Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:24 am BST

PDB ID	:	2J58
Title	:	The structure of Wza
Authors	:	Dong, C.; Naismith, J.H.
Deposited on	:	2006-09-12
Resolution	:	2.25 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
https://www.wwpdb.org/validation/2017/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:

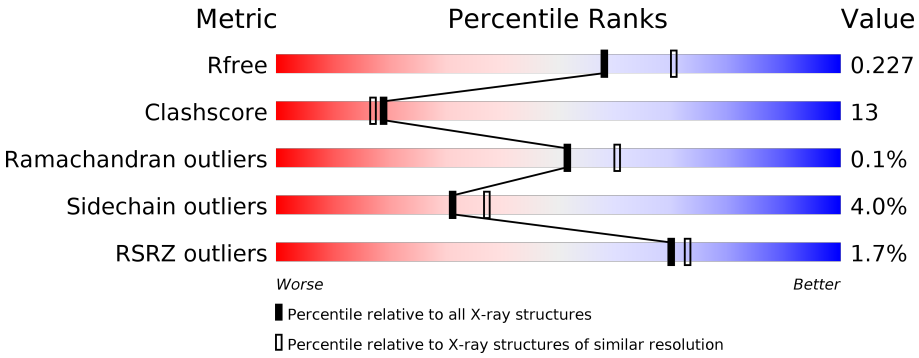
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 respectively. 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 <=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	359	4% 81% 17%
1	B	359	2% 81% 17%
1	C	359	84% 13%
1	D	359	3% 82% 15%
1	E	359	84% 13%
1	F	359	84% 15%

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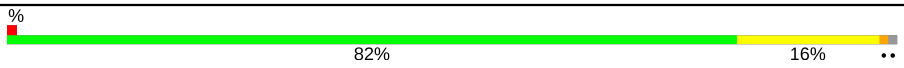
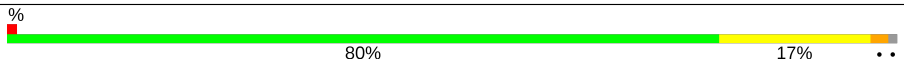
Mol	Chain	Length	Quality of chain
1	G	359	
1	H	359	

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
1	SC2	D	21	-	-	X	-
1	SC2	E	21	-	-	X	-
4	SO4	H	605	-	-	-	X

2 Entry composition (i)

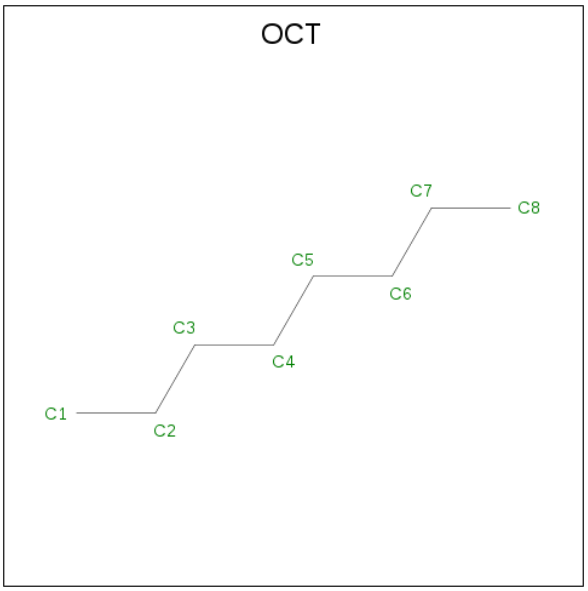
There are 5 unique types of molecules in this entry. The entry contains 23866 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OUTER MEMBRANE LIPOPROTEIN WZA.

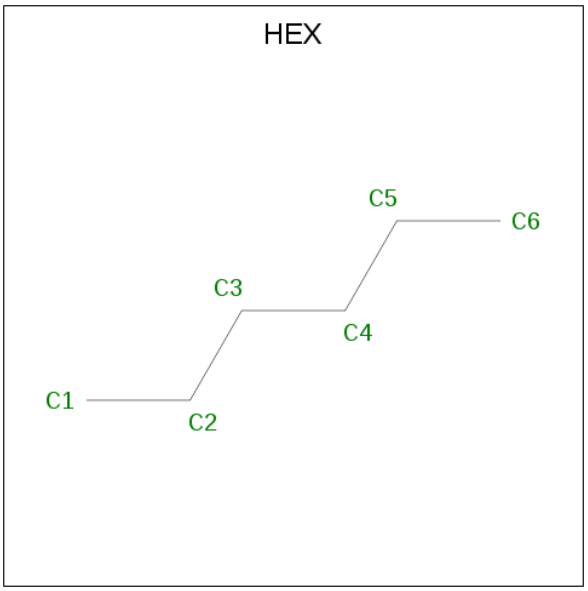
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	B	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	C	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	D	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	E	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	F	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	G	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	H	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			

- Molecule 2 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



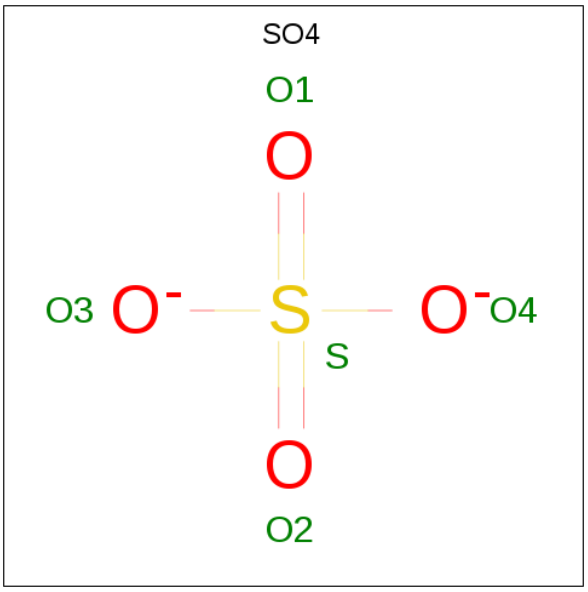
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 8 8	0	0
2	B	1	Total C 8 8	0	0
2	C	1	Total C 8 8	0	0
2	D	1	Total C 8 8	0	0
2	E	1	Total C 8 8	0	0
2	F	1	Total C 8 8	0	0
2	G	1	Total C 8 8	0	0
2	H	1	Total C 8 8	0	0

- Molecule 3 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	C	1	Total C 6 6	0	0
3	D	1	Total C 6 6	0	0
3	E	1	Total C 6 6	0	0
3	F	1	Total C 6 6	0	0
3	G	1	Total C 6 6	0	0
3	H	1	Total C 6 6	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

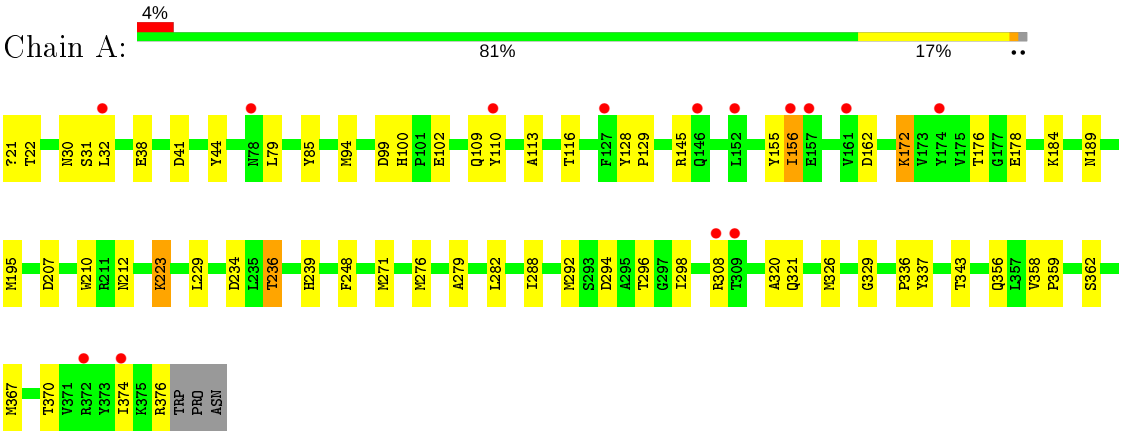
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	167	Total O 167 167	0	0
5	B	199	Total O 199 199	0	0
5	C	229	Total O 229 229	0	0
5	D	157	Total O 157 157	0	0
5	E	191	Total O 191 191	0	0
5	F	231	Total O 231 231	0	0
5	G	227	Total O 227 227	0	0
5	H	233	Total O 233 233	0	0

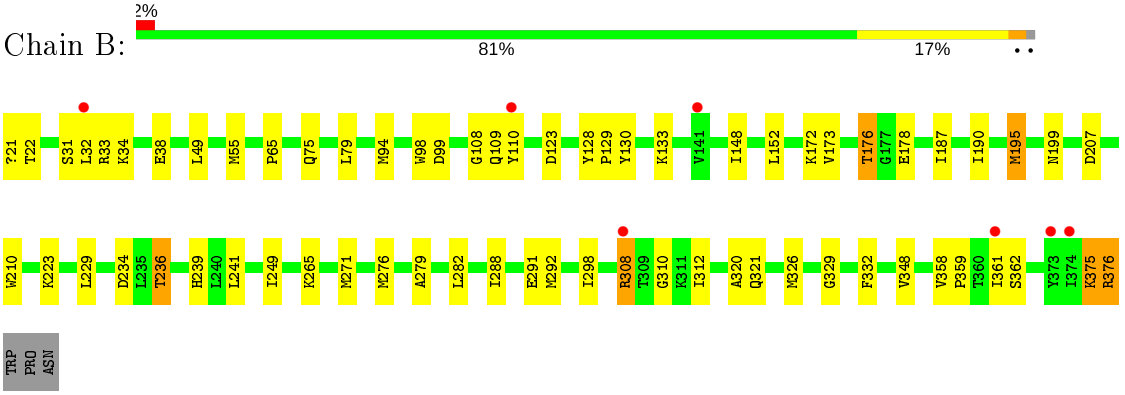
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

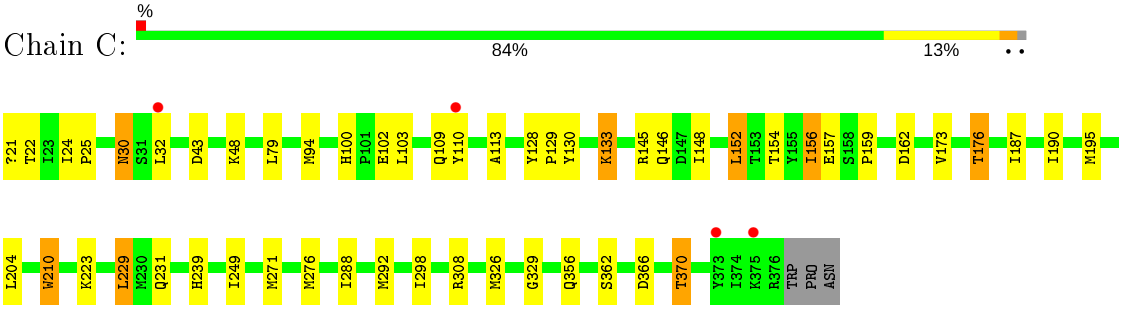
• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA



• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA

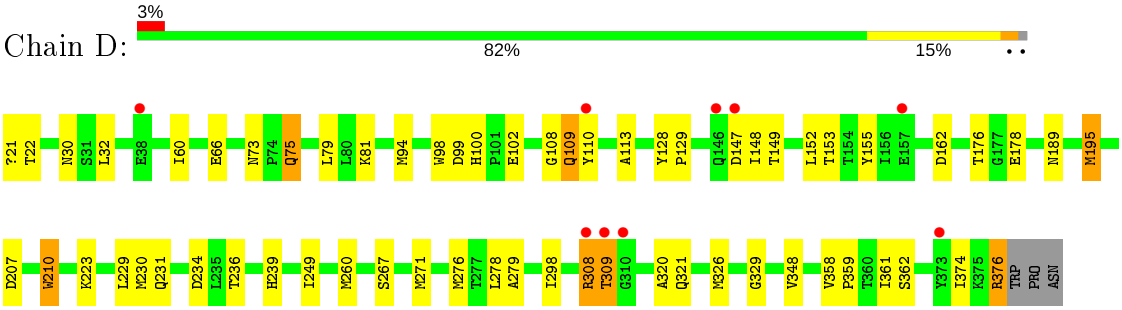


• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA



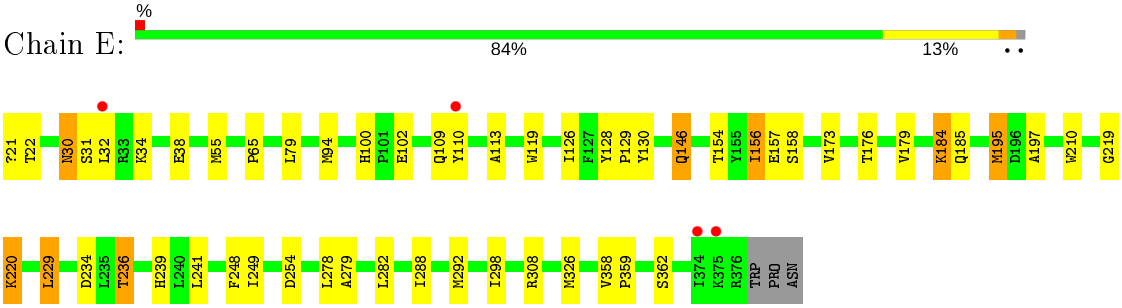
• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA

Chain D:



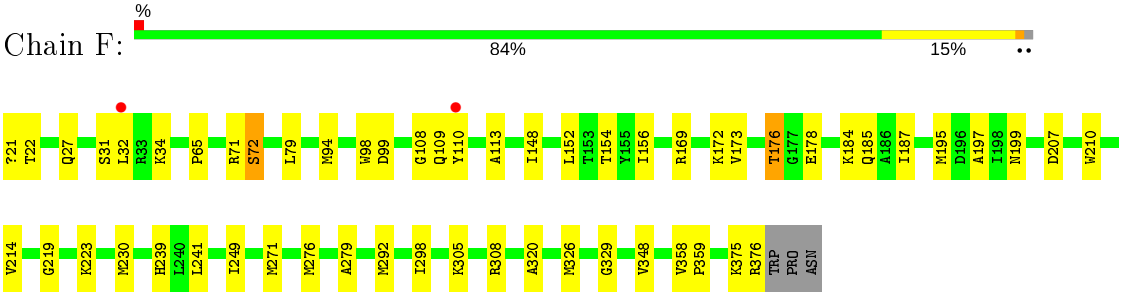
• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA

Chain E:



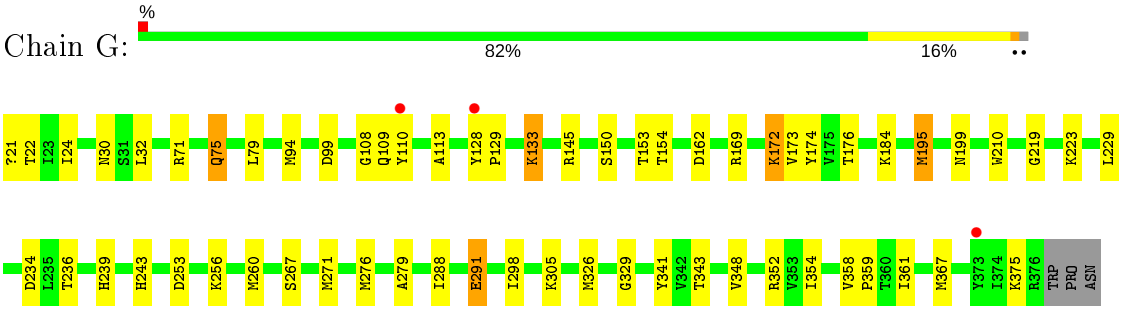
• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA

Chain F:



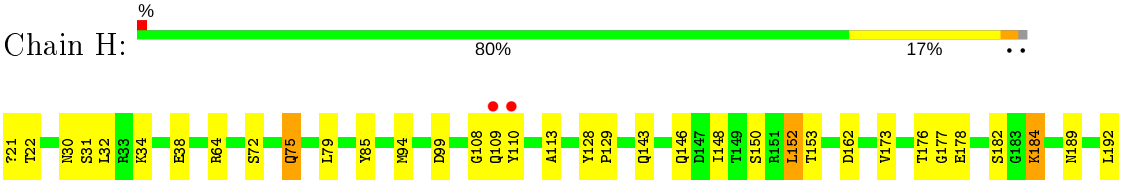
• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA

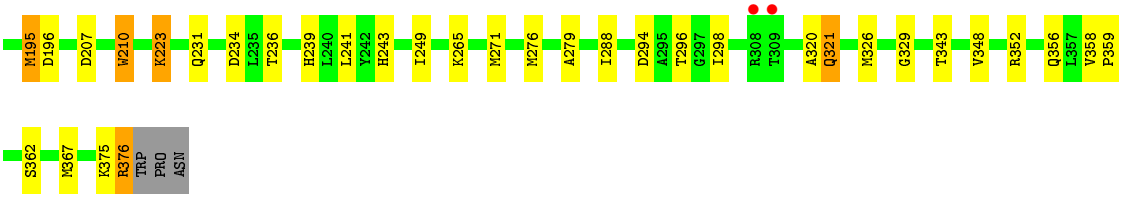
Chain G:



• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA

Chain H:




M195
D196
D207
W210
K223
Q231
D234
L235
T236
H239
L240
L241
Y242
H243
I249
K265
M271
M276
A279
I288
D294
A295
T296
G297
I298
R308
T309
A320
Q321
M326
G329
T343
V348
R352
Q356
L357
V358
P359
S362
M367
K375
R376
TRP
PRO
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.72Å 215.27Å 220.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.83 – 2.25 107.63 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.2 (107.83-2.25) 99.1 (107.63-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.226 0.190 , 0.227	Depositor DCC
R_{free} test set	10588 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23866	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: OCT, HEX, SO4, SC2

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	0.58	4/2785 (0.1%)	0.64	0/3775
1	B	0.56	0/2785	0.65	0/3775
1	C	0.60	0/2785	0.69	0/3775
1	D	0.61	3/2785 (0.1%)	0.65	0/3775
1	E	0.54	0/2785	0.64	0/3775
1	F	0.59	0/2785	0.64	0/3775
1	G	0.58	1/2785 (0.0%)	0.65	0/3775
1	H	0.58	0/2785	0.66	0/3775
All	All	0.58	8/22280 (0.0%)	0.65	0/30200

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	155	TYR	CE2-CZ	11.73	1.53	1.38
1	D	155	TYR	CG-CD2	8.22	1.49	1.39
1	A	155	TYR	CG-CD1	8.19	1.49	1.39
1	D	155	TYR	CG-CD1	7.61	1.49	1.39
1	A	155	TYR	CE2-CZ	7.47	1.48	1.38
1	A	155	TYR	CG-CD2	5.65	1.46	1.39
1	A	155	TYR	CE1-CZ	5.54	1.45	1.38
1	G	291	GLU	CG-CD	5.44	1.60	1.51

There are no bond angle outliers.

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	2755	0	2762	87	0
1	B	2755	0	2762	86	0
1	C	2755	0	2762	76	0
1	D	2755	0	2762	87	0
1	E	2755	0	2762	94	0
1	F	2755	0	2762	93	0
1	G	2755	0	2762	92	0
1	H	2755	0	2762	94	0
2	A	8	0	18	0	0
2	B	8	0	18	1	0
2	C	8	0	18	0	0
2	D	8	0	18	0	0
2	E	8	0	18	0	0
2	F	8	0	18	0	0
2	G	8	0	18	1	0
2	H	8	0	18	0	0
3	A	6	0	14	0	0
3	B	6	0	14	0	0
3	C	6	0	14	0	0
3	D	6	0	14	0	0
3	E	6	0	14	0	0
3	F	6	0	14	0	0
3	G	6	0	14	0	0
3	H	6	0	14	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
4	G	10	0	0	0	0
4	H	10	0	0	0	0
5	A	167	0	0	12	0
5	B	199	0	0	11	0
5	C	229	0	0	13	0
5	D	157	0	0	12	0
5	E	191	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	231	0	0	20	0
5	G	227	0	0	16	0
5	H	233	0	0	21	0
All	All	23866	0	22352	577	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 13.

