



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:01 am BST

PDB ID : 4EFD
Title : Crystal Structure of an M17 aminopeptidase from Trypanosoma Brucei, Tb427tmp.02.4440
Authors : Wernimont, A.K.; Osman, K.T.; Loppnau, P.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Hui, R.; Lin, Y.H.; Structural Genomics Consortium (SGC)
Deposited on : 2012-03-29
Resolution : 2.45 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

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
5	UNX	B	608	-	-	-	X
5	UNX	D	604	-	-	-	X
5	UNX	E	603	-	-	-	X
5	UNX	F	606	-	-	X	X

2 Entry composition [i](#)

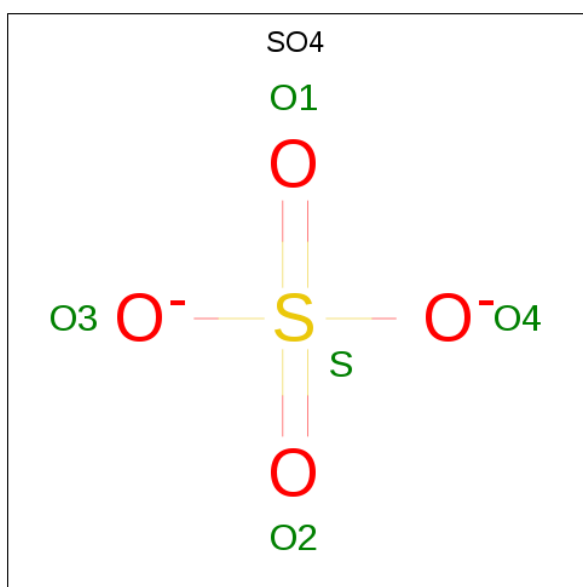
There are 7 unique types of molecules in this entry. The entry contains 23792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	517	Total 3836	C 2423	N 656	O 735	S 22	0	4	0
1	B	515	Total 3819	C 2411	N 648	O 739	S 21	0	9	0
1	C	514	Total 3808	C 2405	N 647	O 734	S 22	0	9	0
1	D	516	Total 3799	C 2401	N 643	O 733	S 22	0	2	0
1	E	515	Total 3809	C 2404	N 651	O 732	S 22	0	3	0
1	F	516	Total 3827	C 2419	N 647	O 739	S 22	0	5	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total X 1 1	0	0
5	E	1	Total X 1 1	0	0
5	B	1	Total X 1 1	0	0
5	C	1	Total X 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total X 1 1	0	0
5	F	1	Total X 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Na 1 1	0	0
6	F	1	Total Na 1 1	0	0

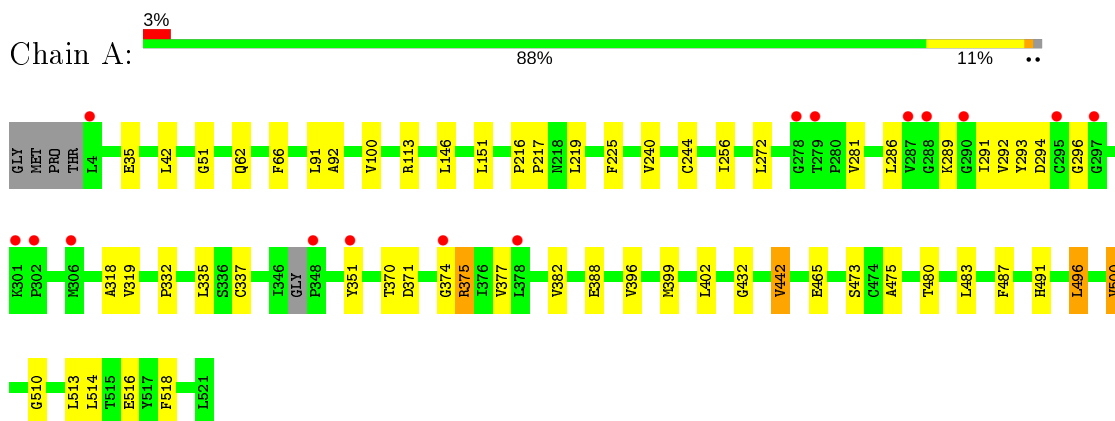
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	100	Total O 100 100	0	0
7	B	131	Total O 131 131	0	0
7	C	82	Total O 82 82	0	0
7	D	97	Total O 97 97	0	0
7	E	161	Total O 162 162	0	1
7	F	198	Total O 198 198	0	0

