



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:50 PM GMT

PDB ID : 3V4T
Title : E. cloacae C115D MURA liganded with UNAG
Authors : Zhu, J.-Y.; Yang, Y.; Schonbrunn, E.
Deposited on : 2011-12-15
Resolution : 2.50 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

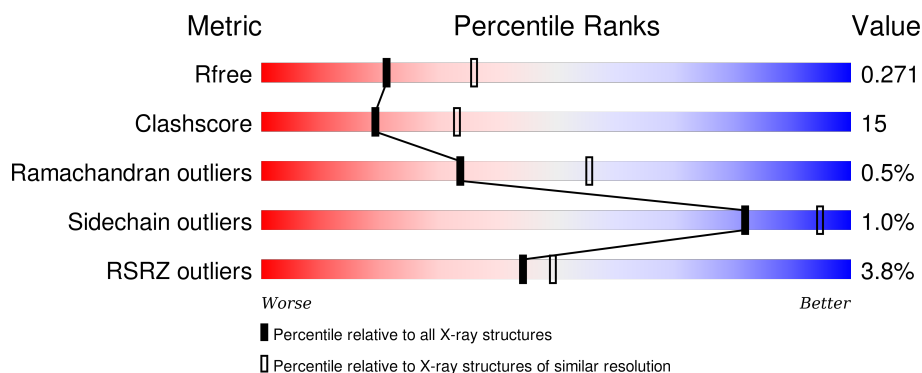
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	419	<div> <div>74%</div> <div>26%</div> </div>
1	B	419	<div>11%</div> <div>61%</div> <div>38%</div> <div>.</div>
1	C	419	<div>2%</div> <div>69%</div> <div>30%</div> <div>.</div>
1	D	419	<div>4%</div> <div>70%</div> <div>29%</div> <div>.</div>
1	E	419	<div>4%</div> <div>68%</div> <div>31%</div> <div>.</div>

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Mol	Chain	Length	Quality of chain
1	F	419	
1	G	419	
1	H	419	

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
3	ACT	A	502	-	-	-	X
3	ACT	A	505	-	-	-	X
3	ACT	B	502	-	-	-	X
3	ACT	C	502	-	-	X	-
3	ACT	C	503	-	-	X	X
3	ACT	D	502	-	-	-	X
3	ACT	E	502	-	-	X	-
3	ACT	F	503	-	-	X	X
3	ACT	H	503	-	-	-	X
3	ACT	H	505	-	-	-	X
3	ACT	H	506	-	-	-	X
4	EDO	A	507	-	-	-	X
4	EDO	A	509	-	-	-	X
4	EDO	B	505	-	-	-	X
4	EDO	C	506	-	-	-	X
4	EDO	D	506	-	-	-	X
4	EDO	D	510	-	-	-	X
4	EDO	E	507	-	-	-	X
4	EDO	F	506	-	-	-	X
4	EDO	F	509	-	-	-	X
4	EDO	G	504	-	-	-	X
4	EDO	G	507	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26190 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	B	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	C	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	D	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	E	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	F	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	G	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	H	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			

There are 16 discrepancies between the modelled and reference sequences:

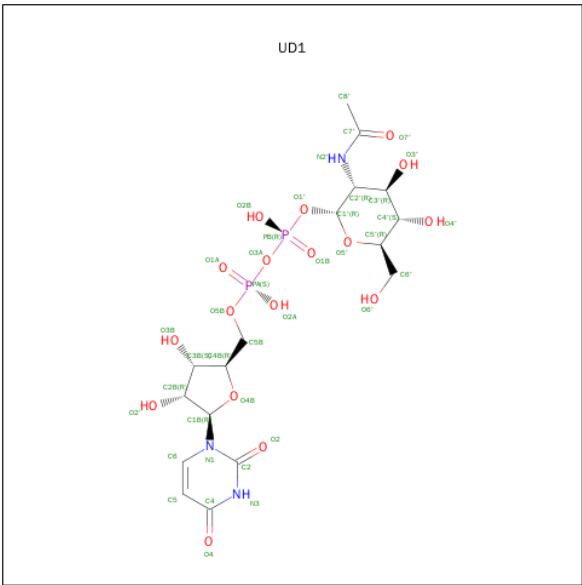
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	SEE REMARK 999	UNP P33038
A	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
B	67	IAS	ASN	SEE REMARK 999	UNP P33038
B	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
C	67	IAS	ASN	SEE REMARK 999	UNP P33038
C	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
D	67	IAS	ASN	SEE REMARK 999	UNP P33038
D	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
E	67	IAS	ASN	SEE REMARK 999	UNP P33038
E	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
F	67	IAS	ASN	SEE REMARK 999	UNP P33038
F	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
G	67	IAS	ASN	SEE REMARK 999	UNP P33038

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Chain	Residue	Modelled	Actual	Comment	Reference
G	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
H	67	IAS	ASN	SEE REMARK 999	UNP P33038
H	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	E	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	F	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	G	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	H	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



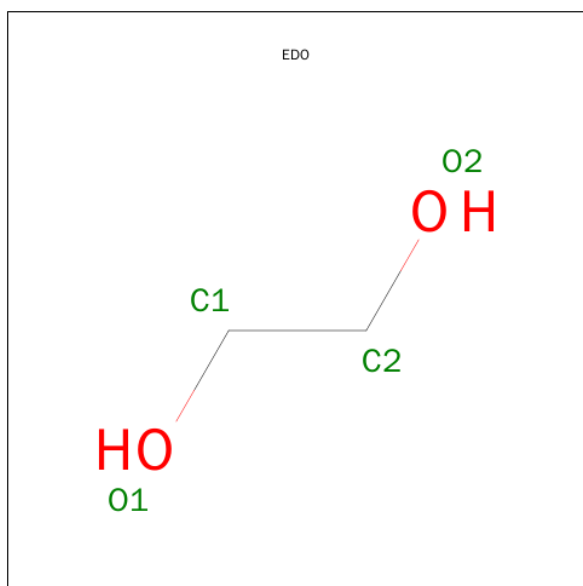
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		

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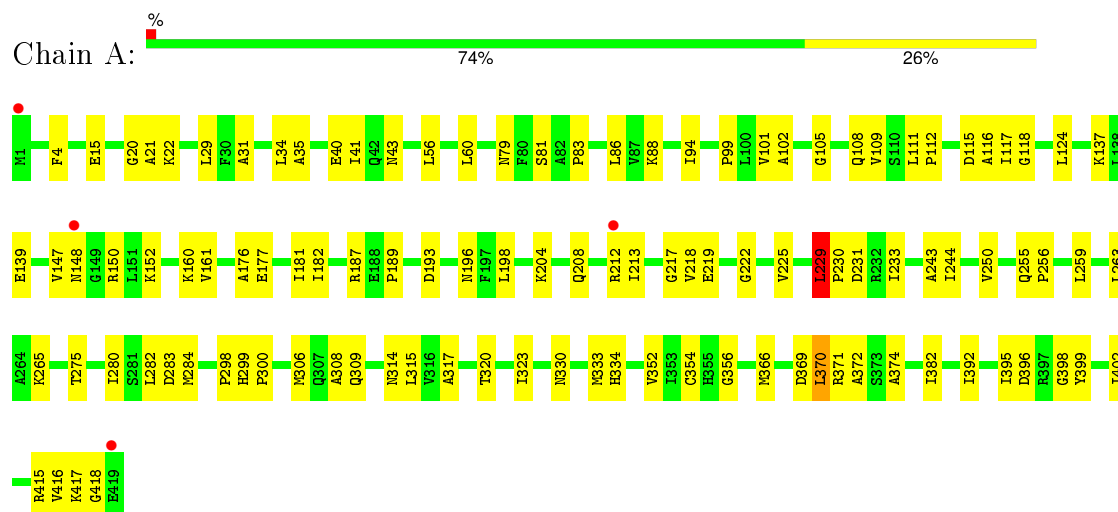
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	33	Total 33	O 33	0	0
5	C	53	Total 53	O 53	0	0
5	D	61	Total 61	O 61	0	0
5	E	66	Total 66	O 66	0	0
5	F	60	Total 60	O 60	0	0
5	G	67	Total 67	O 67	0	0
5	H	63	Total 63	O 63	0	0

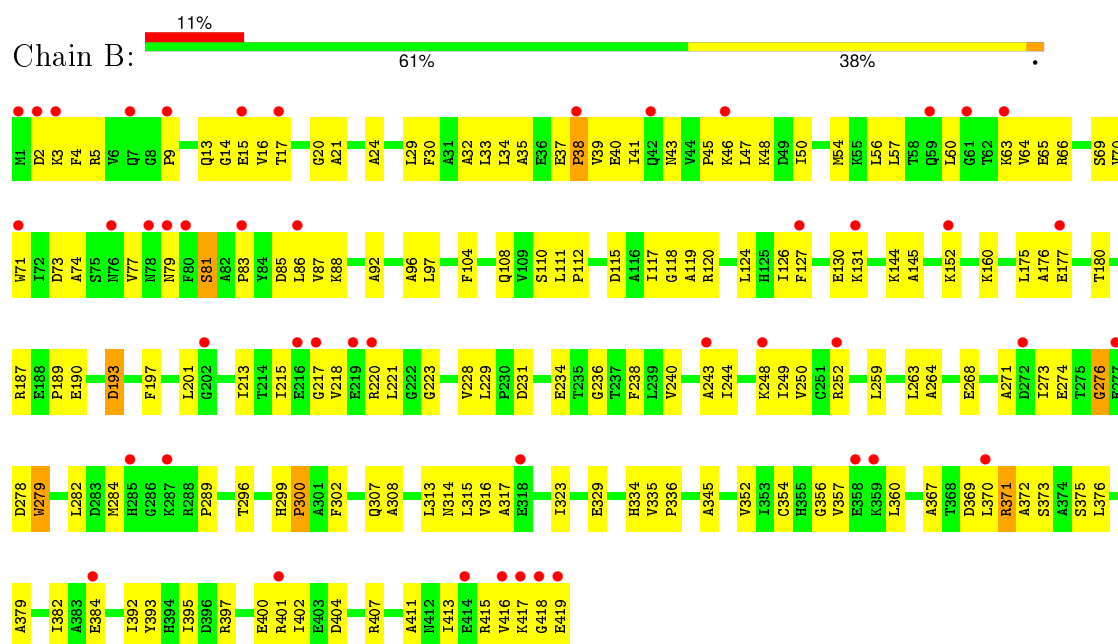
3 Residue-property plots

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.

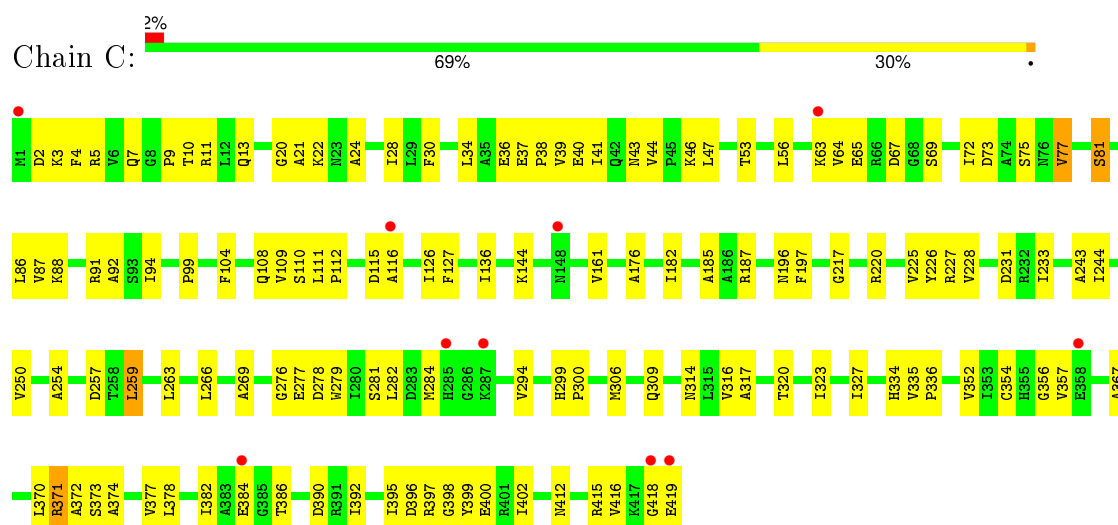
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



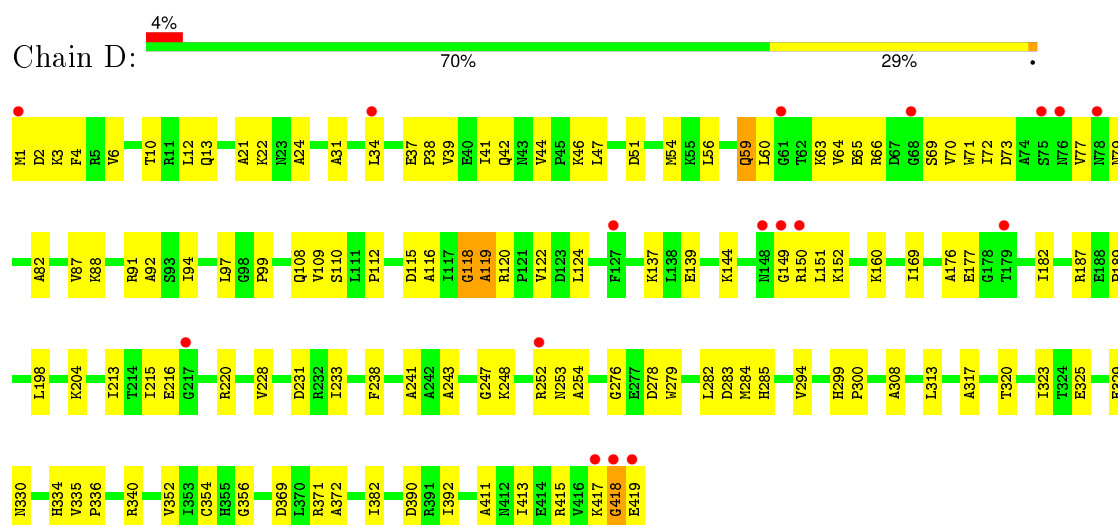
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



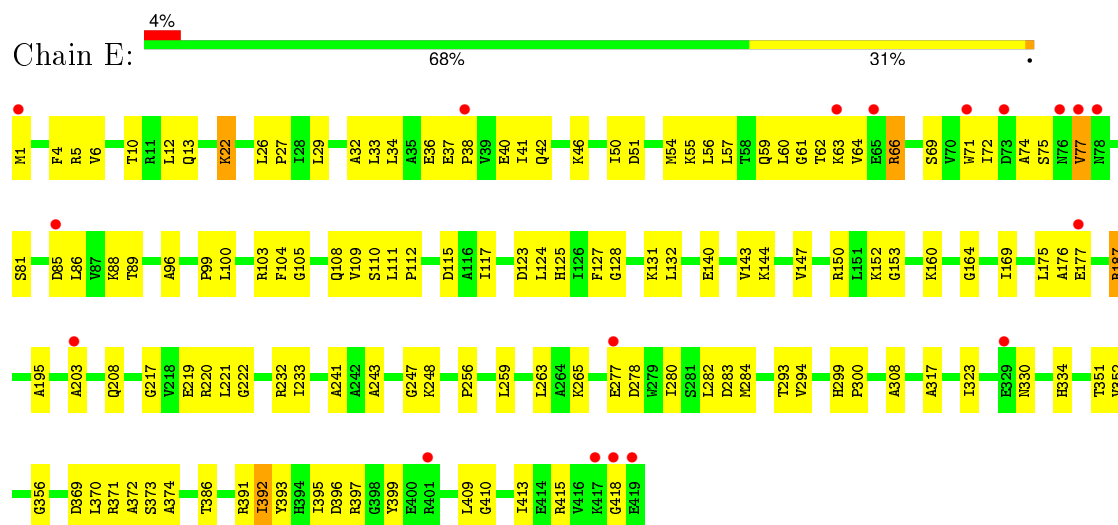
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