All (577) 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:C:326:MSE:CE	1:C:329:GLY:HA3	1.28	1.60
1:A:110:TYR:CZ	1:D:110:TYR:CE1	1.95	1.53
1:E:110:TYR:CZ	1:F:110:TYR:CE1	1.93	1.52
1:B:110:TYR:CE1	1:G:110:TYR:CZ	1.97	1.51
1:B:326:MSE:CE	1:B:329:GLY:HA3	1.41	1.50
1:A:326:MSE:CE	1:A:329:GLY:HA3	1.41	1.46
1:F:21:SC2:HA	1:F:22:THR:N	1.15	1.46
1:C:110:TYR:CE1	1:F:110:TYR:CZ	2.04	1.43
1:G:110:TYR:CE1	1:H:110:TYR:CZ	2.14	1.33
1:D:110:TYR:CZ	1:E:110:TYR:CE1	2.17	1.32
1:C:110:TYR:CZ	1:H:110:TYR:CE1	2.20	1.28
1:A:110:TYR:CE1	1:B:110:TYR:CZ	2.25	1.23
1:E:110:TYR:CE1	1:F:110:TYR:HE1	1.58	1.20
1:A:110:TYR:CE1	1:D:110:TYR:HE1	1.57	1.20
1:C:326:MSE:CE	1:C:329:GLY:CA	2.20	1.18
1:H:326:MSE:CE	1:H:329:GLY:HA3	1.73	1.18
1:C:110:TYR:CE1	1:F:110:TYR:CE2	2.32	1.17
1:A:110:TYR:CE1	1:D:110:TYR:CE1	2.29	1.17
1:E:279:ALA:HA	1:E:326:MSE:HE3	1.27	1.17
1:F:176:THR:HB	5:F:2113:HOH:O	1.44	1.17
1:F:21:SC2:CA	1:F:22:THR:N	2.07	1.15
1:F:279:ALA:CB	1:F:326:MSE:HE2	1.78	1.13
1:B:110:TYR:HE1	1:G:110:TYR:CE1	1.67	1.13
1:G:279:ALA:CB	1:G:326:MSE:HE2	1.77	1.13
1:E:110:TYR:CE2	1:F:110:TYR:CE1	2.36	1.12
1:G:279:ALA:HB2	1:G:326:MSE:HE2	1.16	1.12
1:E:279:ALA:HA	1:E:326:MSE:CE	1.78	1.11
1:F:279:ALA:CA	1:F:326:MSE:HE2	1.80	1.10
1:B:326:MSE:HE3	1:B:329:GLY:HA3	1.31	1.10
1:E:110:TYR:CZ	1:F:110:TYR:HE1	1.50	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:MSE:HE3	1:D:329:GLY:HA3	1.29	1.09
1:B:326:MSE:HE1	1:B:329:GLY:HA3	1.24	1.08
1:C:110:TYR:HE1	1:F:110:TYR:CZ	1.56	1.08
1:B:94:MSE:HE3	5:B:2067:HOH:O	1.50	1.07
1:G:279:ALA:HB2	1:G:326:MSE:CE	1.85	1.07
1:D:110:TYR:CE1	1:E:110:TYR:HE1	1.72	1.07
1:D:195:MSE:HA	1:D:195:MSE:HE3	1.37	1.06
1:B:326:MSE:CE	1:B:329:GLY:CA	2.34	1.06
1:F:279:ALA:HA	1:F:326:MSE:HE2	1.40	1.04
1:F:279:ALA:HB2	1:F:326:MSE:CE	1.88	1.04
1:H:223:LYS:HG3	5:H:2147:HOH:O	1.55	1.04
1:E:110:TYR:CE1	1:F:110:TYR:CE1	2.37	1.03
1:B:110:TYR:CE1	1:G:110:TYR:CE2	2.46	1.03
1:H:326:MSE:HE3	1:H:329:GLY:HA3	1.33	1.03
1:H:176:THR:HB	5:H:2113:HOH:O	1.58	1.03
1:C:326:MSE:HE1	1:C:329:GLY:HA3	1.05	1.03
1:A:326:MSE:HE3	1:A:329:GLY:CA	1.88	1.03
1:B:110:TYR:CE1	1:G:110:TYR:CE1	2.41	1.03
1:A:326:MSE:HE3	1:A:329:GLY:HA3	1.09	1.03
1:G:110:TYR:HE1	1:H:110:TYR:CE1	1.76	1.03
1:A:326:MSE:CE	1:A:329:GLY:CA	2.36	1.02
1:E:282:LEU:HD12	1:E:326:MSE:HE1	1.37	1.02
1:E:195:MSE:HE3	1:E:229:LEU:HD13	1.41	1.02
1:B:308:ARG:HG2	1:B:308:ARG:HH11	1.21	1.02
5:G:2222:HOH:O	1:H:367:MSE:HG2	1.58	1.02
1:C:326:MSE:HE2	1:C:329:GLY:HA3	1.39	1.00
1:G:110:TYR:CE1	1:H:110:TYR:CE1	2.49	1.00
1:D:21:SC2:C	1:D:22:THR:N	2.25	1.00
1:D:195:MSE:HA	1:D:195:MSE:CE	1.92	0.99
1:C:110:TYR:CE1	1:H:110:TYR:HE1	1.79	0.99
1:A:326:MSE:HE1	1:A:329:GLY:HA3	1.44	0.99
1:G:176:THR:HB	5:G:2089:HOH:O	1.61	0.99
1:C:110:TYR:CE1	1:H:110:TYR:CE1	2.51	0.98
1:E:21:SC2:C	1:E:22:THR:N	2.28	0.97
1:A:110:TYR:CE2	1:D:110:TYR:CE1	2.52	0.96
1:H:279:ALA:HB2	1:H:326:MSE:HE2	1.45	0.96
1:B:195:MSE:HA	1:B:195:MSE:HE2	1.44	0.96
1:D:110:TYR:CE1	1:E:110:TYR:CE1	2.48	0.96
1:B:21:SC2:C	1:B:22:THR:N	2.29	0.95
1:E:279:ALA:CA	1:E:326:MSE:HE3	1.97	0.95
5:D:2009:HOH:O	1:F:326:MSE:SE	2.34	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:SER:O	1:G:153:THR:HG22	1.66	0.94
1:B:110:TYR:HE1	1:G:110:TYR:CZ	1.60	0.93
1:A:110:TYR:CZ	1:D:110:TYR:CZ	2.57	0.92
1:E:282:LEU:HD12	1:E:326:MSE:CE	1.99	0.92
1:A:110:TYR:HE1	1:B:110:TYR:CZ	1.85	0.92
1:B:234:ASP:OD1	1:B:236:THR:HB	1.69	0.92
1:D:110:TYR:CE2	1:E:110:TYR:CE1	2.58	0.91
1:H:21:SC2:SG	5:H:2001:HOH:O	2.28	0.91
1:H:38:GLU:HG2	5:H:2013:HOH:O	1.70	0.91
1:E:195:MSE:HE2	1:E:195:MSE:HA	1.50	0.91
1:F:279:ALA:HB2	1:F:326:MSE:HE2	1.44	0.91
1:C:110:TYR:CZ	1:H:110:TYR:HE1	1.86	0.91
1:C:110:TYR:HE1	1:F:110:TYR:CE1	1.89	0.90
1:H:326:MSE:HE1	1:H:329:GLY:HA3	1.50	0.90
1:H:195:MSE:HA	1:H:195:MSE:HE3	1.54	0.90
1:F:279:ALA:CA	1:F:326:MSE:CE	2.49	0.90
5:E:2065:HOH:O	1:F:94:MSE:HE1	1.72	0.90
1:A:110:TYR:OH	1:D:110:TYR:OH	1.89	0.90
1:D:279:ALA:HB2	1:D:326:MSE:HE2	1.50	0.90
1:G:21:SC2:C	1:G:22:THR:N	2.35	0.89
1:H:21:SC2:C	1:H:22:THR:N	2.36	0.89
1:D:326:MSE:CE	1:D:329:GLY:HA3	2.01	0.88
1:B:110:TYR:CZ	1:G:110:TYR:CZ	2.61	0.88
1:C:110:TYR:CE2	1:H:110:TYR:CE1	2.61	0.88
1:E:110:TYR:CZ	1:F:110:TYR:CZ	2.60	0.88
1:H:195:MSE:HA	1:H:195:MSE:CE	2.04	0.88
1:A:234:ASP:OD1	1:A:236:THR:HB	1.73	0.87
1:A:195:MSE:HE3	1:A:229:LEU:HD13	1.56	0.87
1:B:326:MSE:HE3	1:B:329:GLY:CA	2.02	0.87
1:D:279:ALA:CB	1:D:326:MSE:HE2	2.03	0.87
1:A:110:TYR:OH	1:D:110:TYR:CZ	2.27	0.86
1:B:292:MSE:HE1	5:B:2195:HOH:O	1.74	0.86
1:G:195:MSE:CE	1:G:195:MSE:HA	2.04	0.86
1:B:110:TYR:OH	1:G:110:TYR:OH	1.91	0.86
1:C:326:MSE:HE3	1:C:329:GLY:HA3	1.52	0.86
1:G:94:MSE:HG3	5:H:2081:HOH:O	1.74	0.86
1:C:195:MSE:HA	1:C:195:MSE:HE2	1.58	0.86
1:E:110:TYR:OH	1:F:110:TYR:OH	1.92	0.86
1:G:110:TYR:CE1	1:H:110:TYR:CE2	2.63	0.86
1:H:326:MSE:HE3	1:H:329:GLY:CA	2.05	0.86
1:C:176:THR:HB	5:C:2092:HOH:O	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:GLN:HG3	5:H:2075:HOH:O	1.77	0.85
1:A:110:TYR:CE1	1:B:110:TYR:CE2	2.64	0.85
1:C:326:MSE:HE1	1:C:329:GLY:CA	1.97	0.84
1:C:110:TYR:CD1	1:F:110:TYR:CE2	2.64	0.84
1:A:223:LYS:HG2	5:A:2097:HOH:O	1.76	0.84
1:G:223:LYS:HG2	5:G:2128:HOH:O	1.76	0.84
1:D:110:TYR:CZ	1:E:110:TYR:HE1	1.80	0.84
1:F:109:GLN:HB3	5:F:2079:HOH:O	1.76	0.83
1:D:21:SC2:HBC2	1:D:22:THR:N	1.94	0.83
1:E:184:LYS:H	1:E:184:LYS:NZ	1.76	0.83
1:C:21:SC2:O	1:C:22:THR:N	2.11	0.83
1:A:176:THR:HG22	1:A:248:PHE:HD1	1.41	0.82
1:B:110:TYR:CZ	1:G:110:TYR:OH	2.31	0.82
1:G:326:MSE:CE	1:G:329:GLY:HA3	2.10	0.82
1:D:326:MSE:HE3	1:D:329:GLY:CA	2.10	0.82
1:E:176:THR:HG21	1:F:230:MSE:SE	2.30	0.81
1:H:223:LYS:HD2	5:H:2146:HOH:O	1.79	0.81
1:E:176:THR:HG23	5:E:2086:HOH:O	1.80	0.81
1:A:110:TYR:HE1	1:B:110:TYR:CE1	1.98	0.81
1:G:305:LYS:HD3	5:G:2183:HOH:O	1.80	0.81
1:D:239:HIS:HE1	5:D:2091:HOH:O	1.63	0.81
1:A:195:MSE:CE	1:A:229:LEU:HD13	2.11	0.81
1:D:279:ALA:CA	1:D:326:MSE:HE2	2.10	0.81
1:B:110:TYR:CE1	1:G:110:TYR:OH	2.34	0.80
1:C:21:SC2:C	1:C:22:THR:N	2.45	0.79
1:F:279:ALA:HA	1:F:326:MSE:CE	2.09	0.79
1:A:110:TYR:CE1	1:B:110:TYR:CE1	2.69	0.79
1:A:110:TYR:OH	1:D:110:TYR:CE1	2.35	0.79
1:D:308:ARG:HB2	1:D:308:ARG:HH11	1.47	0.79
1:E:236:THR:HG21	5:E:2037:HOH:O	1.83	0.79
1:D:110:TYR:CZ	1:E:110:TYR:CZ	2.70	0.79
1:C:110:TYR:CZ	1:H:110:TYR:CZ	2.70	0.79
1:E:184:LYS:HG2	5:F:2129:HOH:O	1.82	0.78
1:H:94:MSE:HE3	5:H:2104:HOH:O	1.83	0.78
1:G:195:MSE:HA	1:G:195:MSE:HE3	1.65	0.78