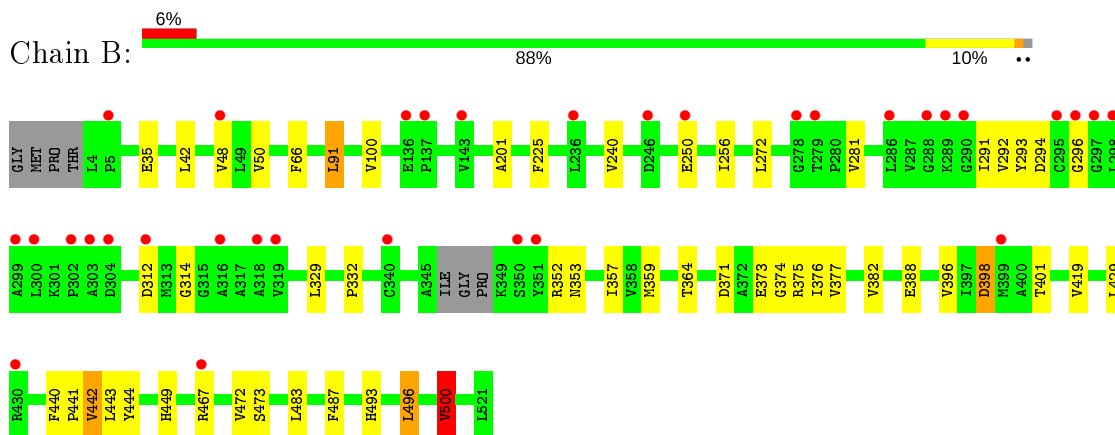
3 Residue-property plots i

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.

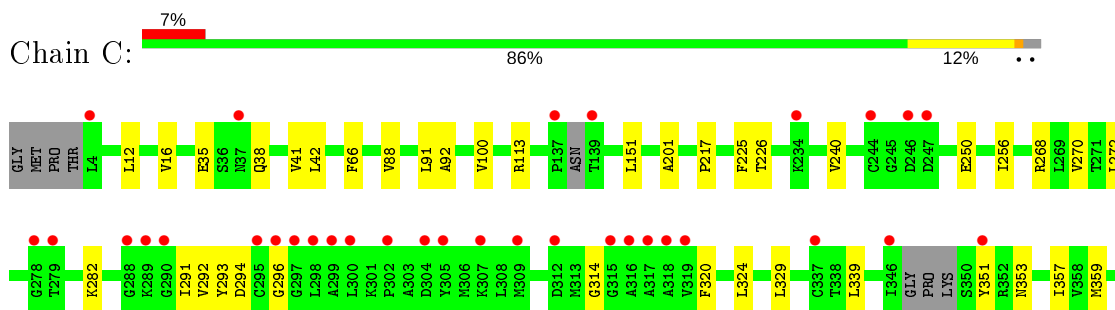
- Molecule 1: Aminopeptidase

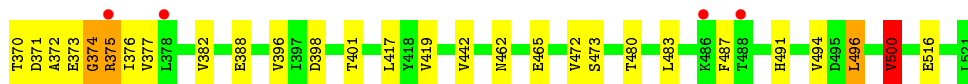


- Molecule 1: Aminopeptidase

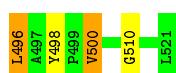
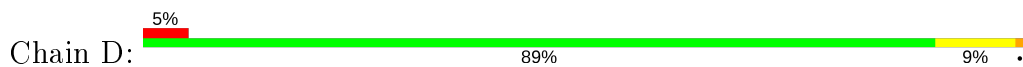


- Molecule 1: Aminopeptidase

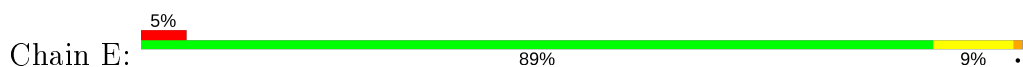




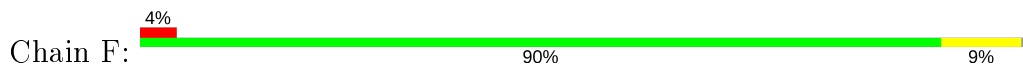
- Molecule 1: Aminopeptidase



- Molecule 1: Aminopeptidase



- Molecule 1: Aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	161.92Å 161.74Å 176.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.45 29.87 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.45) 99.3 (29.87-2.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.45Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.227 , 0.253 0.225 , 0.248	Depositor DCC
R_{free} test set	8455 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.015 for k,h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23792	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, GOL, MN, SO4, NA