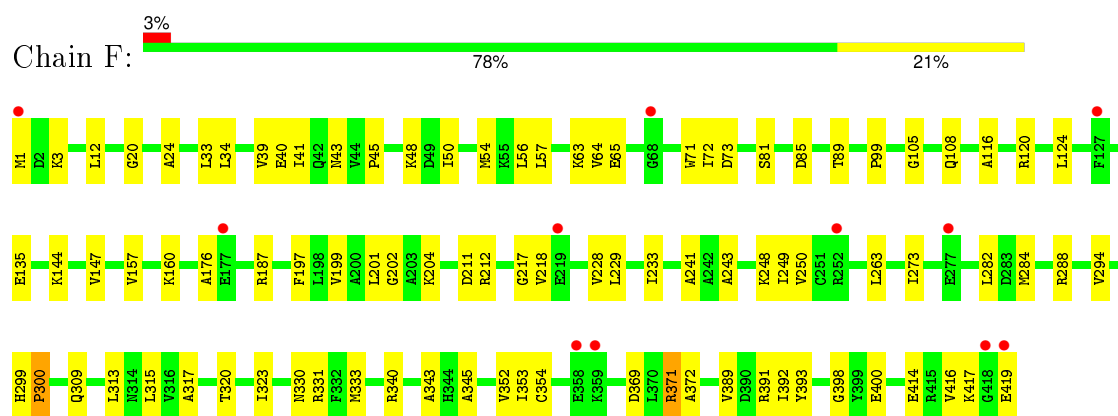
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



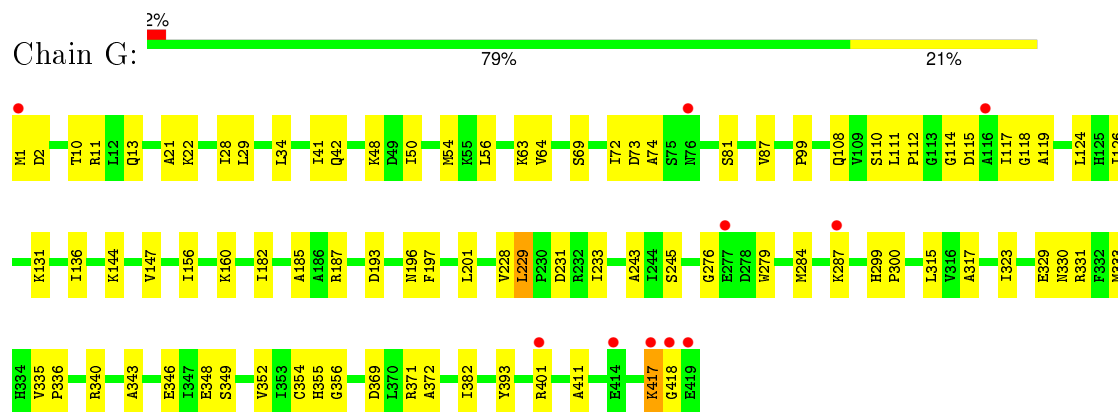
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



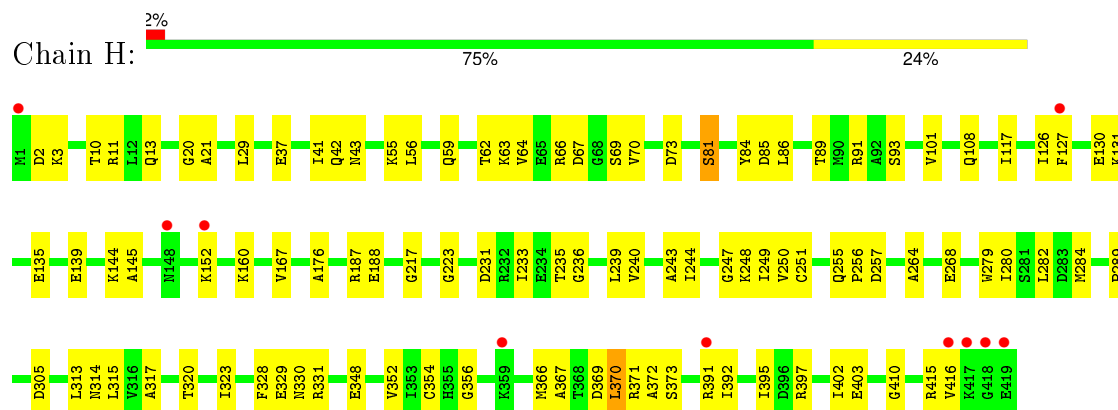
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.05Å 153.14Å 131.68Å 90.00° 102.36° 90.00°	Depositor
Resolution (Å)	19.77 – 2.50 19.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.77-2.50) 99.7 (19.77-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.50Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.208 , 0.271 0.208 , 0.271	Depositor DCC
R_{free} test set	1216 reflections (1.10%)	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.2	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 110457 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26190	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.63% 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: UD1, EDO, IAS, ACT

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	0.56	1/3180 (0.0%)	0.91	1/4308 (0.0%)
1	B	0.53	3/3180 (0.1%)	0.89	2/4308 (0.0%)
1	C	0.49	0/3180	0.88	1/4308 (0.0%)
1	D	0.49	0/3180	0.90	0/4308
1	E	0.50	1/3180 (0.0%)	0.89	1/4308 (0.0%)
1	F	0.51	1/3180 (0.0%)	0.89	0/4308
1	G	0.52	0/3180	0.89	2/4308 (0.0%)
1	H	0.49	0/3180	0.89	2/4308 (0.0%)
All	All	0.51	6/25440 (0.0%)	0.89	9/34464 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	PRO	N-CD	-12.67	1.30	1.47
1	B	300	PRO	N-CD	-12.44	1.30	1.47
1	F	300	PRO	N-CD	-11.88	1.31	1.47
1	B	38	PRO	N-CD	-10.56	1.33	1.47
1	E	277	GLU	CG-CD	5.46	1.60	1.51
1	B	279	TRP	NE1-CE2	-5.03	1.31	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	370	LEU	CA-CB-CG	8.73	135.39	115.30
1	A	229	LEU	CA-CB-CG	6.67	130.64	115.30
1	B	81	SER	N-CA-C	5.83	126.74	111.00
1	G	287	LYS	N-CA-C	5.79	126.63	111.00
1	B	276	GLY	N-CA-C	-5.43	99.53	113.10
1	C	81	SER	N-CA-C	5.19	125.02	111.00
1	G	417	LYS	N-CA-C	5.19	125.02	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	247	GLY	N-CA-C	5.18	126.05	113.10
1	H	81	SER	N-CA-C	5.10	124.77	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3144	0	3215	92	0
1	B	3144	0	3215	136	1
1	C	3144	0	3215	108	0
1	D	3144	0	3215	95	0
1	E	3144	0	3215	112	0
1	F	3144	0	3215	74	0
1	G	3144	0	3215	76	0
1	H	3144	0	3215	99	1
2	A	39	0	25	1	0
2	B	39	0	25	0	0
2	C	39	0	25	0	0
2	D	39	0	25	0	0
2	E	39	0	25	0	0
2	F	39	0	25	0	0
2	G	39	0	25	0	0
2	H	39	0	25	0	0
3	A	16	0	12	0	0
3	B	4	0	3	0	0
3	C	8	0	6	4	0
3	D	8	0	6	0	0
3	E	12	0	9	2	0
3	F	12	0	9	3	0
3	H	20	0	15	2	0
4	A	16	0	24	2	0
4	B	12	0	18	0	0
4	C	16	0	24	0	0
4	D	28	0	42	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	28	0	42	1	0
4	F	20	0	30	1	0
4	G	28	0	42	1	0
4	H	28	0	42	3	0
5	A	67	0	0	0	0
5	B	33	0	0	1	0
5	C	53	0	0	4	0
5	D	61	0	0	1	0
5	E	66	0	0	3	0
5	F	60	0	0	2	0
5	G	67	0	0	5	0
5	H	63	0	0	4	0
All	All	26190	0	26244	784	1