1:E:110:TYR:CE2	1:F:110:TYR:CD1	2.72	0.78
1:B:195:MSE:HA	1:B:195:MSE:CE	2.14	0.78
1:E:195:MSE:HE3	1:E:229:LEU:CD1	2.13	0.78
1:C:110:TYR:CE1	1:F:110:TYR:CE1	2.66	0.77
1:E:110:TYR:OH	1:F:110:TYR:CZ	2.36	0.77
1:D:376:ARG:HG2	5:D:2154:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:LYS:HD3	1:F:199:ASN:CB	2.14	0.77
1:G:110:TYR:CZ	1:H:110:TYR:CZ	2.73	0.77
1:B:195:MSE:HE3	1:B:229:LEU:HD13	1.67	0.76
1:A:21:SC2:O	1:A:22:THR:N	2.18	0.76
1:A:195:MSE:HE3	1:A:229:LEU:CD1	2.16	0.76
1:G:110:TYR:HE1	1:H:110:TYR:CZ	1.80	0.76
1:H:21:SC2:O	1:H:22:THR:N	2.17	0.76
1:F:279:ALA:HB2	1:F:326:MSE:HE3	1.64	0.76
1:E:110:TYR:OH	1:F:110:TYR:CE1	2.39	0.75
5:C:2060:HOH:O	1:H:94:MSE:HE1	1.86	0.75
1:C:110:TYR:CE1	1:F:110:TYR:OH	2.39	0.75
1:A:94:MSE:HE3	5:A:2061:HOH:O	1.87	0.75
1:E:279:ALA:HA	1:E:326:MSE:HE1	1.69	0.75
1:E:234:ASP:OD1	1:E:236:THR:HB	1.87	0.74
1:G:326:MSE:HE3	1:G:329:GLY:HA3	1.69	0.74
1:G:279:ALA:CA	1:G:326:MSE:HE2	2.17	0.73
1:F:154:THR:CG2	5:F:2097:HOH:O	2.36	0.73
1:B:279:ALA:HB2	1:B:326:MSE:HE2	1.70	0.73
1:G:109:GLN:HG2	1:H:108:GLY:HA3	1.71	0.72
1:A:195:MSE:HA	1:A:195:MSE:HE2	1.71	0.72
1:D:260:MSE:HE1	1:E:326:MSE:HE2	1.70	0.72
1:D:110:TYR:OH	1:E:110:TYR:OH	2.02	0.72
1:E:176:THR:HG22	1:E:248:PHE:HD1	1.55	0.72
1:B:110:TYR:CD1	1:G:110:TYR:CE2	2.78	0.71
1:G:223:LYS:CG	5:G:2128:HOH:O	2.36	0.71
5:G:2112:HOH:O	1:H:176:THR:HG23	1.91	0.71
1:C:110:TYR:CD1	1:F:110:TYR:CD2	2.79	0.70
1:E:195:MSE:CE	1:E:229:LEU:HD13	2.19	0.70
1:A:21:SC2:C	1:A:22:THR:N	2.55	0.70
1:C:94:MSE:HE2	1:C:113:ALA:HB3	1.74	0.70
1:D:21:SC2:CB	1:D:22:THR:N	2.55	0.69
1:B:176:THR:HB	5:B:2075:HOH:O	1.91	0.69
1:E:279:ALA:CB	1:E:326:MSE:HE3	2.21	0.69
1:C:239:HIS:HE1	5:C:2129:HOH:O	1.75	0.69
1:E:21:SC2:CA	1:E:22:THR:N	2.55	0.69
1:E:110:TYR:CD2	1:F:110:TYR:CD1	2.79	0.69
1:D:279:ALA:HA	1:D:326:MSE:HE2	1.74	0.69
1:G:358:VAL:CG2	1:G:359:PRO:HD3	2.23	0.69
1:C:110:TYR:CZ	1:F:110:TYR:CZ	2.78	0.69
1:A:110:TYR:CZ	1:D:110:TYR:HE1	1.63	0.68
1:G:199:ASN:HB3	1:H:184:LYS:HD3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:600:OCT:H11	5:G:2067:HOH:O	1.93	0.68
1:H:75:GLN:HB2	5:H:2049:HOH:O	1.93	0.68
1:F:292:MSE:HE1	5:F:2223:HOH:O	1.94	0.68
1:A:212:ASN:HA	1:A:223:LYS:HD2	1.75	0.68
1:G:110:TYR:CZ	1:H:110:TYR:OH	2.46	0.68
1:D:108:GLY:HA3	1:E:109:GLN:HG2	1.76	0.68
5:G:2112:HOH:O	1:H:182:SER:HB3	1.93	0.68
1:E:184:LYS:HD3	1:F:199:ASN:HB3	1.74	0.67
1:E:94:MSE:HE2	1:E:113:ALA:CB	2.24	0.67
1:H:30:ASN:ND2	1:H:32:LEU:HB2	2.09	0.67
1:E:184:LYS:HD3	1:F:199:ASN:HB2	1.75	0.67
1:H:279:ALA:CB	1:H:326:MSE:HE2	2.21	0.67
1:C:190:ILE:HD13	1:F:169:ARG:HB3	1.77	0.67
1:F:239:HIS:HE1	5:F:2154:HOH:O	1.78	0.67
1:H:326:MSE:CE	1:H:329:GLY:CA	2.60	0.67
1:D:234:ASP:OD1	1:D:236:THR:HB	1.95	0.66
1:A:110:TYR:CE2	1:D:110:TYR:CD1	2.83	0.66
1:A:100:HIS:CE1	1:A:156:ILE:HD13	2.31	0.66
1:E:288:ILE:HD11	1:E:298:ILE:HD13	1.78	0.66
1:C:190:ILE:CD1	1:F:169:ARG:HB3	2.27	0.65
1:C:366:ASP:O	1:C:370:THR:HG23	1.96	0.65
1:C:223:LYS:HG2	5:C:2122:HOH:O	1.96	0.65
1:D:308:ARG:C	5:D:2132:HOH:O	2.34	0.65
1:G:288:ILE:HD11	1:G:298:ILE:HD13	1.78	0.65
1:A:176:THR:HG22	1:A:248:PHE:CD1	2.30	0.64
1:D:309:THR:HB	5:D:2133:HOH:O	1.97	0.64
1:D:279:ALA:HB2	1:D:326:MSE:CE	2.24	0.64
1:D:309:THR:N	5:D:2132:HOH:O	2.31	0.64
1:F:279:ALA:CB	1:F:326:MSE:CE	2.51	0.63
1:G:94:MSE:HE2	1:G:113:ALA:CB	2.28	0.63
1:C:94:MSE:HE2	1:C:113:ALA:CB	2.28	0.63
1:C:133:LYS:HD2	5:C:2065:HOH:O	1.97	0.63
1:G:110:TYR:OH	1:H:110:TYR:OH	2.07	0.63
1:A:376:ARG:HG3	5:A:2166:HOH:O	1.99	0.63
1:C:145:ARG:HD2	5:C:2073:HOH:O	1.99	0.62
1:G:172:LYS:HD3	1:G:184:LYS:HD2	1.80	0.62
1:A:367:MSE:SE	1:D:361:ILE:HD12	2.50	0.62
1:C:110:TYR:CZ	1:F:110:TYR:OH	2.49	0.62
1:G:110:TYR:CE1	1:H:110:TYR:OH	2.52	0.62
1:G:75:GLN:HG2	5:G:2042:HOH:O	1.99	0.62
1:D:358:VAL:CG2	1:D:359:PRO:HD3	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:MSE:CE	5:B:2067:HOH:O	2.26	0.62
1:C:100:HIS:HD2	1:C:102:GLU:OE2	1.83	0.62
1:C:176:THR:CB	5:C:2092:HOH:O	2.43	0.61
1:H:150:SER:O	1:H:153:THR:HB	2.00	0.61
1:G:234:ASP:OD1	1:G:236:THR:HB	1.99	0.61
1:A:110:TYR:CZ	1:D:110:TYR:CD1	2.80	0.61
1:B:308:ARG:HG2	1:B:308:ARG:NH1	2.00	0.61
1:E:100:HIS:CE1	1:E:156:ILE:HD13	2.35	0.61
1:E:184:LYS:H	1:E:184:LYS:HZ3	1.49	0.61
1:C:110:TYR:OH	1:H:110:TYR:OH	2.04	0.61
1:A:184:LYS:HD2	5:A:2071:HOH:O	2.01	0.61
1:C:109:GLN:HG2	1:F:108:GLY:HA3	1.82	0.61
1:C:326:MSE:HE2	1:C:329:GLY:CA	2.11	0.61
1:D:94:MSE:HE3	5:D:2052:HOH:O	2.01	0.60
1:A:176:THR:HG21	1:D:230:MSE:SE	2.51	0.60
1:B:292:MSE:HE2	1:B:348:VAL:CG1	2.31	0.60
1:A:279:ALA:HB2	1:A:326:MSE:HE2	1.84	0.60
1:C:94:MSE:HE3	5:C:2081:HOH:O	2.02	0.60
1:D:110:TYR:OH	1:E:110:TYR:CZ	2.52	0.60
1:C:195:MSE:HE3	1:C:229:LEU:HD13	1.84	0.60
1:C:30:ASN:C	1:C:30:ASN:OD1	2.39	0.60
1:C:43:ASP:HB2	5:C:2013:HOH:O	2.01	0.59
5:C:2136:HOH:O	1:F:219:GLY:HA2	2.02	0.59
1:G:326:MSE:HE3	1:G:329:GLY:CA	2.32	0.59
1:H:239:HIS:HE1	5:H:2153:HOH:O	1.84	0.59
1:B:308:ARG:HH11	1:B:308:ARG:CG	2.04	0.59
1:E:195:MSE:CE	1:E:195:MSE:HA	2.26	0.59
1:G:94:MSE:HE3	5:G:2080:HOH:O	2.01	0.59
1:A:362:SER:HB3	5:A:2163:HOH:O	2.01	0.59
1:E:65:PRO:HD3	5:E:2035:HOH:O	2.01	0.59
1:C:195:MSE:CE	1:C:195:MSE:HA	2.32	0.59
1:A:110:TYR:CE1	1:D:110:TYR:CD1	2.90	0.59
1:G:358:VAL:HG23	1:G:359:PRO:HD3	1.84	0.58
5:B:2121:HOH:O	1:G:219:GLY:HA2	2.04	0.58
1:C:110:TYR:OH	1:H:110:TYR:CZ	2.54	0.58
1:H:128:TYR:CG	1:H:129:PRO:HD2	2.38	0.58
1:A:239:HIS:HE1	5:A:2101:HOH:O	1.86	0.58
1:E:94:MSE:HE3	5:E:2077:HOH:O	2.02	0.58
1:G:199:ASN:CB	1:H:184:LYS:HD3	2.34	0.57
1:F:65:PRO:HD3	5:F:2035:HOH:O	2.04	0.57
1:A:110:TYR:CZ	1:B:110:TYR:CZ	2.89	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:ALA:CA	1:G:326:MSE:CE	2.82	0.57
1:F:326:MSE:HE3	1:F:329:GLY:HA3	1.86	0.57
1:B:292:MSE:HE2	1:B:348:VAL:HG13	1.86	0.57
1:C:326:MSE:HE3	1:C:329:GLY:CA	2.18	0.57
1:E:185:GLN:HE22	1:E:197:ALA:HA	1.69	0.57
1:E:358:VAL:CG2	1:E:359:PRO:HD3	2.35	0.57
1:B:110:TYR:CD1	1:G:110:TYR:CD2	2.93	0.57
1:F:21:SC2:C	1:F:22:THR:N	2.68	0.57
1:B:75:GLN:HB2	5:B:2027:HOH:O	2.05	0.57
1:E:358:VAL:HG23	1:E:359:PRO:HD3	1.87	0.57
1:E:176:THR:CG2	1:F:230:MSE:SE	3.03	0.57
1:H:234:ASP:OD1	1:H:236:THR:HB	2.05	0.57
1:B:176:THR:CB	5:B:2075:HOH:O	2.49	0.57
1:E:184:LYS:H	1:E:184:LYS:HZ2	1.53	0.57
1:F:94:MSE:HE3	5:F:2103:HOH:O	2.04	0.57
1:D:223:LYS:HD2	5:D:2082:HOH:O	2.04	0.56
1:D:66:GLU:OE1	1:D:66:GLU:HA	2.04	0.56
1:D:75:GLN:H	1:D:75:GLN:CD	2.08	0.56
1:G:239:HIS:HE1	5:G:2137:HOH:O	1.88	0.56