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	0.28	0/3915	0.45	1/5337 (0.0%)
1	B	0.27	0/3917	0.44	1/5343 (0.0%)
1	C	0.27	0/3885	0.43	1/5302 (0.0%)
1	D	0.28	0/3874	0.45	0/5288
1	E	0.28	0/3887	0.45	0/5299
1	F	0.28	0/3905	0.45	0/5323
All	All	0.28	0/23383	0.45	3/31892 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	500	VAL	CG1-CB-CG2	5.52	119.73	110.90
1	C	500	VAL	CG1-CB-CG2	5.29	119.37	110.90
1	A	500	VAL	CG1-CB-CG2	5.01	118.91	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3836	0	3746	37	0
1	B	3819	0	3716	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3808	0	3669	52	0
1	D	3799	0	3677	40	0
1	E	3809	0	3713	39	0
1	F	3827	0	3731	32	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	F	2	0	0	0	0
4	A	18	0	24	1	0
4	B	18	0	24	0	0
4	C	12	0	16	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	2	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	A	100	0	0	0	0
7	B	131	0	0	0	0
7	C	82	0	0	0	0
7	D	97	0	0	0	0
7	E	162	0	0	1	0
7	F	198	0	0	0	0
All	All	23792	0	22316	236	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (236) 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:372[B]:ALA:O	1:C:375[B]:ARG:HD3	1.35	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375[B]:ARG:CG	1:F:375[B]:ARG:HH11	1.59	1.15
1:F:375[B]:ARG:HH11	1:F:375[B]:ARG:HG2	1.05	1.13
1:E:375[A]:ARG:HH11	1:E:375[A]:ARG:HG2	1.02	1.12
1:B:375[B]:ARG:CD	1:B:375[B]:ARG:H	1.58	1.10
1:C:375[B]:ARG:HD2	1:C:375[B]:ARG:N	1.63	1.08
1:B:375[B]:ARG:HH11	1:B:375[B]:ARG:CG	1.69	1.06
1:B:375[B]:ARG:HG3	1:B:375[B]:ARG:NH1	1.57	1.06
1:E:375[A]:ARG:CD	1:E:375[A]:ARG:H	1.71	1.04
1:D:496:LEU:O	1:D:500:VAL:HG22	1.58	1.04
1:C:496:LEU:O	1:C:500:VAL:HG22	1.58	1.03
1:E:375[A]:ARG:HD2	1:E:375[A]:ARG:H	1.24	1.03
1:D:345:ALA:HB1	1:D:346:ILE:HG23	1.39	1.03
1:B:496:LEU:O	1:B:500:VAL:HG22	1.59	1.02
1:B:375[B]:ARG:HD3	1:B:375[B]:ARG:H	1.26	1.00
1:C:375[B]:ARG:H	1:C:375[B]:ARG:CD	1.74	0.98
1:C:375[B]:ARG:HD2	1:C:375[B]:ARG:H	0.82	0.96
1:E:375[A]:ARG:CG	1:E:375[A]:ARG:HH11	1.77	0.96
1:F:375[B]:ARG:HH12	5:F:606:UNX:UNK	1.02	0.94
1:C:226:THR:HG22	1:C:270:VAL:HG21	1.49	0.94
1:F:375[B]:ARG:HG2	1:F:375[B]:ARG:NH1	1.75	0.93
1:E:375[A]:ARG:HD2	1:E:375[A]:ARG:N	1.84	0.93
1:B:375[B]:ARG:CD	1:B:375[B]:ARG:N	2.35	0.89
1:B:375[B]:ARG:HG3	1:B:375[B]:ARG:HH11	0.77	0.87
1:F:375[B]:ARG:NH1	5:F:606:UNX:UNK	1.70	0.87
1:C:372[B]:ALA:O	1:C:375[B]:ARG:CD	2.22	0.86
1:E:375[A]:ARG:HG2	1:E:375[A]:ARG:NH1	1.84	0.84