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 (784) 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:G:1:MET:O	1:G:418:GLY:HA2	1.20	1.28
1:B:418:GLY:O	1:B:419:GLU:HG3	1.11	1.24
1:A:395:ILE:CD1	1:A:402:ILE:HG21	1.66	1.24
1:C:418:GLY:CA	1:C:419:GLU:O	1.83	1.24
1:A:395:ILE:HD11	1:A:402:ILE:CG2	1.69	1.23
1:C:392:ILE:O	1:C:395:ILE:HG22	1.11	1.22
1:C:418:GLY:HA3	1:C:419:GLU:O	1.40	1.21
1:G:1:MET:O	1:G:418:GLY:CA	1.90	1.20
1:B:418:GLY:O	1:B:419:GLU:CG	1.93	1.16
1:C:392:ILE:O	1:C:395:ILE:CG2	2.03	1.05
1:A:392:ILE:O	1:A:395:ILE:HG22	1.56	1.05
1:C:395:ILE:HD11	1:C:402:ILE:HG21	1.04	1.03
1:B:81:SER:HB3	1:B:108:GLN:HG3	1.42	1.02
1:C:418:GLY:HA2	1:C:419:GLU:O	1.58	1.01
1:D:120:ARG:HH22	4:D:510:EDO:H12	1.26	1.01
1:C:395:ILE:CD1	1:C:402:ILE:HG21	1.92	0.98
1:B:15:GLU:HG2	1:B:250:VAL:HB	1.40	0.98
1:F:108:GLN:HG2	1:F:144:LYS:HG2	1.47	0.97
1:G:118:GLY:HA3	1:G:329:GLU:OE1	1.63	0.97
1:E:34:LEU:HD21	1:E:99:PRO:HA	1.46	0.96
1:C:56:LEU:HB2	1:C:86:LEU:HD13	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ILE:HG21	1:D:371:ARG:HD2	1.48	0.94
1:C:395:ILE:HD11	1:C:402:ILE:CG2	1.97	0.93
1:G:108:GLN:HG2	1:G:144:LYS:HG2	1.51	0.93
1:H:108:GLN:HG2	1:H:144:LYS:HG2	1.51	0.93
1:C:4:PHE:HE2	1:C:395:ILE:HD13	1.34	0.92
1:H:370:LEU:HD12	1:H:397:ARG:HD3	1.51	0.91
1:H:2:ASP:HB3	1:H:392:ILE:HD11	1.53	0.90
1:H:370:LEU:CD1	1:H:397:ARG:HD3	2.03	0.89
1:C:63:LYS:HB3	1:C:73:ASP:HB3	1.55	0.88
1:G:323:ILE:HB	1:G:352:VAL:HG12	1.54	0.87
1:D:369:ASP:HB3	1:D:372:ALA:HB3	1.55	0.87
1:D:94:ILE:HA	1:D:109:VAL:HG11	1.58	0.85
1:D:177:GLU:HG2	4:D:508:EDO:H21	1.58	0.84
1:G:2:ASP:OD1	1:G:417:LYS:HG2	1.78	0.83
1:F:331:ARG:H	3:F:503:ACT:H2	1.43	0.83
1:A:259:LEU:HD12	1:A:263:LEU:HG	1.61	0.82
1:D:41:ILE:O	1:D:69:SER:HB2	1.79	0.82
1:F:369:ASP:HB3	1:F:372:ALA:HB3	1.62	0.82
1:G:1:MET:O	1:G:418:GLY:N	2.12	0.81
1:A:306:MET:HE1	1:A:309:GLN:NE2	1.96	0.81
1:H:42:GLN:HA	1:H:69:SER:HB3	1.62	0.80
1:G:118:GLY:CA	1:G:329:GLU:OE1	2.28	0.80
1:C:367:ALA:HB1	1:C:373:SER:HB3	1.62	0.80
1:B:64:VAL:O	1:B:65:GLU:HG3	1.84	0.77
1:G:243:ALA:HA	1:G:284:MET:HG3	1.67	0.77
1:G:81:SER:HB3	1:G:108:GLN:HB2	1.66	0.77
1:E:243:ALA:HA	1:E:284:MET:CG	2.14	0.77
1:B:47:LEU:HB2	1:B:50:ILE:HG12	1.65	0.77
1:F:212:ARG:HD2	5:F:660:HOH:O	1.83	0.77
1:H:243:ALA:HA	1:H:284:MET:CG	2.15	0.76
1:C:4:PHE:CE2	1:C:395:ILE:HD13	2.20	0.76
1:B:4:PHE:CD1	1:B:392:ILE:HD13	2.20	0.76
1:D:108:GLN:HG2	1:D:144:LYS:HG2	1.69	0.75
1:E:34:LEU:HD21	1:E:99:PRO:CA	2.17	0.75
1:H:108:GLN:CG	1:H:144:LYS:HG2	2.17	0.75
1:B:244:ILE:HD12	1:B:382:ILE:HD13	1.68	0.74
1:C:418:GLY:CA	1:C:419:GLU:C	2.52	0.74
1:E:55:LYS:HE3	1:E:86:LEU:HD21	1.69	0.74
1:C:370:LEU:HG	1:C:371:ARG:HG2	1.70	0.74
1:E:36:GLU:HG2	1:E:103:ARG:HH21	1.53	0.73
1:E:36:GLU:O	1:E:75:SER:HB3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ILE:HG22	1:C:44:VAL:CG2	2.19	0.72
1:G:233:ILE:HG21	1:G:371:ARG:HD2	1.71	0.72
1:E:1:MET:N	1:E:418:GLY:HA2	2.04	0.72
1:F:48:LYS:NZ	1:F:393:TYR:HB2	2.03	0.72
1:D:91:ARG:NH2	1:D:120:ARG:O	2.22	0.72
1:C:257:ASP:HB3	3:C:502:ACT:H1	1.72	0.72
1:D:323:ILE:HB	1:D:352:VAL:CG1	2.20	0.72
1:G:323:ILE:HB	1:G:352:VAL:CG1	2.18	0.71
1:B:37:GLU:HB2	1:B:223:GLY:H	1.55	0.71
1:A:259:LEU:CD1	1:A:263:LEU:HG	2.20	0.71
1:G:48:LYS:NZ	1:G:393:TYR:HB2	2.06	0.71
1:C:3:LYS:HD3	1:C:390:ASP:OD1	1.89	0.71
1:B:259:LEU:HD12	1:B:263:LEU:HG	1.70	0.71
1:E:127:PHE:CZ	1:E:131:LYS:HE2	2.24	0.71
1:A:181:ILE:HG21	1:A:212:ARG:HD2	1.72	0.71
1:F:331:ARG:N	3:F:503:ACT:H2	2.05	0.71
1:B:63:LYS:HB3	1:B:73:ASP:HB3	1.72	0.71
1:F:33:LEU:HD21	1:F:57:LEU:HD22	1.73	0.71
1:H:243:ALA:HA	1:H:284:MET:HG2	1.73	0.70
1:A:29:LEU:HD23	1:A:41:ILE:CD1	2.21	0.70
1:H:315:LEU:HD23	1:H:354:CYS:HB3	1.72	0.70
1:C:9:PRO:HD3	1:C:384:GLU:HG3	1.73	0.70
1:C:108:GLN:HG2	1:C:144:LYS:HG2	1.74	0.70
1:A:334:HIS:HB3	1:A:372:ALA:HB1	1.73	0.70
1:G:10:THR:HG21	1:G:411:ALA:HA	1.71	0.70
1:C:327:ILE:HD12	3:C:503:ACT:H1	1.73	0.70
1:C:7:GLN:HB2	1:C:412:ASN:ND2	2.06	0.70
1:B:4:PHE:CE1	1:B:392:ILE:HD12	2.27	0.70
1:G:346:GLU:OE2	1:G:355:HIS:NE2	2.21	0.70
1:A:395:ILE:CD1	1:A:402:ILE:CG2	2.49	0.69
1:B:21:ALA:HA	1:B:231:ASP:HB2	1.72	0.69
1:D:323:ILE:HB	1:D:352:VAL:HG13	1.73	0.69
1:E:370:LEU:H	1:E:370:LEU:HD23	1.58	0.69
1:A:176:ALA:O	1:A:217:GLY:HA3	1.91	0.69
1:G:333:MET:HG3	5:G:663:HOH:O	1.92	0.68
1:G:315:LEU:HD13	1:G:343:ALA:HB1	1.75	0.68
1:C:176:ALA:O	1:C:217:GLY:HA3	1.92	0.68
1:C:396:ASP:CG	1:C:415:ARG:HH22	1.95	0.68
1:B:418:GLY:O	1:B:419:GLU:CB	2.41	0.68
1:E:22:LYS:HZ1	3:E:502:ACT:H2	1.58	0.68
1:A:229:LEU:HB2	1:A:230:PRO:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LYS:HG2	1:B:418:GLY:N	2.09	0.68
1:C:81:SER:HB3	1:C:108:GLN:HB2	1.75	0.68
1:A:29:LEU:HD23	1:A:41:ILE:HD12	1.74	0.68
1:B:417:LYS:HG2	1:B:418:GLY:H	1.57	0.68
1:E:103:ARG:NH1	1:E:104:PHE:HZ	1.91	0.67
1:E:369:ASP:HB3	1:E:372:ALA:HB3	1.76	0.67
1:E:108:GLN:HG2	1:E:144:LYS:HG2	1.75	0.67
1:F:176:ALA:O	1:F:217:GLY:HA3	1.95	0.67
1:B:4:PHE:CD1	1:B:392:ILE:CD1	2.78	0.67
1:G:243:ALA:HA	1:G:284:MET:CG	2.25	0.66
1:C:416:VAL:HG12	1:C:418:GLY:H	1.60	0.66
1:F:369:ASP:CB	1:F:372:ALA:HB3	2.25	0.66
1:D:149:GLY:O	1:D:150:ARG:HD3	1.96	0.66
1:D:42:GLN:HA	1:D:69:SER:HB3	1.78	0.66
1:E:36:GLU:HG2	1:E:103:ARG:NH2	2.11	0.66
1:H:370:LEU:CD1	1:H:397:ARG:CD	2.74	0.66
1:A:323:ILE:HB	1:A:352:VAL:CG1	2.26	0.66
1:E:105:GLY:HA2	1:E:147:VAL:HG12	1.78	0.66
1:A:229:LEU:HB2	1:A:230:PRO:CD	2.27	0.66
1:H:369:ASP:HB3	1:H:372:ALA:HB3	1.78	0.66
1:A:181:ILE:CG2	1:A:212:ARG:HD2	2.25	0.65
1:F:243:ALA:HA	1:F:284:MET:CG	2.26	0.65
1:A:317:ALA:O	1:A:356:GLY:HA3	1.96	0.65
1:B:176:ALA:O	1:B:217:GLY:HA3	1.95	0.65
1:A:370:LEU:O	1:A:371:ARG:HD2	1.96	0.65
1:B:401:ARG:HG2	5:B:616:HOH:O	1.96	0.65
1:G:126:ILE:HG23	1:G:136:ILE:HD13	1.77	0.65
1:D:137:LYS:HE3	1:D:139:GLU:OE1	1.97	0.65
1:E:243:ALA:HA	1:E:284:MET:HG2	1.78	0.65
1:F:81:SER:HB3	1:F:108:GLN:HB2	1.79	0.65
1:H:395:ILE:HG21	1:H:402:ILE:HG21	1.79	0.64
1:C:396:ASP:OD2	1:C:415:ARG:NH2	2.21	0.64
1:C:227:ARG:HD2	5:C:637:HOH:O	1.97	0.64
1:E:393:TYR:O	1:E:397:ARG:HG3	1.97	0.64
1:H:63:LYS:HB3	1:H:73:ASP:HB3	1.80	0.64
1:A:243:ALA:HA	1:A:284:MET:CG	2.26	0.64
1:E:128:GLY:HA3	1:E:169:ILE:HD11	1.79	0.64
1:B:118:GLY:CA	1:B:329:GLU:OE2	2.46	0.64
1:E:243:ALA:HA	1:E:284:MET:HG3	1.78	0.64
1:F:243:ALA:HA	1:F:284:MET:HG3	1.77	0.64
1:F:3:LYS:HA	1:F:392:ILE:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD12	1:A:112:PRO:HD2	1.80	0.64
1:D:112:PRO:HA	4:D:509:EDO:H22	1.80	0.64
1:D:82:ALA:HB3	1:D:109:VAL:HG13	1.80	0.63
1:B:29:LEU:HD23	1:B:41:ILE:HD12	1.79	0.63
1:D:243:ALA:HA	1:D:284:MET:CG	2.27	0.63
1:H:108:GLN:NE2	1:H:144:LYS:HE2	2.13	0.63
1:B:74:ALA:O	1:B:77:VAL:HG23	1.97	0.63
1:H:41:ILE:O	1:H:69:SER:HB2	1.98	0.63
1:D:38:PRO:HG3	1:D:73:ASP:OD2	1.97	0.63
1:A:243:ALA:HA	1:A:284:MET:HG3	1.80	0.63
1:G:41:ILE:O	1:G:69:SER:HB2	1.99	0.63
1:C:34:LEU:HD21	1:C:99:PRO:HA	1.81	0.63
1:G:29:LEU:HD23	1:G:41:ILE:HD12	1.81	0.63
1:G:196:ASN:HB3	4:G:505:EDO:H12	1.80	0.63
1:C:24:ALA:HB3	1:C:228:VAL:HG13	1.81	0.62
1:H:10:THR:HG21	1:H:410:GLY:O	1.99	0.62
1:B:418:GLY:C	1:B:419:GLU:HG3	2.11	0.62
1:B:34:LEU:HD22	1:B:175:LEU:HD11	1.82	0.62
1:E:282:LEU:HD23	1:E:282:LEU:C	2.20	0.62
1:A:306:MET:CE	1:A:309:GLN:NE2	2.61	0.62
1:B:152:LYS:HD2	1:B:177:GLU:O	1.99	0.62
1:G:369:ASP:HB3	1:G:372:ALA:HB3	1.82	0.62
1:F:204:LYS:HE3	1:F:218:VAL:HG12	1.82	0.62
1:D:108:GLN:HG3	5:D:646:HOH:O	1.98	0.61
1:A:320:THR:HG21	1:C:320:THR:HG21	1.81	0.61
1:E:46:LYS:HG2	1:E:66:ARG:NH1	2.15	0.61
1:G:48:LYS:HZ3	1:G:393:TYR:HB2	1.65	0.61
1:E:22:LYS:NZ	3:E:502:ACT:H2	2.16	0.61
1:G:335:VAL:HB	1:G:336:PRO:HD3	1.83	0.61
1:F:63:LYS:HB3	1:F:73:ASP:HB3	1.81	0.61
1:B:2:ASP:OD2	1:B:415:ARG:HD3	2.01	0.61
1:D:120:ARG:HH22	4:D:510:EDO:C1	2.07	0.61
1:F:323:ILE:HB	1:F:352:VAL:HG13	1.83	0.61
1:D:92:ALA:HA	4:D:504:EDO:H12	1.82	0.61
1:B:39:VAL:HG22	1:B:223:GLY:HA2	1.81	0.60
1:H:370:LEU:HD11	1:H:397:ARG:NE	2.16	0.60
1:H:313:LEU:C	1:H:313:LEU:HD23	2.22	0.60
1:B:334:HIS:HB3	1:B:372:ALA:HB1	1.83	0.60
1:B:3:LYS:HG3	1:B:3:LYS:O	2.02	0.60
1:B:367:ALA:HB1	1:B:373:SER:OG	2.01	0.60
1:D:124:LEU:HD11	1:D:160:LYS:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:PHE:CD2	1:B:413:ILE:HD11	2.36	0.60
1:F:3:LYS:HB2	1:F:389:VAL:O	2.00	0.60
1:B:373:SER:HB3	1:B:395:ILE:HG12	1.83	0.60
1:H:81:SER:HB3	1:H:108:GLN:HB2	1.83	0.60
1:A:369:ASP:C	1:A:371:ARG:H	2.05	0.59
1:H:176:ALA:O	1:H:217:GLY:HA3	2.02	0.59
1:E:41:ILE:O	1:E:69:SER:HB2	2.03	0.59
1:E:5:ARG:NH1	1:E:386:THR:HG21	2.17	0.59
1:A:150:ARG:HH12	1:A:219:GLU:HA	1.67	0.59
1:G:348:GLU:O	1:G:349:SER:HB3	2.03	0.59
1:G:340:ARG:HG2	1:G:340:ARG:HH11	1.66	0.59
1:H:366:MET:CE	1:H:391:ARG:HD2	2.32	0.59
1:E:150:ARG:HB2	1:E:177:GLU:CG	2.30	0.59
1:A:306:MET:HE1	1:A:309:GLN:HE21	1.65	0.59
1:A:204:LYS:HE2	1:A:218:VAL:HG12	1.84	0.59
1:D:63:LYS:HB3	1:D:73:ASP:HB3	1.84	0.59
1:A:40:GLU:HB3	1:A:225:VAL:HG22	1.84	0.59
1:B:48:LYS:HE3	1:B:397:ARG:HG2	1.85	0.59
1:A:116:ALA:O	1:A:330:ASN:ND2	2.35	0.59
1:E:323:ILE:HB	1:E:352:VAL:HG13	1.85	0.59
1:E:152:LYS:HD2	1:E:153:GLY:N	2.18	0.59
1:G:317:ALA:O	1:G:356:GLY:HA3	2.03	0.59
1:B:4:PHE:CE1	1:B:392:ILE:CD1	2.85	0.58
1:C:4:PHE:HE2	1:C:395:ILE:CD1	2.12	0.58
1:A:259:LEU:HD12	1:A:263:LEU:CG	2.31	0.58
1:C:233:ILE:HG23	1:C:306:MET:HE3	1.84	0.58
1:B:34:LEU:HD22	1:B:175:LEU:CD1	2.33	0.58
1:D:64:VAL:HG22	1:D:72:ILE:HD13	1.85	0.58
1:H:243:ALA:HA	1:H:284:MET:HG3	1.84	0.58
1:F:48:LYS:HZ1	1:F:393:TYR:HB2	1.68	0.58
1:C:36:GLU:OE1	1:C:220:ARG:NE	2.35	0.58
1:H:85:ASP:O	1:H:89:THR:HG23	2.03	0.58
1:A:370:LEU:HD12	1:A:370:LEU:O	2.03	0.58
1:H:152:LYS:HE3	5:H:627:HOH:O	2.03	0.58
1:G:1:MET:C	1:G:418:GLY:HA2	2.14	0.57
1:B:4:PHE:H	1:B:392:ILE:HG21	1.68	0.57
1:C:334:HIS:HB3	1:C:372:ALA:HB1	1.85	0.57
1:G:124:LEU:HD11	1:G:160:LYS:HG2	1.85	0.57
1:F:197:PHE:CZ	1:F:201:LEU:HD11	2.40	0.57
1:B:118:GLY:HA3	1:B:329:GLU:OE2	2.03	0.57
1:B:56:LEU:HB2	1:B:86:LEU:HD13	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ILE:HG22	1:D:44:VAL:CG2	2.35	0.57
1:C:259:LEU:HD12	1:C:263:LEU:HG	1.86	0.57
1:D:66:ARG:HB3	1:D:70:VAL:HG22	1.86	0.57
1:F:391:ARG:HB3	1:F:393:TYR:CE2	2.40	0.57
1:E:152:LYS:HD2	1:E:153:GLY:H	1.70	0.57
1:A:333:MET:CE	1:A:333:MET:HA	2.35	0.57
1:E:373:SER:HB2	1:E:395:ILE:CD1	2.35	0.57
1:E:40:GLU:OE2	1:E:71:TRP:NE1	2.38	0.57
1:F:315:LEU:HD21	1:F:345:ALA:HB2	1.85	0.57
1:E:103:ARG:NH1	1:E:104:PHE:CZ	2.72	0.56
1:F:48:LYS:HZ3	1:F:393:TYR:HB2	1.70	0.56
1:A:15:GLU:HG2	1:A:250:VAL:HB	1.86	0.56
1:E:105:GLY:HA2	1:E:147:VAL:CG1	2.33	0.56
1:F:3:LYS:NZ	1:F:419:GLU:C	2.58	0.56
1:E:127:PHE:CE2	1:E:131:LYS:HE2	2.41	0.56
1:C:306:MET:HA	1:C:306:MET:HE2	1.88	0.56
1:A:395:ILE:HD11	1:A:402:ILE:HG21	0.75	0.56
1:D:243:ALA:HA	1:D:284:MET:HG3	1.88	0.56
1:A:395:ILE:HG23	1:A:396:ASP:N	2.21	0.56
1:E:248:LYS:HD2	1:E:283:ASP:OD2	2.05	0.56
1:B:314:ASN:HB3	1:B:354:CYS:HB2	1.87	0.56
1:D:64:VAL:HG22	1:D:72:ILE:CD1	2.36	0.55
1:B:17:THR:HA	1:B:252:ARG:HB2	1.87	0.55
1:A:94:ILE:HA	1:A:109:VAL:HG11	1.88	0.55
1:B:417:LYS:CG	1:B:418:GLY:H	2.19	0.55
1:G:81:SER:HB3	1:G:108:GLN:CB	2.36	0.55
1:B:29:LEU:HD23	1:B:41:ILE:CD1	2.37	0.55
1:H:127:PHE:CE2	1:H:131:LYS:HD2	2.41	0.55
1:E:330:ASN:OD1	1:H:330:ASN:HB2	2.06	0.55
1:B:372:ALA:O	1:B:375:SER:N	2.39	0.55
1:C:250:VAL:HG22	1:C:281:SER:HB2	1.88	0.55
1:C:182:ILE:HG22	1:C:185:ALA:HB2	1.89	0.55
1:A:81:SER:HB3	1:A:108:GLN:HB2	1.89	0.55