1:A:110:TYR:CE1	1:B:110:TYR:OH	2.58	0.56
1:F:223:LYS:HD2	5:F:2142:HOH:O	2.05	0.56
1:B:361:ILE:HG23	1:G:367:MSE:HG3	1.87	0.56
1:G:326:MSE:HE1	1:G:329:GLY:HA3	1.87	0.56
1:G:110:TYR:CD1	1:H:110:TYR:CE2	2.93	0.56
1:A:110:TYR:CD1	1:B:110:TYR:CE2	2.94	0.56
1:D:21:SC2:CA	1:D:22:THR:N	2.69	0.55
1:H:64:ARG:NE	5:H:2042:HOH:O	2.25	0.55
1:G:243:HIS:HB2	5:G:2087:HOH:O	2.07	0.55
1:E:21:SC2:HA	1:E:22:THR:N	2.22	0.55
1:A:110:TYR:CD2	1:D:110:TYR:CD1	2.95	0.55
1:E:239:HIS:HD2	5:E:2061:HOH:O	1.89	0.55
1:G:21:SC2:C	1:G:21:SC2:OT	2.54	0.55
1:G:348:VAL:O	1:G:352:ARG:HG3	2.07	0.55
1:D:149:THR:O	1:D:153:THR:HG23	2.06	0.55
1:C:110:TYR:CZ	1:F:110:TYR:CE2	2.93	0.55
1:H:30:ASN:HB2	5:H:2009:HOH:O	2.06	0.55
1:A:30:ASN:OD1	1:A:32:LEU:HB2	2.07	0.54
1:C:110:TYR:OH	1:F:110:TYR:OH	2.11	0.54
1:G:341:TYR:HE2	1:G:343:THR:HG22	1.72	0.54
1:H:358:VAL:CG2	1:H:359:PRO:HD3	2.37	0.54
1:H:375:LYS:O	1:H:376:ARG:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:SC2:OT	1:C:21:SC2:C	2.56	0.53
1:E:94:MSE:CE	5:E:2077:HOH:O	2.56	0.53
1:C:326:MSE:HE3	1:C:329:GLY:N	2.23	0.53
1:D:308:ARG:CB	1:D:308:ARG:HH11	2.18	0.53
1:H:271:MSE:HA	1:H:276:MSE:HE3	1.89	0.53
1:H:294:ASP:HB3	1:H:343:THR:OG1	2.08	0.53
1:H:210:TRP:HH2	1:H:231:GLN:HE21	1.55	0.53
1:B:358:VAL:CG2	1:B:359:PRO:HD3	2.39	0.53
1:D:358:VAL:HG23	1:D:359:PRO:HD3	1.89	0.53
1:B:31:SER:HA	1:B:34:LYS:HD2	1.90	0.53
1:H:298:ILE:HD12	1:H:320:ALA:HB3	1.90	0.53
1:A:321:GLN:NE2	5:A:2141:HOH:O	2.41	0.53
1:B:195:MSE:HE3	1:B:229:LEU:CD1	2.37	0.53
1:B:110:TYR:CD1	1:G:110:TYR:CZ	2.83	0.53
1:E:100:HIS:HE1	1:E:156:ILE:HD13	1.74	0.53
1:B:110:TYR:CZ	1:G:110:TYR:CE2	2.96	0.52
1:B:326:MSE:HE1	1:B:329:GLY:CA	2.18	0.52
1:D:110:TYR:CE2	1:E:110:TYR:CD1	2.96	0.52
1:F:94:MSE:HE2	1:F:113:ALA:CB	2.38	0.52
1:F:279:ALA:N	1:F:326:MSE:CE	2.72	0.52
1:E:110:TYR:CE2	1:F:110:TYR:CZ	2.92	0.52
1:B:308:ARG:NH1	1:B:308:ARG:CG	2.70	0.52
1:B:148:ILE:O	1:B:152:LEU:HB2	2.10	0.52
1:E:130:TYR:OH	1:F:99:ASP:OD2	2.28	0.52
1:F:326:MSE:CE	1:F:329:GLY:HA3	2.40	0.52
1:A:94:MSE:CE	5:A:2061:HOH:O	2.52	0.52
1:C:326:MSE:HE3	1:C:329:GLY:H	1.74	0.52
1:F:358:VAL:CG2	1:F:359:PRO:HD3	2.40	0.52
1:D:73:ASN:OD1	1:D:75:GLN:HG2	2.10	0.52
1:E:184:LYS:CD	5:F:2129:HOH:O	2.58	0.52
1:A:292:MSE:HE1	5:A:2159:HOH:O	2.10	0.52
1:B:326:MSE:HE3	1:B:329:GLY:N	2.24	0.52
1:F:358:VAL:HG23	1:F:359:PRO:HD3	1.92	0.51
1:F:375:LYS:O	1:F:376:ARG:HB2	2.09	0.51
1:A:94:MSE:HE2	1:A:113:ALA:CB	2.40	0.51
1:C:356:GLN:HE21	1:H:348:VAL:HA	1.74	0.51
1:B:199:ASN:OD1	1:G:176:THR:HG22	2.10	0.51
1:A:358:VAL:HG23	1:A:359:PRO:HD3	1.93	0.51
1:C:292:MSE:HE2	5:F:2226:HOH:O	2.10	0.51
1:C:288:ILE:HD11	1:C:298:ILE:HD13	1.93	0.51
1:D:110:TYR:CD2	1:E:110:TYR:CD1	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:ALA:N	1:F:326:MSE:HE1	2.25	0.51
1:F:94:MSE:CE	5:F:2103:HOH:O	2.58	0.51
1:C:156:ILE:HG13	1:C:159:PRO:HB3	1.93	0.51
1:D:271:MSE:HA	1:D:276:MSE:HE3	1.93	0.51
1:E:184:LYS:HD2	5:F:2129:HOH:O	2.09	0.51
1:B:178:GLU:OE1	1:B:207:ASP:OD1	2.29	0.51
1:G:279:ALA:HA	1:G:326:MSE:HE2	1.93	0.51
1:B:128:TYR:CG	1:B:129:PRO:HD2	2.47	0.50
1:B:298:ILE:HD12	1:B:320:ALA:HB3	1.92	0.50
1:B:32:LEU:O	1:B:33:ARG:HB2	2.10	0.50
1:C:249:ILE:HD12	1:C:249:ILE:N	2.25	0.50
1:E:94:MSE:HE2	1:E:113:ALA:HB1	1.91	0.50
1:A:358:VAL:CG2	1:A:359:PRO:HD3	2.41	0.50
1:A:109:GLN:HG3	1:B:108:GLY:HA3	1.93	0.50
1:C:152:LEU:HG	1:C:156:ILE:HD11	1.94	0.50
1:G:358:VAL:HG22	1:G:359:PRO:HD3	1.93	0.50
1:C:130:TYR:OH	1:H:99:ASP:OD2	2.27	0.50
1:C:110:TYR:CE2	1:H:110:TYR:CD1	2.99	0.50
1:B:190:ILE:HD11	1:G:169:ARG:HD3	1.94	0.50
5:D:2153:HOH:O	1:E:292:MSE:HE3	2.11	0.50
1:E:110:TYR:CG	1:F:110:TYR:CD1	3.00	0.49
1:F:195:MSE:HE1	1:F:230:MSE:HG2	1.92	0.49
1:A:326:MSE:HE3	1:A:329:GLY:N	2.27	0.49
1:B:109:GLN:HG2	1:G:108:GLY:HA3	1.94	0.49
1:F:176:THR:CB	5:F:2113:HOH:O	2.23	0.49
1:E:239:HIS:HE1	5:E:2114:HOH:O	1.96	0.49
1:H:239:HIS:HD2	5:H:2071:HOH:O	1.96	0.49
1:B:249:ILE:N	1:B:249:ILE:HD12	2.27	0.48
1:A:31:SER:O	1:A:32:LEU:C	2.51	0.48
1:B:321:GLN:HG3	5:G:2218:HOH:O	2.13	0.48
1:B:271:MSE:HA	1:B:276:MSE:HE3	1.95	0.48
1:G:288:ILE:HD11	1:G:298:ILE:CD1	2.41	0.48
1:C:110:TYR:CE2	1:H:110:TYR:CZ	2.99	0.48
1:H:148:ILE:O	1:H:152:LEU:HB2	2.14	0.48
1:B:358:VAL:HG23	1:B:359:PRO:HD3	1.94	0.48
1:E:100:HIS:HD2	1:E:102:GLU:OE2	1.95	0.48
1:G:260:MSE:SE	5:H:2005:HOH:O	2.82	0.48
1:C:110:TYR:CD2	1:H:110:TYR:CD1	3.01	0.48
1:F:298:ILE:HD12	1:F:320:ALA:HB3	1.95	0.48
1:E:173:VAL:HG11	1:E:241:LEU:HD13	1.95	0.48
1:H:109:GLN:CG	5:H:2075:HOH:O	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:THR:O	1:A:374:ILE:HG12	2.14	0.48
1:D:308:ARG:NH1	1:D:308:ARG:HB2	2.23	0.48
1:E:288:ILE:HD11	1:E:298:ILE:CD1	2.41	0.48
1:F:72:SER:N	5:F:2042:HOH:O	2.46	0.48
1:A:109:GLN:HG2	5:A:2043:HOH:O	2.14	0.47
1:E:30:ASN:OD1	1:E:32:LEU:HB2	2.14	0.47
1:A:356:GLN:HE21	1:D:348:VAL:HA	1.80	0.47
1:D:189:ASN:HB3	5:D:2019:HOH:O	2.15	0.47
1:E:146:GLN:HA	1:E:146:GLN:HE21	1.78	0.47
1:F:214:VAL:HG22	1:F:223:LYS:HE3	1.95	0.47
1:A:178:GLU:OE1	1:A:207:ASP:OD1	2.32	0.47
1:C:103:LEU:HD21	1:C:130:TYR:HE2	1.78	0.47
5:D:2153:HOH:O	1:E:292:MSE:CE	2.62	0.47
1:G:288:ILE:HD13	1:G:298:ILE:HD11	1.95	0.47
1:H:192:LEU:HD12	1:H:196:ASP:HB2	1.96	0.47
1:D:308:ARG:CB	1:D:308:ARG:NH1	2.77	0.47
1:A:110:TYR:CD1	1:D:110:TYR:CD1	3.02	0.47
1:F:185:GLN:HE22	1:F:197:ALA:HA	1.80	0.47
1:H:176:THR:CB	5:H:2113:HOH:O	2.36	0.47
1:G:291:GLU:HA	1:H:352:ARG:HD3	1.97	0.47
1:A:367:MSE:HG3	1:D:361:ILE:HG23	1.96	0.47
1:G:305:LYS:HE2	5:G:2185:HOH:O	2.14	0.47
1:B:195:MSE:CE	1:B:229:LEU:HD13	2.43	0.47
1:D:374:ILE:O	1:D:374:ILE:HG22	2.14	0.47
1:E:128:TYR:CG	1:E:129:PRO:HD2	2.50	0.47
1:A:176:THR:CG2	1:A:248:PHE:HD1	2.20	0.46
1:E:219:GLY:HA2	5:F:2157:HOH:O	2.15	0.46
1:G:94:MSE:HE2	1:G:113:ALA:HB3	1.96	0.46
1:A:128:TYR:CG	1:A:129:PRO:HD2	2.50	0.46
1:B:282:LEU:HD13	1:B:288:ILE:HD11	1.96	0.46
1:H:288:ILE:HD11	1:H:298:ILE:HD13	1.97	0.46
1:D:30:ASN:OD1	1:D:32:LEU:HB2	2.15	0.46
1:H:249:ILE:HD12	1:H:249:ILE:N	2.29	0.46
1:D:278:LEU:HG	1:D:326:MSE:HE1	1.98	0.46
1:G:195:MSE:HE2	1:G:195:MSE:HA	1.91	0.46
1:A:116:THR:HG22	5:A:2046:HOH:O	2.14	0.46
1:A:85:TYR:HB2	1:A:189:ASN:HA	1.97	0.46
1:F:292:MSE:HE2	1:F:348:VAL:HG13	1.97	0.46
1:H:162:ASP:OD2	5:H:2100:HOH:O	2.20	0.46
1:A:376:ARG:CG	5:A:2166:HOH:O	2.59	0.46
1:D:98:TRP:O	1:D:99:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:ASP:HB2	5:E:2179:HOH:O	2.16	0.46
1:A:298:ILE:HD12	1:A:320:ALA:HB3	1.98	0.45
