU
1	F	123	LEU
1	F	143	THR
1	F	179	VAL
1	F	204	ARG
1	F	208	VAL
1	F	246	THR
1	F	260	ARG
1	F	273	LEU
1	F	274	THR
1	F	300	LEU
1	F	316	CYS
1	F	336	LYS
1	F	377	TRP
1	F	408	MET
1	F	419	GLU
1	F	444	TYR
1	F	452	LEU
1	F	459	GLU

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Mol	Chain	Res	Type
1	F	464	PHE
1	F	479	TRP
1	F	533	LEU
1	F	573	LEU
1	F	614	VAL
1	F	630	LEU
1	F	651	LYS
1	F	657	LEU
1	F	664	ARG
1	F	693	LEU
1	F	735	THR
1	F	736	LEU
1	F	742	VAL
1	F	756	GLU
1	F	759	LEU
1	F	769	THR
1	F	772	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	107	ASN
1	A	125	ASN
1	A	133	GLN
1	A	280	ASN
1	A	517	ASN
1	A	564	GLN
1	A	652	GLN
1	A	697	HIS
1	B	27	GLN
1	B	77	ASN
1	B	517	ASN
1	B	692	ASN
1	C	15	ASN
1	C	27	GLN
1	C	141	GLN
1	C	146	GLN
1	C	177	GLN
1	C	517	ASN
1	C	564	GLN
1	C	652	GLN

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Mol	Chain	Res	Type
1	C	692	ASN
1	C	764	GLN
1	D	27	GLN
1	D	73	GLN
1	D	146	GLN
1	D	212	HIS
1	D	652	GLN
1	D	692	ASN
1	D	764	GLN
1	D	766	ASN
1	E	27	GLN
1	E	73	GLN
1	E	77	ASN
1	E	280	ASN
1	E	287	ASN
1	E	517	ASN
1	E	564	GLN
1	E	652	GLN
1	E	692	ASN
1	E	721	ASN
1	E	745	ASN
1	E	748	GLN
1	E	764	GLN
1	E	766	ASN
1	F	27	GLN
1	F	73	GLN
1	F	125	ASN
1	F	133	GLN
1	F	146	GLN
1	F	280	ASN
1	F	517	ASN
1	F	564	GLN
1	F	652	GLN
1	F	692	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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
2	TRS	A	2001	-	7,7,7	1.21	1 (14%)	9,9,9	0.94	0
2	TRS	A	2002	-	7,7,7	1.11	1 (14%)	9,9,9	1.95	3 (33%)
2	TRS	A	2008	-	7,7,7	1.37	1 (14%)	9,9,9	2.28	3 (33%)
2	TRS	B	2003	-	7,7,7	1.00	0	9,9,9	2.07	4 (44%)
2	TRS	B	2004	-	7,7,7	0.92	1 (14%)	9,9,9	1.26	2 (22%)
2	TRS	C	2005	-	7,7,7	1.21	1 (14%)	9,9,9	1.04	0
2	TRS	C	2006	-	7,7,7	1.14	1 (14%)	9,9,9	1.49	2 (22%)
2	TRS	D	2007	-	7,7,7	0.73	0	9,9,9	1.17	1 (11%)
2	TRS	E	2009	-	7,7,7	1.21	1 (14%)	9,9,9	1.36	1 (11%)
2	TRS	E	2010	-	7,7,7	0.89	1 (14%)	9,9,9	1.22	0
2	TRS	E	2012	-	7,7,7	1.14	1 (14%)	9,9,9	1.18	1 (11%)
2	TRS	F	2011	-	7,7,7	1.16	1 (14%)	9,9,9	0.99	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	TRS	A	2001	-	-	0/9/9/9	0/0/0/0
2	TRS	A	2002	-	-	0/9/9/9	0/0/0/0
2	TRS	A	2008	-	-	0/9/9/9	0/0/0/0
2	TRS	B	2003	-	-	0/9/9/9	0/0/0/0
2	TRS	B	2004	-	-	0/9/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	C	2005	-	-	0/9/9/9	0/0/0/0
2	TRS	C	2006	-	-	0/9/9/9	0/0/0/0
2	TRS	D	2007	-	-	0/9/9/9	0/0/0/0
2	TRS	E	2009	-	-	0/9/9/9	0/0/0/0
2	TRS	E	2010	-	-	0/9/9/9	0/0/0/0
2	TRS	E	2012	-	-	0/9/9/9	0/0/0/0
2	TRS	F	2011	-	-	0/9/9/9	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2008	TRS	C-N	-3.28	1.45	1.50
2	C	2005	TRS	C-N	-3.04	1.46	1.50
2	A	2001	TRS	C-N	-2.91	1.46	1.50
2	F	2011	TRS	C-N	-2.82	1.46	1.50
2	E	2012	TRS	C-N	-2.79	1.46	1.50
2	E	2009	TRS	C-N	-2.64	1.46	1.50
2	A	2002	TRS	C-N	-2.62	1.46	1.50
2	C	2006	TRS	C-N	-2.55	1.46	1.50
2	B	2004	TRS	C-N	-2.29	1.47	1.50
2	E	2010	TRS	C-N	-2.02	1.47	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2008	TRS	C3-C-N	-3.72	101.31	108.09
2	C	2006	TRS	C3-C-N	-3.65	101.44	108.09
2	A	2008	TRS	O2-C2-C	-3.37	104.37	111.18
2	B	2003	TRS	O2-C2-C	-2.92	105.27	111.18