1:D:345:ALA:HB1	1:D:346:ILE:CG2	2.07	0.84
1:A:319:VAL:HG12	1:A:337:CYS:SG	2.22	0.80
1:E:357:ILE:HD11	1:E:359:MET:SD	2.21	0.80
1:D:319:VAL:HG12	1:D:337:CYS:SG	2.21	0.79
1:A:240:VAL:HG22	1:A:272:LEU:HD22	1.67	0.76
1:D:496:LEU:O	1:D:500:VAL:CG2	2.34	0.74
1:F:382:VAL:HG13	1:F:483:LEU:HD23	1.67	0.74
1:B:496:LEU:O	1:B:500:VAL:CG2	2.34	0.74
1:C:496:LEU:O	1:C:500:VAL:CG2	2.34	0.74
1:B:375[B]:ARG:N	1:B:375[B]:ARG:HD2	2.03	0.73
1:E:42:LEU:HD22	1:E:100:VAL:HG11	1.71	0.73
1:B:375[B]:ARG:HD2	1:B:375[B]:ARG:H	1.52	0.72
1:C:372[B]:ALA:O	1:C:374[B]:GLY:N	2.27	0.68
1:C:357:ILE:HD11	1:C:359:MET:SD	2.35	0.67
1:D:240:VAL:HG22	1:D:272:LEU:HD22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375[B]:ARG:CG	1:F:375[B]:ARG:NH1	2.32	0.66
1:F:382:VAL:CG1	1:F:483:LEU:HD23	2.26	0.65
1:F:375[B]:ARG:HH11	1:F:375[B]:ARG:HG3	1.57	0.64
1:B:382:VAL:HG13	1:B:483:LEU:HD23	1.79	0.64
1:B:357:ILE:HD11	1:B:359:MET:SD	2.37	0.64
1:D:314:GLY:HA3	1:D:500:VAL:HG11	1.80	0.64
1:C:88:VAL:HG11	1:C:91:LEU:HD12	1.80	0.63
1:E:382:VAL:HG13	1:E:483:LEU:HD23	1.80	0.63
1:B:240:VAL:HG22	1:B:272:LEU:HD22	1.80	0.63
1:C:35[B]:GLU:C	1:C:35[B]:GLU:OE1	2.36	0.62
1:A:289:LYS:HE3	1:A:374:GLY:HA3	1.81	0.62
1:A:286:LEU:HB3	1:A:319:VAL:HG13	1.82	0.61
1:A:496:LEU:O	1:A:500:VAL:HG12	2.01	0.60
1:E:375[A]:ARG:CG	1:E:375[A]:ARG:NH1	2.47	0.60
1:C:375[B]:ARG:CD	1:C:375[B]:ARG:N	2.45	0.58
1:E:496:LEU:O	1:E:500:VAL:HG12	2.04	0.57
1:F:496:LEU:O	1:F:500:VAL:HG12	2.04	0.57
1:B:382:VAL:CG1	1:B:483:LEU:HD23	2.34	0.57
1:A:382:VAL:CG1	1:A:483:LEU:HD23	2.35	0.57
1:A:113:ARG:NH1	1:D:419:VAL:O	2.39	0.56
1:C:38:GLN:O	1:C:41:VAL:HG22	2.06	0.56
1:F:396:VAL:HG23	1:F:487:PHE:CE1	2.41	0.56
1:C:314:GLY:HA3	1:C:500:VAL:HG11	1.87	0.55
1:D:345:ALA:CB	1:D:346:ILE:HG23	2.26	0.55
1:A:382:VAL:HG13	1:A:483:LEU:HD23	1.89	0.55
1:F:256:ILE:HA	1:F:377:VAL:HG12	1.89	0.55
1:C:374[B]:GLY:C	1:C:376[B]:ILE:N	2.60	0.55
1:D:382:VAL:CG1	1:D:483:LEU:HD23	2.37	0.55
1:B:42:LEU:HD22	1:B:100:VAL:HG11	1.87	0.54
1:E:396:VAL:HG23	1:E:487:PHE:CE1	2.42	0.54
1:E:375[A]:ARG:HD3	1:E:375[A]:ARG:H	1.65	0.54
1:C:382:VAL:HG13	1:C:483:LEU:HD23	1.89	0.54
1:C:256:ILE:HA	1:C:377:VAL:HG12	1.90	0.54
1:C:376[B]:ILE:HD11	1:C:462:ASN:HB2	1.91	0.53
1:D:66:PHE:HA	1:D:91:LEU:HD11	1.91	0.52
1:E:42:LEU:HD13	1:E:91:LEU:HD22	1.90	0.52
1:A:113:ARG:NH2	4:A:605:GOL:O1	2.42	0.52
1:D:256:ILE:HA	1:D:377:VAL:HG12	1.90	0.52
1:C:66:PHE:HA	1:C:91:LEU:HD11	1.92	0.52
1:D:480:THR:HG22	1:D:491:HIS:CD2	2.45	0.51