1:F:298:ILE:CD1	1:F:320:ALA:HB3	2.46	0.45
1:B:123:ASP:OD2	1:B:133:LYS:NZ	2.40	0.45
1:D:249:ILE:HD12	1:D:249:ILE:N	2.31	0.45
1:G:361:ILE:HG23	5:G:2222:HOH:O	2.15	0.45
1:H:296:THR:HG23	1:H:321:GLN:NE2	2.32	0.45
1:D:94:MSE:HE2	1:D:113:ALA:CB	2.47	0.45
1:G:110:TYR:CD1	1:H:110:TYR:CD2	3.04	0.45
1:F:98:TRP:O	1:F:99:ASP:HB2	2.14	0.45
1:C:24:ILE:HA	1:C:25:PRO:HD3	1.80	0.45
1:D:110:TYR:CE2	1:E:110:TYR:CZ	3.03	0.45
1:E:31:SER:HA	1:E:34:LYS:HD2	1.98	0.45
1:A:100:HIS:HE1	1:A:156:ILE:HD13	1.77	0.45
1:C:210:TRP:HH2	1:C:231:GLN:HE21	1.65	0.45
1:A:145:ARG:NH1	1:A:162:ASP:OD1	2.50	0.45
1:F:154:THR:HG22	5:F:2097:HOH:O	2.10	0.45
1:G:279:ALA:CB	1:G:326:MSE:CE	2.61	0.45
1:B:173:VAL:HG23	1:B:187:ILE:HD11	1.99	0.45
1:H:31:SER:HA	1:H:34:LYS:HD2	1.98	0.45
1:C:148:ILE:O	1:C:152:LEU:HB2	2.17	0.45
1:C:94:MSE:CE	5:C:2081:HOH:O	2.62	0.45
1:E:110:TYR:CE1	1:F:110:TYR:CD1	3.03	0.44
1:F:148:ILE:O	1:F:152:LEU:HB2	2.17	0.44
2:B:600:OCT:H71	1:G:24:ILE:HD11	1.99	0.44
1:A:110:TYR:CZ	1:B:110:TYR:OH	2.64	0.44
1:C:271:MSE:HA	1:C:276:MSE:HE3	1.99	0.44
1:F:249:ILE:HD12	1:F:249:ILE:N	2.32	0.44
1:H:223:LYS:CD	5:H:2146:HOH:O	2.53	0.44
1:A:99:ASP:OD2	1:B:130:TYR:OH	2.35	0.44
1:B:75:GLN:CB	5:B:2027:HOH:O	2.64	0.44
1:H:210:TRP:HH2	1:H:231:GLN:NE2	2.13	0.44
1:H:38:GLU:CG	5:H:2013:HOH:O	2.44	0.44
1:A:94:MSE:HE2	1:A:113:ALA:HB3	1.99	0.44
1:E:21:SC2:O	1:E:22:THR:CA	2.65	0.44
1:E:179:VAL:HG13	1:E:249:ILE:HD13	2.00	0.44
1:A:109:GLN:CG	1:B:108:GLY:HA3	2.47	0.44
1:B:190:ILE:HD12	5:B:2087:HOH:O	2.17	0.44
1:D:298:ILE:HD12	1:D:320:ALA:HB3	1.98	0.44
1:B:291:GLU:HB3	1:B:292:MSE:HG3	1.99	0.44
1:D:108:GLY:HA3	1:E:109:GLN:CG	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:SC2:O	1:D:21:SC2:SG	2.76	0.44
1:F:239:HIS:CE1	5:F:2154:HOH:O	2.60	0.44
1:H:358:VAL:HG23	1:H:359:PRO:HD3	2.00	0.44
1:D:148:ILE:O	1:D:152:LEU:HB2	2.17	0.44
1:A:110:TYR:CG	1:D:110:TYR:CD1	3.06	0.44
1:A:41:ASP:O	1:A:44:TYR:HB3	2.18	0.44
1:A:110:TYR:CD1	1:B:110:TYR:CD2	3.06	0.44
1:D:309:THR:CA	5:D:2132:HOH:O	2.66	0.44
1:A:128:TYR:CD1	1:A:129:PRO:HD2	2.53	0.43
1:B:173:VAL:HG11	1:B:241:LEU:HD13	2.00	0.43
1:E:30:ASN:N	1:E:30:ASN:HD22	2.16	0.43
1:D:100:HIS:HD2	1:D:102:GLU:OE2	2.01	0.43
1:H:176:THR:HG22	1:H:177:GLY:N	2.33	0.43
1:E:195:MSE:CA	1:E:195:MSE:HE2	2.35	0.43
1:B:239:HIS:HE1	5:B:2113:HOH:O	2.01	0.43
1:D:128:TYR:CG	1:D:129:PRO:HD2	2.53	0.43
1:A:195:MSE:CE	1:A:195:MSE:HA	2.46	0.43
1:E:30:ASN:H	1:E:30:ASN:HD22	1.66	0.43
1:H:109:GLN:HB2	5:H:2076:HOH:O	2.18	0.43
1:A:110:TYR:CE2	1:D:110:TYR:CZ	2.99	0.43
5:C:2060:HOH:O	1:H:94:MSE:CE	2.57	0.43
1:C:146:GLN:NE2	5:C:2072:HOH:O	2.51	0.43
1:D:358:VAL:HG22	1:D:359:PRO:HD3	1.99	0.43
1:F:94:MSE:HE2	1:F:113:ALA:HB3	2.01	0.43
1:F:223:LYS:HD3	1:F:223:LYS:HA	1.48	0.43
1:H:173:VAL:HG11	1:H:241:LEU:HD13	2.00	0.43
1:A:294:ASP:HB3	1:A:343:THR:HG22	2.00	0.43
1:D:260:MSE:HE1	1:E:326:MSE:CE	2.43	0.43
1:H:358:VAL:HG22	1:H:359:PRO:HD3	2.00	0.43
1:F:172:LYS:HD3	1:F:184:LYS:HE3	2.00	0.43
1:C:204:LEU:HD13	1:C:210:TRP:HB3	2.01	0.42
1:B:110:TYR:CD1	1:G:110:TYR:CE1	3.02	0.42
1:G:75:GLN:HG2	1:G:75:GLN:H	1.41	0.42
1:H:32:LEU:HD12	1:H:32:LEU:HA	1.67	0.42
1:A:296:THR:CG2	1:A:321:GLN:HG3	2.49	0.42
1:B:375:LYS:O	1:B:376:ARG:C	2.57	0.42
1:C:157:GLU:CD	1:C:157:GLU:N	2.73	0.42
1:F:27:GLN:HG2	1:H:320:ALA:O	2.19	0.42
1:D:178:GLU:OE1	1:D:207:ASP:OD1	2.37	0.42
1:G:288:ILE:CD1	1:G:298:ILE:CD1	2.97	0.42
1:H:94:MSE:HE2	1:H:113:ALA:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD22	1:B:310:GLY:O	2.20	0.42
1:A:271:MSE:HA	1:A:276:MSE:HE3	2.00	0.42
1:F:178:GLU:OE1	1:F:207:ASP:OD1	2.37	0.42
1:F:375:LYS:O	1:F:376:ARG:CB	2.68	0.42
1:C:145:ARG:NH1	1:C:162:ASP:OD1	2.53	0.42
1:F:72:SER:CA	5:F:2042:HOH:O	2.67	0.42
1:G:128:TYR:CG	1:G:129:PRO:HD2	2.55	0.42
1:G:133:LYS:HB3	1:G:133:LYS:HE2	1.70	0.42
1:G:94:MSE:HE2	1:G:113:ALA:HB1	2.00	0.42
1:H:243:HIS:HB2	5:H:2111:HOH:O	2.19	0.42
1:G:279:ALA:HA	1:G:326:MSE:CE	2.50	0.41
1:H:178:GLU:OE1	1:H:207:ASP:OD1	2.38	0.41
1:A:172:LYS:HD3	1:A:184:LYS:HD3	2.02	0.41
1:C:128:TYR:CG	1:C:129:PRO:HD2	2.54	0.41
1:G:71:ARG:HD3	1:G:234:ASP:OD1	2.20	0.41
1:B:55:MSE:HE2	1:B:332:PHE:CD1	2.55	0.41
1:C:326:MSE:O	1:C:326:MSE:HE3	2.20	0.41
1:F:71:ARG:C	5:F:2042:HOH:O	2.58	0.41
1:G:288:ILE:CD1	1:G:298:ILE:HD11	2.50	0.41
1:B:65:PRO:HD3	5:B:2021:HOH:O	2.19	0.41
1:D:109:GLN:H	1:D:109:GLN:HG2	1.64	0.41
1:F:31:SER:HA	1:F:34:LYS:HD2	2.02	0.41
1:D:279:ALA:CA	1:D:326:MSE:CE	2.92	0.41
1:G:173:VAL:HG12	1:G:174:TYR:N	2.35	0.41
1:F:173:VAL:HG23	1:F:187:ILE:HD11	2.03	0.41
1:H:279:ALA:CA	1:H:326:MSE:HE2	2.50	0.41
1:D:98:TRP:CZ3	1:D:162:ASP:HB2	2.56	0.41
1:E:119:TRP:O	1:E:126:ILE:HG22	2.21	0.41
1:E:220:LYS:HB3	1:E:220:LYS:HE2	1.74	0.41
1:B:361:ILE:CG2	1:G:367:MSE:HG3	2.50	0.41
1:A:326:MSE:HE2	1:A:329:GLY:HA3	1.73	0.41
1:F:271:MSE:HA	1:F:276:MSE:HE3	2.03	0.41
1:G:94:MSE:CE	5:G:2080:HOH:O	2.64	0.41
1:H:128:TYR:CD1	1:H:129:PRO:HD2	2.56	0.41
1:H:223:LYS:HZ3	1:H:223:LYS:HG2	1.67	0.41
1:A:282:LEU:HD13	1:A:288:ILE:HD11	2.01	0.41
1:G:271:MSE:HA	1:G:276:MSE:HE3	2.03	0.41
1:G:354:ILE:HA	1:G:354:ILE:HD13	1.85	0.41
1:A:336:PRO:O	1:A:337:TYR:HB2	2.21	0.41
1:C:326:MSE:HE2	1:C:329:GLY:C	2.41	0.41
1:G:145:ARG:NH1	1:G:162:ASP:OD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HB3	1:B:312:ILE:HG12	2.02	0.40
1:G:348:VAL:HA	1:H:356:GLN:HE21	1.85	0.40
1:C:173:VAL:HG23	1:C:187:ILE:HD11	2.03	0.40
1:H:143:GLN:HA	1:H:146:GLN:HE21	1.86	0.40
1:B:292:MSE:HE2	1:B:348:VAL:HG11	2.02	0.40
1:D:210:TRP:HH2	1:D:231:GLN:HE21	1.68	0.40
1:E:110:TYR:CD1	1:F:110:TYR:CD1	3.09	0.40
1:F:173:VAL:HG11	1:F:241:LEU:HD13	2.02	0.40
1:H:85:TYR:HB2	1:H:189:ASN:HA	2.03	0.40
1:B:326:MSE:HE3	1:B:329:GLY:H	1.86	0.40
1:B:98:TRP:O	1:B:99:ASP:HB2	2.22	0.40
1:E:55:MSE:HE1	1:E:278:LEU:HD22	2.04	0.40
1:G:253:ASP:O	1:G:256:LYS:HE3	2.21	0.40
1:E:308:ARG:HB2	5:E:2160:HOH:O	2.21	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	353/359 (98%)	344 (98%)	9 (2%)	0	100	100
1	B	353/359 (98%)	345 (98%)	7 (2%)	1 (0%)	41	46
1	C	353/359 (98%)	346 (98%)	7 (2%)	0	100	100
1	D	353/359 (98%)	348 (99%)	5 (1%)	0	100	100
1	E	353/359 (98%)	346 (98%)	7 (2%)	0	100	100
1	F	353/359 (98%)	348 (99%)	5 (1%)	0	100	100
1	G	353/359 (98%)	346 (98%)	6 (2%)	1 (0%)	41	46
1	H	353/359 (98%)	350 (99%)	3 (1%)	0	100	100
All	All	2824/2872 (98%)	2773 (98%)	49 (2%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	375	LYS
1	G	375	LYS