2	E	2009	TRS	O2-C2-C	-2.89	105.34	111.18
2	B	2003	TRS	C3-C-C1	-2.76	104.80	110.78
2	B	2003	TRS	C2-C-N	-2.76	103.07	108.09
2	A	2002	TRS	C3-C-C2	-2.52	105.33	110.78
2	E	2012	TRS	O2-C2-C	-2.36	106.41	111.18
2	D	2007	TRS	O2-C2-C	-2.33	106.46	111.18
2	B	2004	TRS	O2-C2-C	-2.03	107.07	111.18
2	A	2002	TRS	C1-C-N	-2.02	104.42	108.09
2	B	2004	TRS	C3-C-C1	2.07	115.27	110.78
2	C	2006	TRS	C1-C-N	2.21	112.12	108.09
2	B	2003	TRS	C3-C-N	2.24	112.16	108.09
2	A	2002	TRS	C3-C-C1	3.51	118.39	110.78
2	A	2008	TRS	C3-C-C1	3.54	118.44	110.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	TRS	1	0
2	A	2002	TRS	1	0
2	A	2008	TRS	1	0
2	B	2003	TRS	1	0
2	C	2005	TRS	1	0
2	C	2006	TRS	1	0
2	D	2007	TRS	1	0
2	F	2011	TRS	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	773/778 (99%)	-0.44	2 (0%) 94 95	9, 18, 33, 43	0
1	B	773/778 (99%)	-0.43	14 (1%) 71 76	12, 22, 48, 65	0
1	C	773/778 (99%)	-0.44	7 (0%) 85 88	11, 20, 41, 61	0
1	D	773/778 (99%)	-0.57	4 (0%) 91 93	9, 17, 32, 46	0
1	E	773/778 (99%)	-0.43	12 (1%) 74 79	9, 19, 45, 71	0
1	F	773/778 (99%)	-0.22	25 (3%) 51 60	11, 23, 53, 71	0
All	All	4638/4668 (99%)	-0.42	64 (1%) 78 82	9, 20, 42, 71	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	765	GLY	7.7
1	F	719	THR	5.2
1	B	765	GLY	5.0
1	F	766	ASN	5.0
1	E	765	GLY	4.8
1	F	767	ALA	4.8
1	F	742	VAL	4.5
1	E	744	VAL	4.2
1	E	719	THR	4.2
1	F	749	ASP	4.1
1	C	766	ASN	3.9
1	E	767	ALA	3.8
1	E	747	LEU	3.8
1	B	742	VAL	3.7
1	F	764	GLN	3.6
1	F	745	ASN	3.5
1	F	750	GLY	3.5
1	E	764	GLN	3.5
1	B	719	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	754	GLU	3.4
1	C	767	ALA	3.3
1	E	756	GLU	3.2
1	D	765	GLY	3.2
1	F	768	LEU	3.2
1	B	767	ALA	3.1
1	F	723	ILE	3.1
1	B	88	GLN	3.0
1	D	88	GLN	2.9
1	C	749	ASP	2.9
1	B	745	ASN	2.8
1	F	743	LYS	2.8
1	C	719	THR	2.8
1	F	748	GLN	2.7
1	F	747	LEU	2.7
1	F	746	GLY	2.7
1	B	743	LYS	2.6
1	F	722	THR	2.6
1	F	744	VAL	2.6
1	E	766	ASN	2.6
1	A	744	VAL	2.6
1	F	741	VAL	2.4
1	D	719	THR	2.4
1	E	749	ASP	2.4
1	B	723	ILE	2.3
1	A	745	ASN	2.3
1	F	753	ALA	2.2
1	B	772	LEU	2.2
1	D	76	LEU	2.2
1	B	768	LEU	2.2
1	E	722	THR	2.2
1	F	337	ALA	2.2
1	E	733	ASN	2.1
1	C	742	VAL	2.1
1	C	747	LEU	2.1
1	B	749	ASP	2.1
1	F	738	LEU	2.1
1	F	759	LEU	2.1
1	E	695	ASP	2.1
1	B	323	LEU	2.0
1	F	731	ALA	2.0
1	C	741	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	764	GLN	2.0
1	B	766	ASN	2.0
1	F	769	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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
2	TRS	E	2012	8/8	0.94	0.12	5.00	26,27,30,30	0
2	TRS	E	2010	8/8	0.93	0.10	4.48	23,23,26,27	0
2	TRS	C	2006	8/8	0.88	0.12	4.01	29,31,32,33	0
2	TRS	C	2005	8/8	0.94	0.11	3.21	20,21,23,26	0
2	TRS	B	2004	8/8	0.92	0.10	3.05	26,26,28,28	0
2	TRS	A	2002	8/8	0.92	0.11	2.81	28,29,29,32	0
2	TRS	D	2007	8/8	0.96	0.10	2.65	14,16,17,22	0
2	TRS	E	2009	8/8	0.95	0.09	2.54	13,14,16,21	0
2	TRS	A	2008	8/8	0.95	0.10	1.98	25,26,26,27	0
2	TRS	B	2003	8/8	0.95	0.09	1.73	18,18,19,24	0
2	TRS	A	2001	8/8	0.95	0.11	1.57	13,15,16,22	0
2	TRS	F	2011	8/8	0.96	0.10	1.19	18,21,22,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.