1:E:36:GLU:OE1	1:E:220:ARG:HB2	2.07	0.55
1:H:323:ILE:HB	1:H:352:VAL:CG1	2.37	0.55
1:D:56:LEU:HD23	1:D:56:LEU:C	2.26	0.55
1:B:40:GLU:HG3	1:B:71:TRP:NE1	2.22	0.55
1:C:370:LEU:HD11	1:C:399:TYR:CD1	2.42	0.54
1:D:94:ILE:HD12	1:D:122:VAL:HG11	1.89	0.54
3:H:503:ACT:H2	5:H:606:HOH:O	2.07	0.54
1:H:117:ILE:CG2	1:H:331:ARG:HG3	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LYS:HD2	1:D:177:GLU:O	2.07	0.54
1:B:21:ALA:HB2	1:B:231:ASP:HA	1.90	0.54
1:G:64:VAL:HG22	1:G:72:ILE:HD13	1.89	0.54
1:D:313:LEU:C	1:D:313:LEU:HD23	2.27	0.54
1:A:56:LEU:C	1:A:56:LEU:HD23	2.27	0.54
1:E:103:ARG:HH11	1:E:104:PHE:HZ	1.55	0.54
1:B:48:LYS:NZ	1:B:393:TYR:HB2	2.22	0.54
1:E:373:SER:HB2	1:E:395:ILE:HD11	1.89	0.54
1:H:248:LYS:HB3	1:H:248:LYS:NZ	2.23	0.54
1:H:56:LEU:HD23	1:H:56:LEU:C	2.28	0.54
1:F:56:LEU:HD23	1:F:56:LEU:C	2.27	0.54
1:C:77:VAL:HB	1:C:104:PHE:CZ	2.43	0.54
1:E:56:LEU:HD23	1:E:56:LEU:O	2.07	0.54
1:F:323:ILE:HB	1:F:352:VAL:CG1	2.38	0.54
1:E:323:ILE:HB	1:E:352:VAL:CG1	2.37	0.54
1:B:9:PRO:HD3	1:B:384:GLU:HA	1.89	0.54
1:B:126:ILE:O	1:B:130:GLU:HG3	2.07	0.54
1:F:120:ARG:HB3	5:F:622:HOH:O	2.07	0.54
1:B:97:LEU:O	1:B:97:LEU:HD12	2.08	0.53
1:H:188:GLU:N	1:H:188:GLU:OE1	2.41	0.53
1:B:244:ILE:HA	1:B:289:PRO:HG2	1.89	0.53
1:D:299:HIS:ND1	1:D:300:PRO:HA	2.24	0.53
1:C:127:PHE:HB2	5:C:641:HOH:O	2.07	0.53
1:E:124:LEU:HD11	1:E:160:LYS:HG3	1.90	0.53
1:G:56:LEU:HD23	1:G:56:LEU:O	2.08	0.53
1:A:115:ASP:HB3	1:A:118:GLY:O	2.08	0.53
1:C:317:ALA:O	1:C:356:GLY:HA3	2.08	0.53
1:A:31:ALA:HB1	1:A:198:LEU:HD21	1.90	0.53
1:E:150:ARG:HH12	1:E:219:GLU:HA	1.73	0.53
1:G:111:LEU:HD12	1:G:112:PRO:HD2	1.91	0.53
1:B:395:ILE:HG21	1:B:402:ILE:HG21	1.91	0.53
1:H:62:THR:HG22	1:H:64:VAL:HG22	1.90	0.53
1:H:3:LYS:HB2	1:H:416:VAL:HB	1.91	0.53
1:C:299:HIS:CG	1:C:300:PRO:HA	2.43	0.53
1:F:416:VAL:HG12	1:F:417:LYS:N	2.23	0.53
1:H:317:ALA:O	1:H:356:GLY:HA3	2.09	0.53
1:B:317:ALA:O	1:B:356:GLY:HA3	2.09	0.53
1:B:45:PRO:O	1:B:50:ILE:HG13	2.09	0.53
1:E:74:ALA:O	1:E:77:VAL:HG23	2.09	0.53
1:D:46:LYS:HG2	1:D:66:ARG:CZ	2.39	0.53
1:B:46:LYS:N	1:B:400:GLU:OE1	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:ARG:HH12	1:E:386:THR:HG21	1.73	0.52
1:C:233:ILE:HG23	1:C:306:MET:CE	2.39	0.52
1:B:243:ALA:HA	1:B:284:MET:HG3	1.91	0.52
1:A:181:ILE:HG23	1:A:212:ARG:CG	2.40	0.52
1:C:111:LEU:HD12	1:C:112:PRO:HD2	1.90	0.52
1:A:306:MET:HA	1:A:306:MET:HE2	1.91	0.52
1:E:64:VAL:HG13	1:E:72:ILE:HD11	1.91	0.52
1:H:21:ALA:HA	1:H:231:ASP:HB2	1.91	0.52
1:D:118:GLY:O	1:D:119:ALA:HB3	2.09	0.52
1:A:152:LYS:HD2	1:A:177:GLU:O	2.09	0.52
1:C:316:VAL:HG23	1:C:316:VAL:O	2.08	0.52
1:E:150:ARG:HB2	1:E:177:GLU:HG3	1.91	0.52
1:B:97:LEU:HD11	1:B:145:ALA:HB3	1.92	0.52
1:A:416:VAL:HG12	1:A:418:GLY:H	1.74	0.52
1:C:40:GLU:HB3	1:C:225:VAL:HG22	1.92	0.52
1:C:243:ALA:HA	1:C:284:MET:HG3	1.92	0.52
1:B:213:ILE:HG22	1:B:215:ILE:HD11	1.91	0.52
1:B:108:GLN:NE2	1:B:144:LYS:HE2	2.24	0.52
1:B:249:ILE:HG12	1:B:250:VAL:N	2.24	0.52
1:E:299:HIS:CG	1:E:300:PRO:HA	2.45	0.52
1:C:41:ILE:HD11	1:C:197:PHE:CE1	2.45	0.52
1:F:33:LEU:HD21	1:F:57:LEU:CD2	2.38	0.52
1:E:330:ASN:CG	1:H:330:ASN:HB2	2.29	0.52
1:H:370:LEU:HD11	1:H:397:ARG:CZ	2.40	0.52
1:D:1:MET:N	1:D:418:GLY:O	2.43	0.52
1:H:37:GLU:HB2	1:H:223:GLY:N	2.25	0.52
1:B:87:VAL:HG21	1:B:110:SER:HB3	1.91	0.52
1:A:137:LYS:NZ	1:A:139:GLU:OE2	2.42	0.51
1:A:34:LEU:HD21	1:A:99:PRO:HA	1.91	0.51
1:C:126:ILE:HG23	1:C:136:ILE:HG21	1.92	0.51
1:B:119:ALA:N	1:B:329:GLU:OE2	2.44	0.51
1:C:233:ILE:CG2	1:C:306:MET:HE3	2.41	0.51
1:E:330:ASN:HB2	1:H:330:ASN:OD1	2.10	0.51
1:E:111:LEU:HD13	1:E:143:VAL:CG2	2.40	0.51
1:F:105:GLY:HA2	1:F:147:VAL:HG12	1.92	0.51
1:A:101:VAL:HG13	1:A:102:ALA:N	2.25	0.51
1:A:275:THR:HG22	1:A:280:ILE:HG12	1.92	0.51
1:E:278:ASP:OD1	1:E:278:ASP:N	2.42	0.51
1:B:220:ARG:O	1:B:221:LEU:HD23	2.11	0.51
1:E:123:ASP:HA	4:E:508:EDO:H21	1.93	0.51
1:D:4:PHE:HE1	1:D:415:ARG:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HD11	1:A:160:LYS:HG2	1.93	0.51
1:D:204:LYS:HB2	1:D:216:GLU:HB3	1.92	0.51
1:E:57:LEU:O	1:E:62:THR:HB	2.11	0.51
1:E:369:ASP:CB	1:E:372:ALA:HB3	2.40	0.51
1:D:12:LEU:HD12	1:D:241:ALA:HB1	1.92	0.51
1:D:369:ASP:CB	1:D:372:ALA:HB3	2.35	0.51
1:G:299:HIS:ND1	1:G:300:PRO:HA	2.26	0.51
1:D:254:ALA:O	1:D:278:ASP:HA	2.11	0.51
1:C:276:GLY:HA3	1:C:279:TRP:NE1	2.26	0.50
1:A:259:LEU:CD1	1:A:263:LEU:CG	2.88	0.50
1:G:42:GLN:HA	1:G:69:SER:HB3	1.92	0.50
1:D:299:HIS:CG	1:D:300:PRO:HA	2.46	0.50
1:H:240:VAL:O	1:H:244:ILE:HG12	2.12	0.50
1:G:21:ALA:HA	1:G:231:ASP:HB2	1.92	0.50
1:E:115:ASP:OD2	1:E:117:ILE:HG12	2.12	0.50
1:H:282:LEU:C	1:H:282:LEU:HD23	2.32	0.50
1:A:115:ASP:OD2	1:A:116:ALA:N	2.45	0.50
1:G:131:LYS:HD3	1:G:156:ILE:HG23	1.94	0.50
1:D:13:GLN:HA	1:D:248:LYS:O	2.10	0.50
1:F:340:ARG:HG2	1:F:340:ARG:HH11	1.74	0.50
1:B:5:ARG:NE	1:B:416:VAL:HG21	2.26	0.50
1:E:124:LEU:HD11	1:E:160:LYS:CG	2.42	0.50
1:D:10:THR:HG21	1:D:411:ALA:HA	1.92	0.50
1:E:176:ALA:O	1:E:217:GLY:HA3	2.12	0.50
1:C:36:GLU:O	1:C:75:SER:HB3	2.12	0.50
1:H:62:THR:HG22	1:H:64:VAL:CG2	2.42	0.50
1:B:21:ALA:HA	1:B:231:ASP:CB	2.42	0.49
1:A:81:SER:CB	1:A:108:GLN:HB2	2.42	0.49
1:C:294:VAL:HB	1:C:323:ILE:HD13	1.93	0.49
1:B:37:GLU:HB2	1:B:223:GLY:N	2.23	0.49
1:B:180:THR:HB	1:B:215:ILE:HB	1.94	0.49
1:A:21:ALA:HA	1:A:231:ASP:HB2	1.94	0.49
1:F:50:ILE:O	1:F:54:MET:HG3	2.11	0.49
1:B:296:THR:HA	1:B:302:PHE:O	2.12	0.49
1:F:294:VAL:HB	1:F:323:ILE:HD13	1.94	0.49
1:B:48:LYS:HZ2	1:B:393:TYR:HB2	1.76	0.49
1:E:152:LYS:CE	5:E:632:HOH:O	2.60	0.49
1:E:152:LYS:HE3	5:E:632:HOH:O	2.11	0.49
1:H:329:GLU:HG2	1:H:330:ASN:H	1.76	0.49
1:B:35:ALA:O	1:B:74:ALA:HB3	2.13	0.49
1:C:94:ILE:HA	1:C:109:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:TYR:CD2	1:C:402:ILE:HD12	2.47	0.49
1:B:271:ALA:HB2	1:B:284:MET:SD	2.52	0.49
1:E:4:PHE:CD2	1:E:392:ILE:HG21	2.48	0.49
1:G:87:VAL:HG21	1:G:110:SER:HB3	1.95	0.49
1:H:366:MET:HE3	1:H:391:ARG:HD2	1.94	0.49
1:C:357:VAL:HG13	5:C:606:HOH:O	2.11	0.49
1:F:24:ALA:HB3	1:F:228:VAL:HG13	1.93	0.49
1:E:46:LYS:HG2	1:E:66:ARG:CZ	2.43	0.49
1:C:243:ALA:HA	1:C:284:MET:CG	2.43	0.49
1:H:367:ALA:HB1	1:H:373:SER:CB	2.43	0.49
1:F:330:ASN:HB2	1:G:330:ASN:HB2	1.95	0.48
1:C:87:VAL:HG21	1:C:110:SER:HB3	1.94	0.48
1:E:1:MET:H2	1:E:418:GLY:HA2	1.78	0.48
1:B:35:ALA:HB2	1:B:201:LEU:HD13	1.95	0.48
1:G:340:ARG:CG	1:G:340:ARG:HH11	2.26	0.48
1:B:360:LEU:O	1:B:384:GLU:N	2.44	0.48
1:A:282:LEU:HD23	1:A:282:LEU:C	2.34	0.48
1:B:299:HIS:CG	1:B:300:PRO:HA	2.48	0.48
1:D:276:GLY:HA3	1:D:279:TRP:NE1	2.28	0.48
1:E:294:VAL:HB	1:E:323:ILE:HD13	1.96	0.48
1:C:220:ARG:HG3	1:C:220:ARG:HH11	1.78	0.48
1:E:373:SER:CB	1:E:395:ILE:HD11	2.43	0.48
1:D:150:ARG:HG3	4:D:508:EDO:O1	2.14	0.48
1:H:21:ALA:HA	1:H:231:ASP:CB	2.44	0.48
1:D:22:LYS:HD3	1:D:371:ARG:NH1	2.28	0.48
1:B:234:GLU:HG3	1:B:238:PHE:CE2	2.49	0.48
1:F:45:PRO:HA	1:F:400:GLU:OE1	2.14	0.48
1:G:114:GLY:HA2	1:G:119:ALA:O	2.13	0.48
1:H:348:GLU:OE2	1:H:348:GLU:HA	2.13	0.48
1:F:331:ARG:H	3:F:503:ACT:CH3	2.22	0.48
1:G:160:LYS:HE3	5:G:655:HOH:O	2.13	0.48
1:A:83:PRO:HD2	1:A:86:LEU:HD12	1.96	0.48
1:B:117:ILE:HD11	1:B:120:ARG:NH1	2.28	0.48
1:F:330:ASN:CB	1:G:330:ASN:HB2	2.44	0.48
1:C:91:ARG:HG3	5:C:646:HOH:O	2.13	0.48
1:A:233:ILE:HG23	1:A:306:MET:CE	2.44	0.48
1:C:46:LYS:N	1:C:400:GLU:OE1	2.30	0.48
1:D:417:LYS:O	1:D:419:GLU:N	2.41	0.48
1:C:373:SER:O	1:C:377:VAL:HG23	2.13	0.47
1:B:220:ARG:HG3	1:B:220:ARG:HH11	1.79	0.47
1:B:234:GLU:OE2	1:B:238:PHE:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ARG:HG3	1:B:411:ALA:O	2.13	0.47
1:E:308:ALA:HA	1:E:334:HIS:NE2	2.29	0.47
1:C:309:GLN:N	1:C:309:GLN:OE1	2.44	0.47
1:F:320:THR:HG21	1:H:320:THR:HG21	1.96	0.47
1:C:108:GLN:CG	1:C:144:LYS:HG2	2.43	0.47
1:F:3:LYS:HZ1	1:F:419:GLU:C	2.17	0.47
1:D:115:ASP:OD2	1:D:116:ALA:N	2.48	0.47
1:C:88:LYS:HE3	1:C:88:LYS:HB3	1.40	0.47
1:B:60:LEU:HD22	1:B:79:ASN:O	2.15	0.47
1:D:37:GLU:OE2	1:D:220:ARG:NH2	2.47	0.47
1:B:30:PHE:CE1	1:B:96:ALA:HB2	2.49	0.47
1:B:276:GLY:HA3	1:B:279:TRP:NE1	2.29	0.47
1:C:37:GLU:HB3	1:C:38:PRO:CD	2.44	0.47
1:E:56:LEU:C	1:E:56:LEU:HD23	2.34	0.47
1:E:64:VAL:HG13	1:E:72:ILE:CD1	2.45	0.47
1:B:273:ILE:O	1:B:274:GLU:HG2	2.15	0.47
1:D:37:GLU:O	1:D:39:VAL:HG23	2.14	0.47
1:H:369:ASP:CB	1:H:372:ALA:HB3	2.43	0.47
1:E:125:HIS:CE1	1:E:164:GLY:C	2.88	0.47
1:C:276:GLY:HA3	1:C:279:TRP:CE2	2.48	0.47
1:E:6:VAL:HG22	1:E:413:ILE:HG13	1.96	0.47
1:D:91:ARG:NH2	1:D:120:ARG:HB3	2.30	0.47
1:E:96:ALA:O	1:E:99:PRO:HD2	2.14	0.47
1:G:108:GLN:HG3	5:G:635:HOH:O	2.15	0.47
1:D:97:LEU:HB2	1:D:109:VAL:HG21	1.97	0.47
1:G:333:MET:O	1:G:336:PRO:HD2	2.15	0.47
1:E:128:GLY:HA3	1:E:169:ILE:CD1	2.45	0.47
1:E:42:GLN:HA	1:E:69:SER:CB	2.45	0.47
1:H:248:LYS:CB	1:H:248:LYS:NZ	2.78	0.47
1:B:282:LEU:HD21	1:B:284:MET:HG2	1.95	0.47
1:E:111:LEU:HD13	1:E:143:VAL:HG21	1.97	0.47
1:A:282:LEU:HD23	1:A:283:ASP:N	2.30	0.47
1:B:299:HIS:ND1	1:B:300:PRO:HA	2.30	0.47
1:B:13:GLN:HA	1:B:248:LYS:O	2.15	0.47
1:H:255:GLN:HG2	1:H:257:ASP:OD1	2.14	0.47
1:D:6:VAL:HG22	1:D:413:ILE:HG13	1.96	0.47
1:E:10:THR:HG21	1:E:410:GLY:O	2.15	0.47
1:H:81:SER:CB	1:H:108:GLN:HB2	2.44	0.47
1:A:20:GLY:HA3	1:A:43:ASN:O	2.15	0.47
1:D:22:LYS:HB2	1:D:47:LEU:CD1	2.44	0.47
1:H:29:LEU:HD23	1:H:41:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:HB	1:A:352:VAL:HG13	1.97	0.47
1:C:299:HIS:ND1	1:C:300:PRO:HA	2.30	0.47
1:C:115:ASP:CG	1:C:116:ALA:H	2.17	0.47
1:E:103:ARG:HB2	1:E:175:LEU:CD1	2.44	0.47
1:F:248:LYS:HA	1:F:282:LEU:O	2.15	0.47
1:F:85:ASP:O	1:F:89:THR:HG23	2.15	0.47
1:D:169:ILE:HG22	1:D:182:ILE:HD11	1.97	0.47
1:B:124:LEU:HD11	1:B:160:LYS:HG2	1.95	0.47
1:H:370:LEU:HD11	1:H:397:ARG:CD	2.43	0.46
1:B:236:GLY:O	1:B:240:VAL:HG23	2.15	0.46
1:H:251:CYS:O	1:H:279:TRP:HA	2.15	0.46
1:D:325:GLU:CG	1:D:329:GLU:H	2.28	0.46
1:G:74:ALA:HB3	5:G:637:HOH:O	2.15	0.46
1:H:233:ILE:HD12	1:H:305:ASP:HB2	1.95	0.46
1:C:277:GLU:HG3	3:C:502:ACT:O	2.15	0.46
1:C:3:LYS:CD	1:C:390:ASP:OD1	2.62	0.46
1:G:369:ASP:CB	1:G:372:ALA:HB3	2.45	0.46
1:B:273:ILE:HG22	1:B:274:GLU:N	2.30	0.46
1:D:325:GLU:HG3	1:D:329:GLU:H	1.80	0.46
1:F:233:ILE:HG21	1:F:371:ARG:CD	2.46	0.46
1:C:323:ILE:HB	1:C:352:VAL:HG12	1.97	0.46
1:A:315:LEU:HD23	1:A:354:CYS:HB3	1.96	0.46
1:F:249:ILE:HG12	1:F:250:VAL:N	2.30	0.46
1:D:243:ALA:HA	1:D:284:MET:HG2	1.96	0.46
1:E:59:GLN:C	1:E:61:GLY:H	2.18	0.46
1:F:157:VAL:O	4:F:509:EDO:H22	2.15	0.46
1:G:63:LYS:HB3	1:G:73:ASP:HB3	1.97	0.46
1:B:41:ILE:O	1:B:69:SER:HB2	2.16	0.46
1:F:41:ILE:HG23	1:F:228:VAL:HG23	1.97	0.46
1:D:116:ALA:O	1:D:330:ASN:ND2	2.38	0.46
1:D:60:LEU:O	1:D:77:VAL:HG13	2.16	0.46
1:C:266:LEU:O	1:C:269:ALA:HB3	2.16	0.46
1:B:282:LEU:HD23	1:B:282:LEU:C	2.35	0.46
1:F:288:ARG:NH2	1:F:317:ALA:O	2.48	0.46
1:H:160:LYS:HA	5:H:653:HOH:O	2.16	0.46
1:H:84:TYR:CE1	4:H:507:EDO:H12	2.50	0.46
1:H:108:GLN:CD	1:H:144:LYS:HE2	2.36	0.46
1:E:1:MET:H3	1:E:418:GLY:HA2	1.76	0.46
1:D:417:LYS:C	1:D:419:GLU:H	2.18	0.46
1:F:353:ILE:HD12	1:F:353:ILE:N	2.31	0.46
1:E:88:LYS:HG2	1:E:88:LYS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:ASP:CG	1:G:229:LEU:HD22	2.36	0.46
1:D:21:ALA:HA	1:D:231:ASP:HB2	1.98	0.46
1:B:37:GLU:O	1:B:38:PRO:C	2.53	0.46
1:H:264:ALA:O	1:H:268:GLU:HG3	2.16	0.46
1:H:66:ARG:HB3	1:H:70:VAL:HG22	1.97	0.46
1:C:367:ALA:CB	1:C:373:SER:HB3	2.40	0.46
1:E:36:GLU:OE1	1:E:220:ARG:NE	2.49	0.46
1:G:331:ARG:NH2	1:G:371:ARG:HB2	2.30	0.46
1:H:320:THR:HA	1:H:354:CYS:O	2.16	0.46
1:G:315:LEU:HD23	1:G:354:CYS:HB3	1.98	0.46