5.3.2 Protein sidechains (i)

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	304/297 (102%)	295 (97%)	9 (3%)	41	50
1	B	304/297 (102%)	292 (96%)	12 (4%)	32	38
1	C	304/297 (102%)	290 (95%)	14 (5%)	27	30
1	D	304/297 (102%)	288 (95%)	16 (5%)	22	23
1	E	304/297 (102%)	289 (95%)	15 (5%)	25	27
1	F	304/297 (102%)	296 (97%)	8 (3%)	46	55
1	G	304/297 (102%)	292 (96%)	12 (4%)	32	38
1	H	304/297 (102%)	292 (96%)	12 (4%)	32	38
All	All	2432/2376 (102%)	2334 (96%)	98 (4%)	31	37

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	79	LEU
1	A	102	GLU
1	A	156	ILE
1	A	172	LYS
1	A	210	TRP
1	A	223	LYS
1	A	236	THR
1	A	308	ARG
1	B	38	GLU
1	B	79	LEU
1	B	172	LYS

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Mol	Chain	Res	Type
1	B	176	THR
1	B	195	MSE
1	B	210	TRP
1	B	223	LYS
1	B	236	THR
1	B	265	LYS
1	B	308	ARG
1	B	362	SER
1	B	376	ARG
1	C	30	ASN
1	C	32	LEU
1	C	48	LYS
1	C	79	LEU
1	C	133	LYS
1	C	152	LEU
1	C	154	THR
1	C	156	ILE
1	C	176	THR
1	C	210	TRP
1	C	229	LEU
1	C	308	ARG
1	C	362	SER
1	C	370	THR
1	D	60	ILE
1	D	75	GLN
1	D	79	LEU
1	D	81	LYS
1	D	109	GLN
1	D	147	ASP
1	D	176	THR
1	D	195	MSE
1	D	210	TRP
1	D	229	LEU
1	D	267	SER
1	D	308	ARG
1	D	309	THR
1	D	321	GLN
1	D	362	SER
1	D	376	ARG
1	E	30	ASN
1	E	38	GLU
1	E	79	LEU

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Mol	Chain	Res	Type
1	E	146	GLN
1	E	154	THR
1	E	156	ILE
1	E	157	GLU
1	E	158	SER
1	E	184	LYS
1	E	195	MSE
1	E	210	TRP
1	E	220	LYS
1	E	229	LEU
1	E	236	THR
1	E	362	SER
1	F	32	LEU
1	F	72	SER
1	F	79	LEU
1	F	156	ILE
1	F	176	THR
1	F	210	TRP
1	F	305	LYS
1	F	308	ARG
1	G	30	ASN
1	G	32	LEU
1	G	75	GLN
1	G	79	LEU
1	G	99	ASP
1	G	133	LYS
1	G	154	THR
1	G	172	LYS
1	G	195	MSE
1	G	210	TRP
1	G	229	LEU
1	G	267	SER
1	H	72	SER
1	H	75	GLN
1	H	79	LEU
1	H	152	LEU
1	H	184	LYS
1	H	195	MSE
1	H	210	TRP
1	H	223	LYS
1	H	265	LYS
1	H	321	GLN

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Mol	Chain	Res	Type
1	H	362	SER
1	H	376	ARG

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	62	GLN
1	A	100	HIS
1	A	109	GLN
1	A	218	ASN
1	A	231	GLN
1	A	239	HIS
1	A	243	HIS
1	A	356	GLN
1	B	135	GLN
1	B	218	ASN
1	B	231	GLN
1	B	239	HIS
1	B	243	HIS
1	B	356	GLN
1	C	75	GLN
1	C	100	HIS
1	C	135	GLN
1	C	218	ASN
1	C	231	GLN
1	C	239	HIS
1	C	321	GLN
1	C	356	GLN
1	D	100	HIS
1	D	218	ASN
1	D	231	GLN
1	D	356	GLN
1	E	62	GLN
1	E	100	HIS
1	E	118	ASN
1	E	121	ASN
1	E	146	GLN
1	E	171	GLN
1	E	185	GLN
1	E	218	ASN
1	E	239	HIS
1	F	118	ASN

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Mol	Chain	Res	Type
1	F	185	GLN
1	F	218	ASN
1	F	231	GLN
1	F	239	HIS
1	F	356	GLN
1	G	118	ASN
1	G	218	ASN
1	G	239	HIS
1	G	243	HIS
1	H	30	ASN
1	H	109	GLN
1	H	118	ASN
1	H	146	GLN
1	H	218	ASN
1	H	231	GLN
1	H	243	HIS
1	H	321	GLN
1	H	351	ASN
1	H	356	GLN

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	SC2	H	21	-	7,8,9	0.97	0	9,9,11	2.11	3 (33%)
1	SC2	A	21	-	7,8,9	0.80	0	9,9,11	1.28	1 (11%)
1	SC2	C	21	-	7,8,9	1.06	1 (14%)	9,9,11	1.66	4 (44%)
1	SC2	B	21	1	7,8,9	1.02	0	9,9,11	1.36	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SC2	E	21	1	7,8,9	0.93	0	9,9,11	1.37	1 (11%)
1	SC2	D	21	1	7,8,9	1.04	1 (14%)	9,9,11	0.91	0
1	SC2	G	21	1	7,8,9	1.06	0	9,9,11	1.14	1 (11%)
1	SC2	F	21	-	7,8,9	0.88	0	9,9,11	1.80	1 (11%)

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	SC2	H	21	-	-	3/7/8/10	-
1	SC2	A	21	-	-	2/7/8/10	-
1	SC2	C	21	-	-	3/7/8/10	-
1	SC2	B	21	1	-	4/7/8/10	-
1	SC2	E	21	1	-	0/7/8/10	-
1	SC2	D	21	1	-	2/7/8/10	-
1	SC2	G	21	1	-	3/7/8/10	-
1	SC2	F	21	-	-	3/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	SC2	CM-CT	2.31	1.55	1.50
1	D	21	SC2	CM-CT	2.12	1.54	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	21	SC2	CA-CB-SG	-4.19	109.49	114.19
1	H	21	SC2	CB-CA-N	-3.49	106.31	111.28
1	A	21	SC2	CA-CB-SG	-2.71	111.15	114.19
1	E	21	SC2	CB-CA-N	-2.71	107.43	111.28
1	C	21	SC2	CA-CB-SG	-2.60	111.27	114.19
1	H	21	SC2	CA-CB-SG	-2.59	111.28	114.19
1	H	21	SC2	CB-CA-C	-2.47	105.27	111.31
1	C	21	SC2	CB-CA-N	-2.41	107.85	111.28
1	G	21	SC2	CB-CA-N	-2.29	108.02	111.28
1	C	21	SC2	CB-CA-C	-2.18	105.97	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	21	SC2	CB-CA-N	-2.15	108.22	111.28
1	C	21	SC2	O-C-CA	-2.05	119.40	124.78

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	21	SC2	C-CA-CB-SG
1	H	21	SC2	N-CA-CB-SG
1	H	21	SC2	C-CA-N-CT
1	A	21	SC2	C-CA-CB-SG
1	A	21	SC2	N-CA-CB-SG
1	C	21	SC2	N-CA-CB-SG
1	C	21	SC2	C-CA-N-CT
1	B	21	SC2	O-C-CA-CB
1	B	21	SC2	C-CA-CB-SG
1	B	21	SC2	N-CA-CB-SG
1	B	21	SC2	C-CA-N-CT
1	D	21	SC2	C-CA-N-CT
1	G	21	SC2	C-CA-CB-SG
1	G	21	SC2	N-CA-CB-SG
1	G	21	SC2	C-CA-N-CT
1	F	21	SC2	N-CA-CB-SG
1	D	21	SC2	CB-CA-N-CT
1	F	21	SC2	C-CA-N-CT
1	C	21	SC2	C-CA-CB-SG
1	F	21	SC2	CB-CA-N-CT