1:B:213:ILE:HG22	1:B:215:ILE:CD1	2.45	0.46
1:H:249:ILE:HG12	1:H:250:VAL:N	2.31	0.46
1:A:147:VAL:HG13	1:A:147:VAL:O	2.16	0.46
1:B:14:GLY:O	1:B:249:ILE:HA	2.16	0.45
1:D:39:VAL:HG12	1:D:41:ILE:HD12	1.98	0.45
1:H:248:LYS:HZ3	1:H:248:LYS:HB3	1.80	0.45
1:D:213:ILE:HG22	1:D:215:ILE:HD11	1.97	0.45
1:F:299:HIS:CG	1:F:300:PRO:HA	2.51	0.45
1:C:20:GLY:HA3	1:C:43:ASN:O	2.16	0.45
1:C:47:LEU:HB3	1:C:397:ARG:O	2.16	0.45
1:D:51:ASP:HA	1:D:54:MET:CE	2.46	0.45
1:D:42:GLN:HA	1:D:69:SER:CB	2.46	0.45
1:G:48:LYS:HZ1	1:G:393:TYR:HB2	1.81	0.45
1:F:416:VAL:CG1	1:F:417:LYS:N	2.79	0.45
1:D:12:LEU:O	1:D:247:GLY:HA3	2.16	0.45
1:B:20:GLY:HA3	1:B:43:ASN:O	2.16	0.45
1:H:126:ILE:O	1:H:130:GLU:HG3	2.16	0.45
1:A:4:PHE:HE2	1:A:395:ILE:HD13	1.80	0.45
1:G:28:ILE:HD12	1:G:228:VAL:HG22	1.99	0.45
1:F:124:LEU:HD11	1:F:160:LYS:HG2	1.97	0.45
1:E:26:LEU:N	1:E:27:PRO:HD2	2.32	0.45
1:F:34:LEU:HD21	1:F:99:PRO:HA	1.97	0.45
1:B:85:ASP:HA	1:B:88:LYS:HE2	1.97	0.45
1:H:367:ALA:HB1	1:H:373:SER:HB2	1.97	0.45
1:B:335:VAL:HB	1:B:336:PRO:CD	2.47	0.45
1:F:116:ALA:HB1	1:F:333:MET:HE1	1.98	0.45
1:H:20:GLY:HA3	1:H:43:ASN:O	2.16	0.45
1:F:313:LEU:HD23	1:F:313:LEU:C	2.37	0.45
1:F:108:GLN:HG2	1:F:144:LYS:CG	2.34	0.45
1:D:59:GLN:OE1	1:D:79:ASN:ND2	2.49	0.45
1:B:376:LEU:O	1:B:379:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:299:HIS:CG	1:G:300:PRO:HA	2.51	0.45
1:G:115:ASP:OD2	1:G:117:ILE:HG12	2.17	0.45
1:A:105:GLY:HA2	1:A:147:VAL:CG1	2.47	0.45
1:B:316:VAL:HG23	1:B:316:VAL:O	2.17	0.45
1:B:111:LEU:HD12	1:B:112:PRO:HD2	1.98	0.45
1:C:22:LYS:HD2	1:C:398:GLY:HA2	1.97	0.45
1:F:309:GLN:OE1	1:F:309:GLN:N	2.39	0.45
1:G:108:GLN:CD	1:G:144:LYS:HE2	2.37	0.45
1:E:5:ARG:NH1	5:E:641:HOH:O	2.40	0.45
1:G:11:ARG:HD3	1:G:13:GLN:OE1	2.17	0.45
1:G:197:PHE:CZ	1:G:201:LEU:HD11	2.52	0.45
1:G:401:ARG:HA	5:G:642:HOH:O	2.17	0.45
1:H:59:GLN:NE2	1:H:86:LEU:HD11	2.32	0.44
1:F:299:HIS:ND1	1:F:300:PRO:HA	2.32	0.44
1:C:21:ALA:HA	1:C:231:ASP:HB2	1.98	0.44
1:D:31:ALA:HB1	1:D:198:LEU:HD21	1.98	0.44
1:C:395:ILE:HG23	1:C:396:ASP:N	2.32	0.44
1:C:220:ARG:HG3	1:C:220:ARG:NH1	2.33	0.44
1:E:265:LYS:HE3	1:E:293:THR:O	2.17	0.44
1:E:374:ALA:HB2	1:E:399:TYR:CE1	2.52	0.44
1:G:276:GLY:HA3	1:G:279:TRP:CE2	2.53	0.44
1:F:12:LEU:CD1	1:F:241:ALA:HB1	2.46	0.44
1:E:187:ARG:HD2	1:F:211:ASP:OD2	2.17	0.44
1:H:314:ASN:HD22	1:H:323:ILE:HD11	1.82	0.44
1:B:115:ASP:HB3	1:B:120:ARG:HD3	2.00	0.44
1:G:34:LEU:HD21	1:G:99:PRO:HA	2.00	0.44
1:F:64:VAL:HG13	1:F:72:ILE:HD13	2.00	0.44
1:G:331:ARG:HG2	1:G:331:ARG:O	2.18	0.44
1:A:181:ILE:HG23	1:A:212:ARG:HG3	1.99	0.44
1:G:131:LYS:HE3	1:G:156:ILE:HG12	2.00	0.44
1:B:5:ARG:HE	1:B:416:VAL:HG21	1.81	0.44
1:B:87:VAL:HG11	1:B:110:SER:O	2.17	0.44
1:B:218:VAL:HG21	1:B:221:LEU:HD21	2.00	0.44
1:E:37:GLU:HB3	1:E:38:PRO:CD	2.48	0.44
1:B:127:PHE:CZ	1:B:131:LYS:HE3	2.53	0.44
1:E:50:ILE:O	1:E:54:MET:HG3	2.17	0.44
1:H:167:VAL:HG12	4:H:508:EDO:H22	1.98	0.44
1:D:320:THR:HA	1:D:354:CYS:O	2.16	0.44
1:B:81:SER:CB	1:B:108:GLN:HG3	2.30	0.44
1:H:392:ILE:HD12	1:H:415:ARG:NH1	2.33	0.44
1:B:372:ALA:O	1:B:373:SER:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:LEU:HD11	1:D:160:LYS:CG	2.48	0.44
1:H:367:ALA:CB	1:H:373:SER:HB2	2.48	0.44
1:A:366:MET:CE	1:D:88:LYS:HD2	2.48	0.44
1:H:13:GLN:HA	1:H:248:LYS:O	2.18	0.44
1:E:109:VAL:HG12	1:E:110:SER:O	2.17	0.44
1:H:11:ARG:HD3	1:H:247:GLY:HA2	2.00	0.44
1:E:233:ILE:HG21	1:E:371:ARG:HD3	2.00	0.44
1:C:374:ALA:O	1:C:378:LEU:HG	2.18	0.44
1:G:193:ASP:CB	1:G:229:LEU:HD22	2.48	0.43
1:H:101:VAL:HG11	1:H:145:ALA:HB3	2.00	0.43
1:E:12:LEU:HD12	1:E:241:ALA:HB1	2.00	0.43
1:F:369:ASP:CG	1:F:372:ALA:HB3	2.38	0.43
1:H:67:IAS:CG	1:H:69:SER:N	2.81	0.43
1:B:308:ALA:HA	1:B:334:HIS:NE2	2.32	0.43
1:G:64:VAL:HG22	1:G:72:ILE:CD1	2.49	0.43
1:B:193:ASP:CG	1:B:229:LEU:HD22	2.38	0.43
1:F:39:VAL:HG12	1:F:40:GLU:N	2.32	0.43
1:A:374:ALA:HB2	1:A:399:TYR:CE1	2.53	0.43
1:D:3:LYS:HE2	1:D:390:ASP:OD1	2.18	0.43
1:B:24:ALA:HB3	1:B:228:VAL:HG13	1.99	0.43
1:A:395:ILE:CG2	1:A:396:ASP:N	2.81	0.43
1:B:108:GLN:HB3	1:B:144:LYS:HG2	1.99	0.43
1:D:41:ILE:HG22	1:D:44:VAL:HG23	1.99	0.43
1:A:323:ILE:HB	1:A:352:VAL:HG12	1.98	0.43
1:D:340:ARG:HG2	1:D:340:ARG:HH11	1.83	0.43
1:F:320:THR:HA	1:F:354:CYS:O	2.19	0.43
1:B:16:VAL:CG1	1:B:249:ILE:HD11	2.48	0.43
1:A:244:ILE:HD12	1:A:382:ILE:HD13	2.01	0.43
1:G:56:LEU:HD23	1:G:56:LEU:C	2.39	0.43
1:B:220:ARG:HG3	1:B:220:ARG:NH1	2.33	0.43
1:D:87:VAL:HG11	1:D:110:SER:O	2.18	0.43
1:E:396:ASP:CG	1:E:415:ARG:HH22	2.22	0.43
1:E:1:MET:C	1:E:418:GLY:HA2	2.39	0.43
1:D:335:VAL:HB	1:D:336:PRO:CD	2.48	0.43
1:H:289:PRO:HD3	5:H:601:HOH:O	2.18	0.43
1:B:416:VAL:HG12	1:B:417:LYS:N	2.33	0.43
1:E:256:PRO:HG3	1:E:280:ILE:HG13	2.00	0.43
1:A:22:LYS:HD3	1:A:398:GLY:HA2	2.01	0.43
1:A:35:ALA:HB1	1:A:222:GLY:O	2.19	0.43
1:G:371:ARG:HD3	1:G:371:ARG:HA	1.75	0.43
1:D:189:PRO:HD3	1:D:299:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ALA:O	1:D:356:GLY:HA3	2.18	0.43
1:A:265:LYS:HA	1:A:265:LYS:HD3	1.78	0.43
1:D:151:LEU:O	1:D:176:ALA:HB1	2.19	0.43
1:A:308:ALA:HA	1:A:334:HIS:NE2	2.34	0.42
1:B:32:ALA:O	1:B:34:LEU:N	2.52	0.42
1:D:238:PHE:O	1:D:241:ALA:HB3	2.19	0.42
1:C:64:VAL:HG13	1:C:72:ILE:CD1	2.49	0.42
1:C:335:VAL:HB	1:C:336:PRO:CD	2.49	0.42
1:A:161:VAL:HG11	1:A:298:PRO:HB3	2.00	0.42
1:A:4:PHE:HE1	1:A:415:ARG:HB2	1.83	0.42
1:G:118:GLY:HA2	1:G:329:GLU:OE1	2.14	0.42
1:A:182:ILE:O	1:A:212:ARG:HA	2.19	0.42
1:E:63:LYS:O	1:E:72:ILE:HA	2.19	0.42
1:E:51:ASP:HA	1:E:54:MET:HE2	2.01	0.42
1:D:2:ASP:HB3	1:D:392:ILE:HD11	2.01	0.42
1:B:315:LEU:O	1:B:357:VAL:HG22	2.18	0.42
1:D:94:ILE:CD1	1:D:122:VAL:HG11	2.49	0.42
1:F:33:LEU:CD2	1:F:57:LEU:HD22	2.46	0.42
1:B:323:ILE:HB	1:B:352:VAL:HG13	2.01	0.42
1:E:85:ASP:O	1:E:89:THR:HG23	2.19	0.42
1:E:259:LEU:HD12	1:E:263:LEU:HG	2.01	0.42
1:C:254:ALA:O	1:C:278:ASP:HA	2.20	0.42
1:C:282:LEU:HD23	1:C:282:LEU:C	2.40	0.42
1:E:29:LEU:O	1:E:32:ALA:HB3	2.20	0.42
1:A:230:PRO:HG2	1:A:255:GLN:HB2	2.01	0.42
1:A:117:ILE:HG21	1:A:369:ASP:OD2	2.19	0.42
1:E:323:ILE:O	1:E:351:THR:HA	2.20	0.42
1:E:265:LYS:HA	1:E:265:LYS:HD3	1.84	0.42
1:H:235:THR:O	1:H:239:LEU:HG	2.19	0.42
1:D:308:ALA:HA	1:D:334:HIS:NE2	2.34	0.42
1:C:30:PHE:CZ	1:C:53:THR:HG23	2.54	0.42
1:H:402:ILE:HG23	1:H:403:GLU:N	2.35	0.42
1:B:315:LEU:HD21	1:B:345:ALA:HB2	2.01	0.42
1:E:232:ARG:HB2	1:E:259:LEU:HD23	2.01	0.42
1:B:313:LEU:C	1:B:313:LEU:HD23	2.40	0.42
1:C:370:LEU:HD11	1:C:399:TYR:CE1	2.54	0.42
1:H:42:GLN:HA	1:H:69:SER:CB	2.41	0.42
1:F:414:GLU:HG2	1:F:416:VAL:HG23	2.02	0.42
1:F:64:VAL:C	1:F:65:GLU:HG3	2.40	0.42
1:F:20:GLY:HA3	1:F:43:ASN:O	2.19	0.42
1:C:11:ARG:HD3	1:C:13:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ILE:HA	1:C:144:LYS:O	2.20	0.42
1:A:21:ALA:HA	1:A:231:ASP:CB	2.49	0.42
1:D:34:LEU:HD21	1:D:99:PRO:HA	2.00	0.42
1:B:77:VAL:HB	1:B:104:PHE:CZ	2.55	0.42
1:A:333:MET:HE3	1:A:333:MET:HA	2.00	0.42
1:B:264:ALA:O	1:B:268:GLU:HG3	2.19	0.42
1:C:5:ARG:NH1	1:C:386:THR:HG21	2.35	0.42
1:H:370:LEU:HD12	1:H:397:ARG:CD	2.35	0.42
1:H:2:ASP:HB3	1:H:392:ILE:CD1	2.38	0.42
1:C:28:ILE:HG23	1:C:197:PHE:CD2	2.54	0.42
1:C:24:ALA:CB	1:C:228:VAL:HG13	2.48	0.42
1:E:111:LEU:HA	1:E:112:PRO:HD3	1.90	0.42
1:D:213:ILE:HG22	1:D:215:ILE:CD1	2.50	0.42
1:H:91:ARG:C	1:H:93:SER:H	2.23	0.42
1:G:182:ILE:HG22	1:G:185:ALA:HB2	2.00	0.42
1:E:132:LEU:HA	1:E:132:LEU:HD23	1.87	0.42
1:C:244:ILE:HD12	1:C:382:ILE:HD13	2.01	0.42
1:E:317:ALA:O	1:E:356:GLY:HA3	2.20	0.42
1:B:4:PHE:CE2	1:B:413:ILE:HD11	2.55	0.42
1:D:294:VAL:HB	1:D:323:ILE:HD13	2.00	0.42
1:B:83:PRO:CG	1:B:86:LEU:HD12	2.50	0.42
1:D:382:ILE:HD12	4:D:507:EDO:H22	2.01	0.42
1:A:189:PRO:HD3	1:A:299:HIS:CD2	2.55	0.42
1:H:55:LYS:HA	4:H:510:EDO:H22	2.02	0.42
1:C:392:ILE:HB	1:C:395:ILE:HG21	2.01	0.41
1:B:197:PHE:O	1:B:201:LEU:HG	2.20	0.41
1:C:64:VAL:O	1:C:65:GLU:HG3	2.20	0.41
1:E:103:ARG:HG2	1:E:104:PHE:CE1	2.54	0.41
1:E:81:SER:HB3	1:E:108:GLN:HB2	2.02	0.41
1:F:282:LEU:C	1:F:282:LEU:HD23	2.40	0.41
1:H:66:ARG:CB	1:H:70:VAL:HG22	2.50	0.41
2:A:501:UD1:H5'2	4:A:507:EDO:O2	2.20	0.41
1:H:256:PRO:HG3	1:H:280:ILE:CG1	2.50	0.41
1:B:369:ASP:C	1:B:371:ARG:H	2.23	0.41
1:H:117:ILE:HG22	1:H:331:ARG:HG3	2.01	0.41
1:H:56:LEU:HB2	1:H:86:LEU:HD13	2.02	0.41
1:B:189:PRO:HD3	1:B:299:HIS:CD2	2.55	0.41
1:B:30:PHE:HE1	1:B:96:ALA:HB2	1.85	0.41
1:B:273:ILE:CG2	1:B:274:GLU:N	2.84	0.41
1:G:245:SER:HB3	1:G:382:ILE:HG22	2.01	0.41
1:H:2:ASP:C	1:H:392:ILE:HG12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:366:MET:HE2	1:H:391:ARG:HD2	2.01	0.41
1:A:81:SER:HA	1:A:108:GLN:O	2.20	0.41
1:A:298:PRO:HA	4:A:507:EDO:H11	2.03	0.41
1:E:203:ALA:HB2	1:E:221:LEU:HD21	2.03	0.41
1:G:22:LYS:HD3	1:G:371:ARG:NH2	2.35	0.41
1:H:236:GLY:O	1:H:240:VAL:HG23	2.20	0.41
1:C:37:GLU:HB3	1:C:38:PRO:HD2	2.02	0.41
1:E:195:ALA:HB3	1:E:208:GLN:HG3	2.02	0.41
1:G:50:ILE:O	1:G:54:MET:HG3	2.20	0.41
1:H:29:LEU:HD23	1:H:41:ILE:HD13	2.03	0.41
1:B:415:ARG:HG2	1:B:415:ARG:O	2.19	0.41
1:F:199:VAL:O	1:F:202:GLY:N	2.49	0.41
1:A:88:LYS:HG2	1:A:88:LYS:O	2.21	0.41
1:D:282:LEU:HD23	1:D:282:LEU:C	2.40	0.41
1:B:54:MET:HG2	1:B:64:VAL:HG11	2.02	0.41
1:C:161:VAL:O	3:C:503:ACT:H2	2.21	0.41
1:F:204:LYS:HG3	1:F:218:VAL:HG11	2.02	0.41
1:A:208:GLN:HA	1:A:213:ILE:HG12	2.03	0.41
1:D:252:ARG:O	1:D:253:ASN:HB2	2.21	0.41
1:H:370:LEU:HD12	1:H:397:ARG:HB2	2.03	0.41
1:D:12:LEU:CD1	1:D:241:ALA:HB1	2.51	0.41
1:C:196:ASN:HB2	1:C:226:TYR:OH	2.20	0.41
1:D:65:GLU:HG3	1:D:71:TRP:HB2	2.02	0.41
1:B:66:ARG:HD2	1:B:70:VAL:HG22	2.03	0.41
1:A:60:LEU:HA	1:A:79:ASN:HB3	2.03	0.41
1:C:392:ILE:C	1:C:395:ILE:HG22	2.15	0.41
1:C:39:VAL:HG12	1:C:41:ILE:CD1	2.50	0.41
1:B:373:SER:HB3	1:B:395:ILE:CG1	2.51	0.41
1:E:42:GLN:HA	1:E:69:SER:HB2	2.02	0.41
1:A:256:PRO:HG3	1:A:280:ILE:HG12	2.02	0.41
1:G:131:LYS:HB3	1:G:131:LYS:HE3	1.94	0.41
1:F:371:ARG:NH2	1:F:398:GLY:O	2.54	0.41
1:C:314:ASN:HB3	1:C:354:CYS:HB2	2.03	0.41
1:E:13:GLN:O	1:E:409:LEU:HA	2.21	0.41
1:B:16:VAL:HG11	1:B:249:ILE:HD11	2.03	0.41
1:H:370:LEU:CD1	1:H:397:ARG:CZ	2.99	0.41
1:G:340:ARG:NH1	1:G:340:ARG:CG	2.83	0.41
1:H:91:ARG:C	1:H:93:SER:N	2.73	0.41
1:F:263:LEU:HD22	1:F:273:ILE:HD13	2.02	0.41
1:D:283:ASP:OD2	1:D:285:HIS:CE1	2.74	0.41
1:C:67:IAS:CG	1:C:69:SER:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ASP:HB3	1:C:392:ILE:HD11	2.03	0.40
1:C:4:PHE:CD1	1:C:392:ILE:HD13	2.56	0.40
1:D:91:ARG:NH2	1:D:120:ARG:CB	2.84	0.40
1:A:369:ASP:C	1:A:371:ARG:N	2.74	0.40
1:E:330:ASN:HB2	1:H:330:ASN:CG	2.42	0.40
1:H:117:ILE:HD12	1:H:328:PHE:CD2	2.56	0.40
1:H:56:LEU:HD23	1:H:56:LEU:O	2.20	0.40
1:E:57:LEU:O	1:E:62:THR:CB	2.69	0.40
1:B:57:LEU:HD23	1:B:57:LEU:HA	1.92	0.40
1:H:63:LYS:HG2	3:H:504:ACT:H3	2.03	0.40
1:F:315:LEU:HD22	1:F:343:ALA:HB1	2.01	0.40
1:A:196:ASN:OD1	1:A:208:GLN:NE2	2.55	0.40
1:E:33:LEU:HD13	1:E:100:LEU:HD21	2.03	0.40
1:G:147:VAL:HG13	1:G:147:VAL:O	2.20	0.40
1:C:367:ALA:HB1	1:C:373:SER:CB	2.44	0.40
1:A:314:ASN:ND2	1:A:323:ILE:HD11	2.36	0.40
1:B:190:GLU:N	1:B:190:GLU:OE1	2.50	0.40
1:A:4:PHE:HA	1:A:4:PHE:HD1	1.79	0.40
1:A:233:ILE:HG23	1:A:306:MET:HE3	2.03	0.40
1:F:1:MET:CE	1:F:391:ARG:HG2	2.50	0.40
1:B:401:ARG:HB3	1:B:404:ASP:OD2	2.21	0.40
1:B:395:ILE:HG21	1:B:402:ILE:CG2	2.52	0.40
1:D:24:ALA:HB3	1:D:228:VAL:HG13	2.03	0.40
1:C:4:PHE:CG	1:C:392:ILE:HG21	2.56	0.40
1:F:40:GLU:CD	1:F:71:TRP:HE1	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:GLU:O	1:H:139:GLU:OE2[2_456]	1.89	0.31

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	415/419 (99%)	398 (96%)	14 (3%)	3 (1%)	26	46
1	B	415/419 (99%)	386 (93%)	26 (6%)	3 (1%)	26	46
1	C	415/419 (99%)	404 (97%)	9 (2%)	2 (0%)	34	55
1	D	415/419 (99%)	398 (96%)	14 (3%)	3 (1%)	26	46
1	E	415/419 (99%)	389 (94%)	21 (5%)	5 (1%)	16	29
1	F	415/419 (99%)	399 (96%)	16 (4%)	0	100	100
1	G	415/419 (99%)	400 (96%)	15 (4%)	0	100	100
1	H	415/419 (99%)	397 (96%)	18 (4%)	0	100	100
All	All	3320/3352 (99%)	3171 (96%)	133 (4%)	16 (0%)	34	55

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	119	ALA
1	E	60	LEU
1	E	77	VAL
1	B	33	LEU
1	A	417	LYS
1	B	92	ALA
1	B	370	LEU
1	C	92	ALA
1	D	118	GLY
1	E	140	GLU
1	A	148	ASN
1	A	370	LEU
1	D	418	GLY
1	E	222	GLY
1	C	77	VAL
1	E	392	ILE

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	329/329 (100%)	326 (99%)	3 (1%)	84	95
1	B	329/329 (100%)	324 (98%)	5 (2%)	72	91
1	C	329/329 (100%)	325 (99%)	4 (1%)	78	93
1	D	329/329 (100%)	327 (99%)	2 (1%)	90	97
1	E	329/329 (100%)	325 (99%)	4 (1%)	78	93
1	F	329/329 (100%)	325 (99%)	4 (1%)	78	93
1	G	329/329 (100%)	327 (99%)	2 (1%)	90	97
1	H	329/329 (100%)	326 (99%)	3 (1%)	84	95
All	All	2632/2632 (100%)	2605 (99%)	27 (1%)	82	95

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ARG
1	A	193	ASP
1	A	229	LEU
1	B	187	ARG
1	B	193	ASP
1	B	278	ASP
1	B	307	GLN
1	B	371	ARG
1	C	10	THR
1	C	187	ARG
1	C	259	LEU
1	C	371	ARG
1	D	59	GLN
1	D	187	ARG
1	E	22	LYS
1	E	66	ARG
1	E	187	ARG
1	E	391	ARG
1	F	135	GLU
1	F	187	ARG
1	F	229	LEU
1	F	371	ARG
1	G	187	ARG
1	G	229	LEU
1	H	135	GLU
1	H	187	ARG
1	H	371	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	79	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z > 2$
1	IAS	A	67	1	4,7,8	0.57	0	1,8,10	1.20	0
1	IAS	B	67	1	4,7,8	0.53	0	1,8,10	1.29	0
1	IAS	C	67	1	4,7,8	0.59	0	1,8,10	1.33	0
1	IAS	D	67	1	4,7,8	0.70	0	1,8,10	1.11	0
1	IAS	E	67	1	4,7,8	0.60	0	1,8,10	1.26	0
1	IAS	F	67	1	4,7,8	0.64	0	1,8,10	1.43	0
1	IAS	G	67	1	4,7,8	0.75	0	1,8,10	1.26	0
1	IAS	H	67	1	4,7,8	0.61	0	1,8,10	1.21	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
1	IAS	A	67	1	-	0/3/7/8	0/0/0/0
1	IAS	B	67	1	-	0/3/7/8	0/0/0/0
1	IAS	C	67	1	-	0/3/7/8	0/0/0/0
1	IAS	D	67	1	-	0/3/7/8	0/0/0/0
1	IAS	E	67	1	-	0/3/7/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IAS	F	67	1	-	0/3/7/8	0/0/0/0
1	IAS	G	67	1	-	0/3/7/8	0/0/0/0
1	IAS	H	67	1	-	0/3/7/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	67	IAS	1	0
1	H	67	IAS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