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	21	SC2	3	0
1	A	21	SC2	2	0
1	C	21	SC2	3	0
1	B	21	SC2	1	0
1	E	21	SC2	4	0
1	D	21	SC2	5	0
1	G	21	SC2	2	0
1	F	21	SC2	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OCT	A	600	-	7,7,7	0.54	0	6,6,6	0.36	0
4	SO4	G	605	-	4,4,4	0.17	0	6,6,6	0.14	0
2	OCT	C	600	-	7,7,7	0.58	0	6,6,6	0.27	0
2	OCT	F	600	-	7,7,7	0.49	0	6,6,6	0.36	0
4	SO4	A	605	-	4,4,4	0.14	0	6,6,6	0.20	0
4	SO4	B	605	-	4,4,4	0.13	0	6,6,6	0.19	0
4	SO4	D	605	-	4,4,4	0.14	0	6,6,6	0.12	0
3	HEX	F	601	-	5,5,5	0.38	0	4,4,4	0.37	0
2	OCT	H	600	-	7,7,7	0.55	0	6,6,6	0.30	0
4	SO4	E	602	-	4,4,4	0.19	0	6,6,6	0.41	0
2	OCT	B	600	-	7,7,7	0.59	0	6,6,6	0.33	0
4	SO4	E	605	-	4,4,4	0.13	0	6,6,6	0.16	0
4	SO4	C	605	-	4,4,4	0.14	0	6,6,6	0.11	0
4	SO4	C	602	-	4,4,4	0.22	0	6,6,6	0.27	0
4	SO4	H	602	-	4,4,4	0.14	0	6,6,6	0.25	0
3	HEX	B	601	-	5,5,5	0.44	0	4,4,4	0.32	0
3	HEX	A	601	-	5,5,5	0.49	0	4,4,4	0.39	0
3	HEX	G	601	-	5,5,5	0.52	0	4,4,4	0.28	0
4	SO4	G	602	-	4,4,4	0.15	0	6,6,6	0.44	0
3	HEX	H	601	-	5,5,5	0.48	0	4,4,4	0.27	0
4	SO4	B	602	-	4,4,4	0.17	0	6,6,6	0.42	0
4	SO4	D	602	-	4,4,4	0.16	0	6,6,6	0.33	0
3	HEX	E	601	-	5,5,5	0.42	0	4,4,4	0.27	0
4	SO4	A	602	-	4,4,4	0.22	0	6,6,6	0.44	0
2	OCT	E	600	-	7,7,7	0.56	0	6,6,6	0.31	0
4	SO4	F	605	-	4,4,4	0.12	0	6,6,6	0.18	0
2	OCT	D	600	-	7,7,7	0.47	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OCT	G	600	-	7,7,7	0.57	0	6,6,6	0.30	0
4	SO4	H	605	-	4,4,4	0.14	0	6,6,6	0.23	0
4	SO4	F	602	-	4,4,4	0.21	0	6,6,6	0.37	0
3	HEX	D	601	-	5,5,5	0.50	0	4,4,4	0.24	0
3	HEX	C	601	-	5,5,5	0.54	0	4,4,4	0.27	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	OCT	H	600	-	-	2/5/5/5	-
2	OCT	A	600	-	-	2/5/5/5	-
3	HEX	H	601	-	-	0/3/3/3	-
2	OCT	B	600	-	-	2/5/5/5	-
2	OCT	E	600	-	-	2/5/5/5	-
2	OCT	C	600	-	-	2/5/5/5	-
2	OCT	F	600	-	-	3/5/5/5	-
2	OCT	D	600	-	-	3/5/5/5	-
2	OCT	G	600	-	-	2/5/5/5	-
3	HEX	D	601	-	-	0/3/3/3	-
3	HEX	C	601	-	-	0/3/3/3	-
3	HEX	B	601	-	-	0/3/3/3	-
3	HEX	A	601	-	-	0/3/3/3	-
3	HEX	G	601	-	-	2/3/3/3	-
3	HEX	F	601	-	-	0/3/3/3	-
3	HEX	E	601	-	-	1/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	600	OCT	C2-C3-C4-C5
2	G	600	OCT	C3-C4-C5-C6
2	C	600	OCT	C2-C3-C4-C5
3	E	601	HEX	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	B	600	OCT	C3-C4-C5-C6
2	H	600	OCT	C3-C4-C5-C6
2	B	600	OCT	C2-C3-C4-C5
2	D	600	OCT	C3-C4-C5-C6
2	C	600	OCT	C1-C2-C3-C4
2	D	600	OCT	C2-C3-C4-C5
2	A	600	OCT	C1-C2-C3-C4
2	F	600	OCT	C1-C2-C3-C4
2	D	600	OCT	C1-C2-C3-C4
2	E	600	OCT	C1-C2-C3-C4
2	G	600	OCT	C1-C2-C3-C4
2	E	600	OCT	C3-C4-C5-C6
2	H	600	OCT	C1-C2-C3-C4
2	F	600	OCT	C3-C4-C5-C6
3	G	601	HEX	C3-C4-C5-C6
2	A	600	OCT	C4-C5-C6-C7
3	G	601	HEX	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	OCT	1	0
2	G	600	OCT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1
1	D	1
1	E	1
1	H	1
1	B	1
1	C	1

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Mol	Chain	Number of breaks
1	A	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	21:SC2	C	22:THR	N	2.68
1	A	21:SC2	C	22:THR	N	2.55
1	C	21:SC2	C	22:THR	N	2.45
1	H	21:SC2	C	22:THR	N	2.36
1	G	21:SC2	C	22:THR	N	2.35
1	B	21:SC2	C	22:THR	N	2.29
1	E	21:SC2	C	22:THR	N	2.28
1	D	21:SC2	C	22:THR	N	2.25

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, 95^{th} 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	345/359 (96%)	0.31	14 (4%)	37 40	29, 34, 45, 57	1 (0%)
1	B	345/359 (96%)	0.24	7 (2%)	65 68	28, 34, 44, 58	1 (0%)
1	C	345/359 (96%)	0.26	4 (1%)	79 81	28, 34, 43, 58	1 (0%)
1	D	345/359 (96%)	0.26	9 (2%)	56 59	28, 34, 43, 57	1 (0%)
1	E	345/359 (96%)	0.20	4 (1%)	79 81	29, 34, 45, 57	1 (0%)
1	F	345/359 (96%)	0.19	2 (0%)	89 89	29, 34, 45, 58	1 (0%)
1	G	345/359 (96%)	0.25	3 (0%)	84 85	29, 34, 45, 58	1 (0%)
1	H	345/359 (96%)	0.26	4 (1%)	79 81	29, 34, 43, 57	1 (0%)
All	All	2760/2872 (96%)	0.25	47 (1%)	70 73	28, 34, 45, 58	8 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	110	TYR	4.3
1	A	308	ARG	4.0
1	E	110	TYR	4.0
1	D	308	ARG	3.9
1	A	110	TYR	3.8
1	A	146	GLN	3.6
1	G	373	TYR	3.5
1	D	146	GLN	3.4
1	C	110	TYR	3.3
1	B	374	ILE	3.3
1	B	32	LEU	3.2
1	C	32	LEU	3.1
1	A	309	THR	3.0
1	A	32	LEU	2.9
1	F	32	LEU	2.9
1	G	110	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	309	THR	2.9
1	A	374	ILE	2.8
1	E	32	LEU	2.7
1	H	110	TYR	2.7
1	D	147	ASP	2.7
1	H	109	GLN	2.7
1	B	110	TYR	2.6
1	C	375	LYS	2.6
1	H	308	ARG	2.6
1	B	308	ARG	2.5
1	D	110	TYR	2.5
1	D	310	GLY	2.4
1	H	309	THR	2.4
1	A	157	GLU	2.4
1	A	152	LEU	2.3
1	D	157	GLU	2.3
1	D	38	GLU	2.3
1	A	372	ARG	2.2
1	G	128	TYR	2.2
1	E	375	LYS	2.2
1	A	127	PHE	2.2
1	D	373	TYR	2.2
1	C	373	TYR	2.2
1	B	373	TYR	2.1
1	A	161	VAL	2.1
1	B	141	VAL	2.1
1	A	174	TYR	2.1
1	A	78	ASN	2.1
1	B	361	ILE	2.1
1	E	374	ILE	2.1
1	A	156	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
1	SC2	G	21	9/10	0.76	0.27	72,74,75,75	0
1	SC2	H	21	9/10	0.77	0.21	67,68,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SC2	B	21	9/10	0.78	0.25	69,70,71,71	0
1	SC2	F	21	9/10	0.81	0.23	77,78,78,78	0
1	SC2	C	21	9/10	0.83	0.18	73,74,75,75	0
1	SC2	A	21	9/10	0.84	0.20	75,76,76,78	0
1	SC2	D	21	9/10	0.88	0.22	70,71,71,71	0
1	SC2	E	21	9/10	0.89	0.16	57,59,59,61	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. 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	B-factors(Å^2)	Q<0.9
2	OCT	G	600	8/8	0.71	0.22	50,58,62,62	0
2	OCT	B	600	8/8	0.73	0.22	53,54,58,58	0
2	OCT	A	600	8/8	0.77	0.18	48,54,55,55	0
4	SO4	B	605	5/5	0.77	0.36	122,122,122,122	0
2	OCT	H	600	8/8	0.78	0.20	55,57,59,59	0
4	SO4	H	605	5/5	0.79	0.40	111,111,111,111	0
2	OCT	D	600	8/8	0.80	0.21	55,56,58,59	0
4	SO4	C	605	5/5	0.80	0.38	100,100,101,101	0
3	HEX	G	601	6/6	0.80	0.17	43,44,46,46	0
2	OCT	E	600	8/8	0.81	0.18	52,52,53,54	0
3	HEX	D	601	6/6	0.82	0.14	46,46,47,48	0
4	SO4	D	605	5/5	0.83	0.32	114,114,115,115	0
2	OCT	C	600	8/8	0.83	0.15	44,46,47,48	0
4	SO4	G	605	5/5	0.84	0.39	98,99,99,99	0
2	OCT	F	600	8/8	0.85	0.14	55,56,58,58	0
4	SO4	F	605	5/5	0.85	0.32	99,99,99,100	0
3	HEX	H	601	6/6	0.87	0.16	50,51,51,51	0
4	SO4	A	605	5/5	0.89	0.28	92,93,93,94	0
3	HEX	B	601	6/6	0.90	0.12	46,48,49,50	0
4	SO4	E	605	5/5	0.91	0.36	96,96,96,97	0
3	HEX	F	601	6/6	0.92	0.14	48,48,49,51	0
3	HEX	A	601	6/6	0.92	0.11	39,40,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEX	C	601	6/6	0.92	0.13	43,43,44,44	0
3	HEX	E	601	6/6	0.93	0.14	50,50,52,53	0
4	SO4	A	602	5/5	0.98	0.14	48,50,51,51	0
4	SO4	B	602	5/5	0.98	0.18	52,52,53,53	0
4	SO4	H	602	5/5	0.99	0.13	41,42,43,45	0
4	SO4	E	602	5/5	0.99	0.11	37,42,44,45	0
4	SO4	F	602	5/5	0.99	0.11	37,37,40,41	0
4	SO4	D	602	5/5	0.99	0.14	49,50,53,53	0
4	SO4	G	602	5/5	0.99	0.11	42,43,43,45	0
4	SO4	C	602	5/5	1.00	0.12	35,35,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.