72 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	UD1	A	501	-	32,41,41	1.85	10 (31%)	46,62,62	2.19	7 (15%)
3	ACT	A	502	-	1,3,3	3.05	1 (100%)	0,3,3	0.00	-
3	ACT	A	503	-	1,3,3	1.88	0	0,3,3	0.00	-
3	ACT	A	504	-	1,3,3	2.31	1 (100%)	0,3,3	0.00	-
3	ACT	A	505	-	1,3,3	2.31	1 (100%)	0,3,3	0.00	-
4	EDO	A	506	-	3,3,3	0.55	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	507	-	3,3,3	0.47	0	2,2,2	0.46	0
4	EDO	A	508	-	3,3,3	0.51	0	2,2,2	0.39	0
4	EDO	A	509	-	3,3,3	0.55	0	2,2,2	0.41	0
2	UD1	B	501	-	32,41,41	1.87	12 (37%)	46,62,62	2.21	8 (17%)
3	ACT	B	502	-	1,3,3	2.20	1 (100%)	0,3,3	0.00	-
4	EDO	B	503	-	3,3,3	0.37	0	2,2,2	0.54	0
4	EDO	B	504	-	3,3,3	0.45	0	2,2,2	0.43	0
4	EDO	B	505	-	3,3,3	0.43	0	2,2,2	0.45	0
2	UD1	C	501	-	32,41,41	1.92	9 (28%)	46,62,62	2.17	7 (15%)
3	ACT	C	502	-	1,3,3	1.99	0	0,3,3	0.00	-
3	ACT	C	503	-	1,3,3	2.61	1 (100%)	0,3,3	0.00	-
4	EDO	C	504	-	3,3,3	0.45	0	2,2,2	0.39	0
4	EDO	C	505	-	3,3,3	0.61	0	2,2,2	0.33	0
4	EDO	C	506	-	3,3,3	0.54	0	2,2,2	0.37	0
4	EDO	C	507	-	3,3,3	0.52	0	2,2,2	0.40	0
2	UD1	D	501	-	32,41,41	1.90	10 (31%)	46,62,62	2.22	7 (15%)
3	ACT	D	502	-	1,3,3	2.34	1 (100%)	0,3,3	0.00	-
3	ACT	D	503	-	1,3,3	1.93	0	0,3,3	0.00	-
4	EDO	D	504	-	3,3,3	0.42	0	2,2,2	0.50	0
4	EDO	D	505	-	3,3,3	0.36	0	2,2,2	0.47	0
4	EDO	D	506	-	3,3,3	0.65	0	2,2,2	0.29	0
4	EDO	D	507	-	3,3,3	0.46	0	2,2,2	0.41	0
4	EDO	D	508	-	3,3,3	0.58	0	2,2,2	0.31	0
4	EDO	D	509	-	3,3,3	0.46	0	2,2,2	0.41	0
4	EDO	D	510	-	3,3,3	0.55	0	2,2,2	0.43	0
2	UD1	E	501	-	32,41,41	1.88	10 (31%)	46,62,62	2.24	7 (15%)
3	ACT	E	502	-	1,3,3	1.55	0	0,3,3	0.00	-
3	ACT	E	503	-	1,3,3	1.94	0	0,3,3	0.00	-
3	ACT	E	504	-	1,3,3	1.97	0	0,3,3	0.00	-
4	EDO	E	505	-	3,3,3	0.52	0	2,2,2	0.40	0
4	EDO	E	506	-	3,3,3	0.57	0	2,2,2	0.34	0
4	EDO	E	507	-	3,3,3	0.63	0	2,2,2	0.33	0
4	EDO	E	508	-	3,3,3	0.55	0	2,2,2	0.33	0
4	EDO	E	509	-	3,3,3	0.37	0	2,2,2	0.44	0
4	EDO	E	510	-	3,3,3	0.60	0	2,2,2	0.29	0
4	EDO	E	511	-	3,3,3	0.54	0	2,2,2	0.37	0
2	UD1	F	501	-	32,41,41	1.83	10 (31%)	46,62,62	2.21	6 (13%)
3	ACT	F	502	-	1,3,3	2.26	1 (100%)	0,3,3	0.00	-
3	ACT	F	503	-	1,3,3	1.54	0	0,3,3	0.00	-
3	ACT	F	504	-	1,3,3	2.40	1 (100%)	0,3,3	0.00	-
4	EDO	F	505	-	3,3,3	0.47	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	F	506	-	3,3,3	0.49	0	2,2,2	0.42	0
4	EDO	F	507	-	3,3,3	0.50	0	2,2,2	0.37	0
4	EDO	F	508	-	3,3,3	0.50	0	2,2,2	0.40	0
4	EDO	F	509	-	3,3,3	0.57	0	2,2,2	0.42	0
2	UD1	G	501	-	32,41,41	1.80	8 (25%)	46,62,62	2.23	7 (15%)
4	EDO	G	502	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	G	503	-	3,3,3	0.49	0	2,2,2	0.43	0
4	EDO	G	504	-	3,3,3	0.60	0	2,2,2	0.33	0
4	EDO	G	505	-	3,3,3	0.49	0	2,2,2	0.41	0
4	EDO	G	506	-	3,3,3	0.55	0	2,2,2	0.37	0
4	EDO	G	507	-	3,3,3	0.58	0	2,2,2	0.32	0
4	EDO	G	508	-	3,3,3	0.88	0	2,2,2	0.39	0
2	UD1	H	501	-	32,41,41	1.95	10 (31%)	46,62,62	2.31	8 (17%)
3	ACT	H	502	-	1,3,3	1.95	0	0,3,3	0.00	-
3	ACT	H	503	-	1,3,3	0.54	0	0,3,3	0.00	-
3	ACT	H	504	-	1,3,3	1.22	0	0,3,3	0.00	-
3	ACT	H	505	-	1,3,3	2.27	1 (100%)	0,3,3	0.00	-
3	ACT	H	506	-	1,3,3	2.56	1 (100%)	0,3,3	0.00	-
4	EDO	H	507	-	3,3,3	0.48	0	2,2,2	0.37	0
4	EDO	H	508	-	3,3,3	0.59	0	2,2,2	0.35	0
4	EDO	H	509	-	3,3,3	0.52	0	2,2,2	0.38	0
4	EDO	H	510	-	3,3,3	0.52	0	2,2,2	0.39	0
4	EDO	H	511	-	3,3,3	0.52	0	2,2,2	0.41	0
4	EDO	H	512	-	3,3,3	0.53	0	2,2,2	0.42	0
4	EDO	H	513	-	3,3,3	0.55	0	2,2,2	0.38	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	UD1	A	501	-	-	0/22/63/63	0/3/3/3
3	ACT	A	502	-	-	0/0/0/0	0/0/0/0
3	ACT	A	503	-	-	0/0/0/0	0/0/0/0
3	ACT	A	504	-	-	0/0/0/0	0/0/0/0
3	ACT	A	505	-	-	0/0/0/0	0/0/0/0
4	EDO	A	506	-	-	0/1/1/1	0/0/0/0
4	EDO	A	507	-	-	0/1/1/1	0/0/0/0
4	EDO	A	508	-	-	0/1/1/1	0/0/0/0
4	EDO	A	509	-	-	0/1/1/1	0/0/0/0
2	UD1	B	501	-	-	0/22/63/63	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	B	502	-	-	0/0/0/0	0/0/0/0
4	EDO	B	503	-	-	0/1/1/1	0/0/0/0
4	EDO	B	504	-	-	0/1/1/1	0/0/0/0
4	EDO	B	505	-	-	0/1/1/1	0/0/0/0
2	UD1	C	501	-	-	0/22/63/63	0/3/3/3
3	ACT	C	502	-	-	0/0/0/0	0/0/0/0
3	ACT	C	503	-	-	0/0/0/0	0/0/0/0
4	EDO	C	504	-	-	0/1/1/1	0/0/0/0
4	EDO	C	505	-	-	0/1/1/1	0/0/0/0
4	EDO	C	506	-	-	0/1/1/1	0/0/0/0
4	EDO	C	507	-	-	0/1/1/1	0/0/0/0
2	UD1	D	501	-	-	0/22/63/63	0/3/3/3
3	ACT	D	502	-	-	0/0/0/0	0/0/0/0
3	ACT	D	503	-	-	0/0/0/0	0/0/0/0
4	EDO	D	504	-	-	0/1/1/1	0/0/0/0
4	EDO	D	505	-	-	0/1/1/1	0/0/0/0
4	EDO	D	506	-	-	0/1/1/1	0/0/0/0
4	EDO	D	507	-	-	0/1/1/1	0/0/0/0
4	EDO	D	508	-	-	0/1/1/1	0/0/0/0
4	EDO	D	509	-	-	0/1/1/1	0/0/0/0
4	EDO	D	510	-	-	0/1/1/1	0/0/0/0
2	UD1	E	501	-	-	0/22/63/63	0/3/3/3
3	ACT	E	502	-	-	0/0/0/0	0/0/0/0
3	ACT	E	503	-	-	0/0/0/0	0/0/0/0
3	ACT	E	504	-	-	0/0/0/0	0/0/0/0
4	EDO	E	505	-	-	0/1/1/1	0/0/0/0
4	EDO	E	506	-	-	0/1/1/1	0/0/0/0
4	EDO	E	507	-	-	0/1/1/1	0/0/0/0
4	EDO	E	508	-	-	0/1/1/1	0/0/0/0
4	EDO	E	509	-	-	0/1/1/1	0/0/0/0
4	EDO	E	510	-	-	0/1/1/1	0/0/0/0
4	EDO	E	511	-	-	0/1/1/1	0/0/0/0
2	UD1	F	501	-	-	0/22/63/63	0/3/3/3
3	ACT	F	502	-	-	0/0/0/0	0/0/0/0
3	ACT	F	503	-	-	0/0/0/0	0/0/0/0
3	ACT	F	504	-	-	0/0/0/0	0/0/0/0
4	EDO	F	505	-	-	0/1/1/1	0/0/0/0
4	EDO	F	506	-	-	0/1/1/1	0/0/0/0
4	EDO	F	507	-	-	0/1/1/1	0/0/0/0
4	EDO	F	508	-	-	0/1/1/1	0/0/0/0
4	EDO	F	509	-	-	0/1/1/1	0/0/0/0
2	UD1	G	501	-	-	0/22/63/63	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	G	502	-	-	0/1/1/1	0/0/0/0
4	EDO	G	503	-	-	0/1/1/1	0/0/0/0
4	EDO	G	504	-	-	0/1/1/1	0/0/0/0
4	EDO	G	505	-	-	0/1/1/1	0/0/0/0
4	EDO	G	506	-	-	0/1/1/1	0/0/0/0
4	EDO	G	507	-	-	0/1/1/1	0/0/0/0
4	EDO	G	508	-	-	0/1/1/1	0/0/0/0
2	UD1	H	501	-	-	0/22/63/63	0/3/3/3
3	ACT	H	502	-	-	0/0/0/0	0/0/0/0
3	ACT	H	503	-	-	0/0/0/0	0/0/0/0
3	ACT	H	504	-	-	0/0/0/0	0/0/0/0
3	ACT	H	505	-	-	0/0/0/0	0/0/0/0
3	ACT	H	506	-	-	0/0/0/0	0/0/0/0
4	EDO	H	507	-	-	0/1/1/1	0/0/0/0
4	EDO	H	508	-	-	0/1/1/1	0/0/0/0
4	EDO	H	509	-	-	0/1/1/1	0/0/0/0
4	EDO	H	510	-	-	0/1/1/1	0/0/0/0
4	EDO	H	511	-	-	0/1/1/1	0/0/0/0
4	EDO	H	512	-	-	0/1/1/1	0/0/0/0
4	EDO	H	513	-	-	0/1/1/1	0/0/0/0

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	UD1	PB-O2B	-2.89	1.42	1.54
2	H	501	UD1	PB-O1B	-2.75	1.41	1.51
2	G	501	UD1	PB-O2B	-2.73	1.43	1.54
2	A	501	UD1	PB-O2B	-2.56	1.44	1.54
2	E	501	UD1	PB-O2B	-2.52	1.44	1.54
2	F	501	UD1	PB-O2B	-2.52	1.44	1.54
2	D	501	UD1	PB-O2B	-2.39	1.44	1.54
2	F	501	UD1	PB-O1B	-2.38	1.42	1.51
2	G	501	UD1	PB-O1B	-2.37	1.42	1.51
2	B	501	UD1	PB-O2B	-2.32	1.45	1.54
2	H	501	UD1	PB-O2B	-2.32	1.45	1.54
2	F	501	UD1	PA-O2A	-2.32	1.45	1.54
2	C	501	UD1	PB-O1B	-2.29	1.42	1.51
2	D	501	UD1	PB-O1B	-2.14	1.43	1.51
2	E	501	UD1	PB-O1B	-2.13	1.43	1.51
2	A	501	UD1	PA-O2A	-2.09	1.46	1.54
2	C	501	UD1	O3'-C3'	2.03	1.47	1.43
2	F	501	UD1	O3'-C3'	2.06	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	UD1	C1'-C2'	2.07	1.56	1.53
2	B	501	UD1	C3B-C4B	2.07	1.58	1.53
2	F	501	UD1	C8'-C7'	2.09	1.54	1.50
2	D	501	UD1	C3B-C4B	2.10	1.58	1.53
2	E	501	UD1	O5'-C1'	2.11	1.47	1.41
2	D	501	UD1	O5'-C1'	2.14	1.47	1.41
2	G	501	UD1	O3'-C3'	2.14	1.48	1.43
2	B	501	UD1	O3'-C3'	2.17	1.48	1.43
2	B	501	UD1	O4'-C4'	2.19	1.48	1.43
2	B	501	UD1	O2'-C2B	2.20	1.48	1.43
3	B	502	ACT	CH3-C	2.20	1.51	1.48
2	E	501	UD1	O3'-C3'	2.23	1.48	1.43
2	A	501	UD1	C2'-N2'	2.23	1.49	1.45
2	H	501	UD1	C8'-C7'	2.24	1.55	1.50
3	F	502	ACT	CH3-C	2.26	1.52	1.48
2	B	501	UD1	C8'-C7'	2.26	1.55	1.50
3	H	505	ACT	CH3-C	2.27	1.52	1.48
3	A	504	ACT	CH3-C	2.31	1.52	1.48
2	F	501	UD1	O5'-C5'	2.31	1.50	1.44
3	A	505	ACT	CH3-C	2.31	1.52	1.48
3	D	502	ACT	CH3-C	2.34	1.52	1.48
2	F	501	UD1	O3B-C3B	2.35	1.48	1.43
2	B	501	UD1	C4'-C5'	2.37	1.58	1.53
2	H	501	UD1	O3B-C3B	2.37	1.48	1.43
2	C	501	UD1	O5'-C5'	2.37	1.50	1.44
2	H	501	UD1	C1'-C2'	2.40	1.57	1.53
3	F	504	ACT	CH3-C	2.40	1.52	1.48
2	E	501	UD1	C8'-C7'	2.41	1.55	1.50
2	D	501	UD1	O3'-C3'	2.42	1.48	1.43
2	H	501	UD1	O2'-C2B	2.43	1.48	1.43
2	D	501	UD1	O2'-C2B	2.43	1.48	1.43
2	E	501	UD1	O2'-C2B	2.45	1.48	1.43
2	A	501	UD1	O3B-C3B	2.47	1.48	1.43
2	A	501	UD1	C8'-C7'	2.49	1.55	1.50
2	H	501	UD1	O5'-C5'	2.50	1.50	1.44
2	C	501	UD1	C8'-C7'	2.51	1.55	1.50
2	C	501	UD1	O2'-C2B	2.54	1.49	1.43
2	G	501	UD1	O2'-C2B	2.54	1.49	1.43
2	G	501	UD1	C8'-C7'	2.54	1.55	1.50
2	D	501	UD1	C8'-C7'	2.56	1.55	1.50
3	H	506	ACT	CH3-C	2.56	1.52	1.48
2	A	501	UD1	O4'-C4'	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	UD1	O3B-C3B	2.59	1.49	1.43
2	B	501	UD1	O5'-C5'	2.60	1.50	1.44
3	C	503	ACT	CH3-C	2.61	1.52	1.48
2	B	501	UD1	O3B-C3B	2.66	1.49	1.43
2	E	501	UD1	O5'-C5'	2.70	1.51	1.44
2	G	501	UD1	O5'-C5'	2.75	1.51	1.44
2	F	501	UD1	O2'-C2B	2.75	1.49	1.43
2	H	501	UD1	O3'-C3'	2.76	1.49	1.43
2	A	501	UD1	O2'-C2B	2.77	1.49	1.43
2	E	501	UD1	O3B-C3B	2.98	1.50	1.43
3	A	502	ACT	CH3-C	3.05	1.53	1.48
2	B	501	UD1	C4-N3	3.11	1.38	1.33
2	F	501	UD1	C4-N3	3.28	1.39	1.33
2	D	501	UD1	O5'-C5'	3.29	1.52	1.44
2	A	501	UD1	O5'-C5'	3.29	1.52	1.44
2	E	501	UD1	C4-N3	3.39	1.39	1.33
2	G	501	UD1	C4-N3	3.50	1.39	1.33
2	H	501	UD1	C4-N3	3.63	1.39	1.33
2	A	501	UD1	C4-N3	3.76	1.40	1.33
2	A	501	UD1	C6-N1	4.13	1.41	1.35
2	D	501	UD1	C4-N3	4.17	1.40	1.33
2	C	501	UD1	C4-N3	4.22	1.40	1.33
2	F	501	UD1	C6-N1	4.50	1.42	1.35
2	G	501	UD1	C6-N1	4.58	1.42	1.35
2	B	501	UD1	C6-N1	4.65	1.42	1.35
2	D	501	UD1	C6-N1	4.68	1.42	1.35
2	E	501	UD1	C6-N1	4.81	1.42	1.35
2	C	501	UD1	C6-N1	5.28	1.43	1.35
2	H	501	UD1	C6-N1	5.36	1.43	1.35

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	UD1	C5-C4-N3	-3.10	115.17	123.12
2	B	501	UD1	C5-C4-N3	-3.05	115.29	123.12
2	A	501	UD1	C5-C4-N3	-3.04	115.33	123.12
2	G	501	UD1	C5-C4-N3	-3.01	115.41	123.12
2	D	501	UD1	C5-C4-N3	-2.98	115.47	123.12
2	H	501	UD1	C5-C4-N3	-2.96	115.52	123.12
2	E	501	UD1	C5-C4-N3	-2.94	115.58	123.12
2	F	501	UD1	C5-C4-N3	-2.87	115.77	123.12
2	H	501	UD1	C4'-C3'-C2'	-2.33	107.20	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	UD1	C2B-C3B-C4B	-2.04	98.41	102.61
2	B	501	UD1	O2B-PB-O3A	2.01	114.19	105.09
2	H	501	UD1	O2B-PB-O3A	2.07	114.46	105.09
2	C	501	UD1	O2A-PA-O3A	2.08	114.54	105.09
2	D	501	UD1	O2B-PB-O3A	2.11	114.68	105.09
2	E	501	UD1	O2B-PB-O3A	2.14	114.80	105.09
2	G	501	UD1	O2B-PB-O3A	2.15	114.87	105.09
2	H	501	UD1	O2A-PA-O3A	2.20	115.08	105.09
2	A	501	UD1	O2B-PB-O3A	2.24	115.26	105.09
2	F	501	UD1	O2A-PA-O3A	2.25	115.32	105.09
2	D	501	UD1	O2A-PA-O3A	2.31	115.56	105.09
2	C	501	UD1	O2B-PB-O3A	2.33	115.67	105.09
2	A	501	UD1	O2A-PA-O3A	2.36	115.78	105.09
2	E	501	UD1	O2A-PA-O3A	2.41	116.05	105.09
2	B	501	UD1	O2A-PA-O3A	2.48	116.34	105.09
2	G	501	UD1	O2A-PA-O3A	2.48	116.35	105.09
2	G	501	UD1	O2'-C2B-C3B	2.63	120.37	111.83
2	F	501	UD1	O3B-C3B-C4B	2.73	119.25	111.05
2	D	501	UD1	O2'-C2B-C3B	2.74	120.74	111.83
2	C	501	UD1	O3A-PA-O5B	2.78	110.32	102.94
2	C	501	UD1	O2'-C2B-C3B	2.80	120.92	111.83
2	H	501	UD1	O2'-C2B-C3B	2.80	120.93	111.83
2	E	501	UD1	O2'-C2B-C3B	2.84	121.08	111.83
2	A	501	UD1	O3B-C3B-C4B	2.91	119.77	111.05
2	B	501	UD1	O2'-C2B-C3B	2.91	121.29	111.83
2	F	501	UD1	O2'-C2B-C3B	2.91	121.30	111.83
2	C	501	UD1	O3B-C3B-C4B	2.94	119.86	111.05
2	E	501	UD1	O3B-C3B-C4B	2.94	119.87	111.05
2	A	501	UD1	O2'-C2B-C3B	2.95	121.42	111.83
2	D	501	UD1	O3B-C3B-C4B	3.00	120.05	111.05
2	G	501	UD1	O3B-C3B-C4B	3.04	120.17	111.05
2	B	501	UD1	O3A-PA-O5B	3.10	111.15	102.94
2	G	501	UD1	O3A-PA-O5B	3.17	111.36	102.94
2	A	501	UD1	O3A-PA-O5B	3.28	111.64	102.94
2	B	501	UD1	O3B-C3B-C4B	3.32	121.00	111.05
2	H	501	UD1	O3B-C3B-C4B	3.34	121.06	111.05
2	D	501	UD1	O3A-PA-O5B	3.44	112.07	102.94
2	F	501	UD1	O3A-PA-O5B	3.63	112.58	102.94
2	E	501	UD1	O3A-PA-O5B	3.68	112.71	102.94
2	H	501	UD1	O3A-PA-O5B	4.35	114.47	102.94
2	C	501	UD1	C4-N3-C2	11.48	125.51	114.14
2	D	501	UD1	C4-N3-C2	11.53	125.56	114.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	UD1	C4-N3-C2	11.54	125.57	114.14
2	B	501	UD1	C4-N3-C2	11.58	125.61	114.14
2	E	501	UD1	C4-N3-C2	11.70	125.72	114.14
2	F	501	UD1	C4-N3-C2	11.72	125.75	114.14
2	G	501	UD1	C4-N3-C2	11.91	125.93	114.14
2	H	501	UD1	C4-N3-C2	12.13	126.15	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	UD1	1	0
4	A	507	EDO	2	0
3	C	502	ACT	2	0
3	C	503	ACT	2	0
4	D	504	EDO	1	0
4	D	507	EDO	1	0
4	D	508	EDO	2	0
4	D	509	EDO	1	0
4	D	510	EDO	2	0
3	E	502	ACT	2	0
4	E	508	EDO	1	0
3	F	503	ACT	3	0
4	F	509	EDO	1	0
4	G	505	EDO	1	0
3	H	503	ACT	1	0
3	H	504	ACT	1	0
4	H	507	EDO	1	0
4	H	508	EDO	1	0
4	H	510	EDO	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	418/419 (99%)	-0.09	4 (0%) 84 86	22, 36, 52, 87	0
1	B	418/419 (99%)	0.59	47 (11%) 7 7	30, 53, 75, 94	0
1	C	418/419 (99%)	0.04	10 (2%) 62 66	24, 42, 58, 81	0
1	D	418/419 (99%)	0.04	17 (4%) 41 46	22, 39, 58, 83	0
1	E	418/419 (99%)	0.16	18 (4%) 39 44	19, 42, 71, 92	0
1	F	418/419 (99%)	0.00	11 (2%) 59 63	24, 40, 58, 84	0
1	G	418/419 (99%)	0.03	10 (2%) 62 66	22, 39, 56, 93	0
1	H	418/419 (99%)	-0.03	10 (2%) 62 66	19, 36, 52, 89	0
All	All	3344/3352 (99%)	0.09	127 (3%) 44 49	19, 40, 64, 94	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	GLY	10.7
1	C	419	GLU	10.6
1	H	419	GLU	7.5
1	B	419	GLU	7.5
1	H	418	GLY	6.7
1	B	417	LYS	6.6
1	G	419	GLU	6.6
1	H	417	LYS	5.8
1	F	419	GLU	5.6
1	E	418	GLY	5.5
1	G	418	GLY	5.2
1	A	419	GLU	4.9
1	E	419	GLU	4.8
1	A	1	MET	4.5
1	B	287	LYS	4.3
1	B	277	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	418	GLY	4.2
1	E	277	GLU	4.2
1	D	419	GLU	4.1
1	E	63	LYS	4.0
1	E	417	LYS	4.0
1	D	418	GLY	4.0
1	C	1	MET	3.8
1	D	1	MET	3.8
1	C	287	LYS	3.7
1	H	1	MET	3.7
1	B	359	LYS	3.7
1	D	148	ASN	3.6
1	D	76	ASN	3.6
1	B	401	ARG	3.6
1	E	65	GLU	3.6
1	D	149	GLY	3.6
1	B	38	PRO	3.5
1	E	329	GLU	3.5
1	F	277	GLU	3.4
1	B	71	TRP	3.3
1	E	71	TRP	3.3
1	B	61	GLY	3.2
1	B	63	LYS	3.2
1	B	2	ASP	3.2
1	F	1	MET	3.2
1	B	358	GLU	3.2
1	B	83	PRO	3.1
1	F	127	PHE	3.1
1	G	417	LYS	3.1
1	E	38	PRO	3.1
1	C	418	GLY	3.1
1	F	177	GLU	3.1
1	B	285	HIS	3.1
1	E	1	MET	3.1
1	B	416	VAL	3.1
1	B	248	LYS	3.0
1	B	127	PHE	3.0
1	E	85	ASP	3.0
1	G	1	MET	3.0
1	B	80	PHE	3.0
1	E	401	ARG	2.9
1	F	219	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	63	LYS	2.8
1	E	76	ASN	2.8
1	B	76	ASN	2.7
1	B	79	ASN	2.7
1	H	391	ARG	2.7
1	B	202	GLY	2.7
1	F	358	GLU	2.7
1	B	78	ASN	2.7
1	B	384	GLU	2.7
1	B	15	GLU	2.6
1	F	68	GLY	2.6
1	A	212	ARG	2.6
1	B	219	GLU	2.6
1	D	75	SER	2.6
1	D	252	ARG	2.5
1	G	76	ASN	2.5
1	B	86	LEU	2.5
1	E	78	ASN	2.5
1	B	42	GLN	2.5
1	E	203	ALA	2.5
1	B	252	ARG	2.4
1	D	417	LYS	2.4
1	D	34	LEU	2.4
1	G	116	ALA	2.4
1	B	46	LYS	2.4
1	B	217	GLY	2.4
1	C	384	GLU	2.4
1	B	7	GLN	2.4
1	C	358	GLU	2.4
1	B	243	ALA	2.4
1	C	285	HIS	2.4
1	A	148	ASN	2.3
1	F	359	LYS	2.3
1	E	77	VAL	2.3
1	B	9	PRO	2.3
1	D	217	GLY	2.3
1	G	277	GLU	2.3
1	H	416	VAL	2.3
1	B	318	GLU	2.3
1	H	148	ASN	2.3
1	C	116	ALA	2.3
1	D	78	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	177	GLU	2.2
1	B	272	ASP	2.2
1	B	370	LEU	2.2
1	D	150	ARG	2.2
1	B	59	GLN	2.2
1	E	73	ASP	2.2
1	G	401	ARG	2.2
1	H	152	LYS	2.2
1	B	1	MET	2.2
1	D	127	PHE	2.2
1	B	3	LYS	2.2
1	B	152	LYS	2.2
1	B	220	ARG	2.1
1	B	216	GLU	2.1
1	F	252	ARG	2.1
1	D	179	THR	2.1
1	C	148	ASN	2.1
1	B	177	GLU	2.1
1	H	127	PHE	2.1
1	G	414	GLU	2.1
1	H	359	LYS	2.1
1	B	131	LYS	2.0
1	D	61	GLY	2.0
1	G	287	LYS	2.0
1	D	68	GLY	2.0
1	B	414	GLU	2.0
1	B	17	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
1	IAS	G	67	8/9	0.93	0.20	-	36,38,41,42	0
1	IAS	H	67	8/9	0.97	0.12	-	34,35,37,38	0
1	IAS	E	67	8/9	0.86	0.30	-	68,70,71,72	0
1	IAS	C	67	8/9	0.93	0.20	-	49,52,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	IAS	A	67	8/9	0.93	0.11	-	34,36,37,37	0
1	IAS	F	67	8/9	0.92	0.24	-	59,60,62,64	0
1	IAS	D	67	8/9	0.86	0.27	-	56,57,61,62	0
1	IAS	B	67	8/9	0.92	0.36	-	73,74,76,76	0

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(\AA^2)	Q<0.9
4	EDO	A	507	4/4	0.96	0.42	20.06	35,35,37,40	0
3	ACT	C	503	4/4	0.88	0.36	12.75	52,53,55,56	0
3	ACT	H	505	4/4	0.81	0.31	8.81	57,58,59,60	0
3	ACT	A	505	4/4	0.67	0.39	8.25	72,72,73,73	0
3	ACT	F	503	4/4	0.85	0.36	7.66	49,52,52,52	0
4	EDO	D	506	4/4	0.89	0.27	7.64	48,50,52,53	0
3	ACT	B	502	4/4	0.87	0.23	6.85	69,71,71,71	0
4	EDO	A	509	4/4	0.89	0.27	6.23	55,56,56,56	0
4	EDO	C	506	4/4	0.92	0.22	6.11	55,57,57,58	0
4	EDO	E	507	4/4	0.89	0.24	5.66	45,46,47,47	0
4	EDO	F	509	4/4	0.86	0.25	5.52	44,45,47,49	0
3	ACT	H	503	4/4	0.94	0.19	3.61	42,45,46,47	0
4	EDO	G	507	4/4	0.85	0.21	3.35	48,49,50,51	0
4	EDO	G	504	4/4	0.88	0.18	3.10	45,45,46,47	0
4	EDO	F	506	4/4	0.84	0.17	3.03	59,59,61,61	0
4	EDO	B	505	4/4	0.88	0.30	3.00	59,59,59,60	0
3	ACT	A	502	4/4	0.71	0.25	2.54	47,51,51,51	0
3	ACT	H	506	4/4	0.86	0.20	2.39	57,57,58,58	0
3	ACT	D	502	4/4	0.84	0.22	2.22	52,54,55,56	0
4	EDO	D	510	4/4	0.86	0.20	2.08	44,47,48,51	0
4	EDO	D	507	4/4	0.84	0.28	1.46	58,59,59,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	G	506	4/4	0.74	0.29	1.45	57,58,58,58	0
4	EDO	A	506	4/4	0.94	0.17	1.43	32,34,35,39	0
4	EDO	E	506	4/4	0.88	0.21	1.27	48,48,50,52	0
4	EDO	B	503	4/4	0.92	0.18	1.25	44,44,44,48	0
3	ACT	H	504	4/4	0.89	0.24	1.24	58,58,58,59	0
4	EDO	D	504	4/4	0.95	0.17	1.23	39,40,41,43	0
4	EDO	F	505	4/4	0.97	0.15	1.12	43,44,44,45	0
4	EDO	C	504	4/4	0.98	0.16	1.08	37,37,37,37	0
4	EDO	G	508	4/4	0.88	0.25	0.95	46,47,48,49	0
4	EDO	D	509	4/4	0.96	0.16	0.93	61,62,62,62	0
4	EDO	E	509	4/4	0.96	0.14	0.79	45,46,47,49	0
4	EDO	F	507	4/4	0.86	0.18	0.56	60,63,63,64	0
3	ACT	A	504	4/4	0.92	0.19	0.53	52,54,54,56	0
4	EDO	C	505	4/4	0.83	0.19	0.40	51,54,55,56	0
4	EDO	G	502	4/4	0.97	0.13	0.38	35,36,37,39	0
3	ACT	E	502	4/4	0.92	0.16	0.32	63,64,64,65	0
4	EDO	D	505	4/4	0.93	0.15	0.20	48,49,49,51	0
4	EDO	H	508	4/4	0.95	0.16	0.19	50,52,52,52	0
4	EDO	H	512	4/4	0.95	0.15	0.17	34,36,36,39	0
4	EDO	H	511	4/4	0.89	0.17	-0.04	54,56,57,58	0
4	EDO	H	507	4/4	0.95	0.12	-0.40	42,42,43,44	0
2	UD1	A	501	39/39	0.97	0.11	-0.47	18,29,37,41	0
2	UD1	E	501	39/39	0.97	0.11	-0.48	23,30,35,35	0
2	UD1	H	501	39/39	0.97	0.11	-0.53	27,32,39,40	0
4	EDO	B	504	4/4	0.94	0.15	-0.61	59,60,61,61	0
2	UD1	G	501	39/39	0.97	0.11	-0.65	25,30,42,44	0
2	UD1	D	501	39/39	0.97	0.11	-0.69	18,28,37,37	0
2	UD1	F	501	39/39	0.98	0.11	-0.77	24,32,37,40	0
4	EDO	E	505	4/4	0.91	0.12	-0.83	51,55,55,57	0
2	UD1	C	501	39/39	0.98	0.11	-0.90	24,29,37,40	0
2	UD1	B	501	39/39	0.97	0.12	-0.93	31,38,42,44	0
4	EDO	D	508	4/4	0.72	0.19	-0.94	58,59,60,60	0
4	EDO	A	508	4/4	0.96	0.11	-1.08	53,53,54,54	0
4	EDO	E	511	4/4	0.85	0.15	-1.38	62,64,65,65	0
3	ACT	F	502	4/4	0.77	0.47	-	69,69,70,70	0
3	ACT	H	502	4/4	0.89	0.32	-	55,57,58,58	0
3	ACT	A	503	4/4	0.81	0.35	-	67,68,68,69	0
3	ACT	E	503	4/4	0.90	0.32	-	74,75,75,75	0
4	EDO	H	513	4/4	0.91	0.32	-	56,56,56,57	0
4	EDO	H	509	4/4	0.89	0.18	-	58,58,59,61	0
3	ACT	D	503	4/4	0.90	0.23	-	68,68,69,69	0
3	ACT	E	504	4/4	0.71	0.41	-	81,81,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	E	510	4/4	0.78	0.45	-	59,62,63,63	0
4	EDO	H	510	4/4	0.83	0.27	-	56,58,59,60	0
3	ACT	F	504	4/4	0.87	0.29	-	68,70,70,70	0
4	EDO	E	508	4/4	0.78	0.22	-	54,54,55,55	0
4	EDO	G	505	4/4	0.79	0.30	-	62,63,64,64	0
3	ACT	C	502	4/4	0.78	0.35	-	74,75,75,76	0
4	EDO	C	507	4/4	0.93	0.32	-	54,54,54,54	0
4	EDO	G	503	4/4	0.91	0.15	-	51,51,51,53	0
4	EDO	F	508	4/4	0.85	0.24	-	59,62,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.