1:F:292:VAL:HG12	1:F:293:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLY:O	1:A:377:VAL:HG22	2.11	0.51
1:A:35[B]:GLU:HA	1:A:35[B]:GLU:OE1	2.10	0.51
1:E:292:VAL:HG12	1:E:293:TYR:CD2	2.46	0.51
1:A:42:LEU:HD13	1:A:91:LEU:HD22	1.91	0.51
1:A:66:PHE:HA	1:A:91:LEU:HD11	1.93	0.51
1:D:401:THR:CG2	1:D:500:VAL:HG21	2.40	0.51
1:D:292:VAL:HG12	1:D:293:TYR:CD2	2.46	0.50
1:E:382:VAL:CG1	1:E:483:LEU:HD23	2.41	0.50
1:B:292:VAL:HG12	1:B:293:TYR:CD2	2.46	0.50
1:B:66:PHE:HA	1:B:91:LEU:HD11	1.91	0.50
1:D:319:VAL:CG1	1:D:337:CYS:SG	2.97	0.50
1:A:351:TYR:O	1:A:370:THR:HG21	2.12	0.50
1:F:66:PHE:HA	1:F:91:LEU:HD11	1.94	0.50
1:A:292:VAL:HG12	1:A:293:TYR:CD2	2.46	0.50
1:B:373:GLU:HG2	1:B:376:ILE:HD12	1.94	0.49
1:B:396:VAL:HG23	1:B:487:PHE:CE1	2.46	0.49
1:E:392:THR:HG22	1:E:486:LYS:HE3	1.94	0.49
1:D:402:LEU:HD23	1:D:475:ALA:HB1	1.95	0.49
1:B:314:GLY:HA3	1:B:500:VAL:HG11	1.95	0.49
1:C:292:VAL:HG12	1:C:293:TYR:CD2	2.47	0.49
1:C:374[B]:GLY:C	1:C:376[B]:ILE:H	2.16	0.49
1:C:374[B]:GLY:O	1:C:376[B]:ILE:N	2.46	0.49
1:D:396:VAL:HG23	1:D:487:PHE:CE1	2.47	0.49
1:B:352:ARG:NH2	1:B:373:GLU:OE1	2.45	0.49
1:B:353[B]:ASN:HD22	1:D:309:MET:CE	2.26	0.49
1:B:401:THR:CG2	1:B:500:VAL:HG21	2.42	0.48
1:B:401:THR:HG22	1:B:500:VAL:HG21	1.95	0.48
1:C:401:THR:HG22	1:C:500:VAL:HG21	1.95	0.48
1:C:442:VAL:HG12	1:C:473:SER:OG	2.14	0.48
1:A:217:PRO:HB3	1:A:292:VAL:HG13	1.96	0.48
1:D:401:THR:HG22	1:D:500:VAL:HG21	1.96	0.48
1:D:286:LEU:HB3	1:D:319:VAL:HG13	1.96	0.48
1:D:375:ARG:HG3	1:D:375:ARG:HH11	1.79	0.48
1:C:442:VAL:HG11	1:C:472:VAL:HB	1.95	0.48
1:C:382:VAL:CG1	1:C:483:LEU:HD23	2.45	0.47
1:D:318:ALA:HB1	1:D:510:GLY:HA3	1.96	0.47
1:A:296:GLY:HA3	1:A:371:ASP:HB3	1.96	0.47
1:C:201:ALA:HB3	1:C:329:LEU:HD11	1.95	0.47
1:C:374[B]:GLY:O	1:C:377:VAL:HG22	2.14	0.47
1:D:382:VAL:HG13	1:D:483:LEU:HD23	1.96	0.47
1:E:387:ASN:HA	1:E:486:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:437:GLU:CD	1:E:512:ALA:HB3	2.35	0.47
1:B:353[B]:ASN:HD22	1:D:309:MET:HE2	1.79	0.47
1:D:240:VAL:HG22	1:D:272:LEU:CD2	2.44	0.47
1:A:399:MET:SD	1:A:514:LEU:HD11	2.55	0.46
1:C:35[A]:GLU:HA	1:C:35[A]:GLU:OE2	2.15	0.46
1:B:364:THR:HG21	1:D:167:ALA:HB1	1.98	0.46
1:F:262:ALA:HB2	1:F:351:TYR:HE2	1.80	0.46
1:F:42:LEU:HD23	1:F:91:LEU:HD22	1.97	0.46
1:A:151:LEU:HD13	1:A:516:GLU:OE1	2.15	0.46
1:E:48:VAL:HG12	1:E:50:VAL:HG23	1.97	0.46
1:F:346:ILE:HD12	1:F:346:ILE:N	2.29	0.46
1:B:296:GLY:HA3	1:B:371:ASP:HB3	1.96	0.46
1:E:217:PRO:HB3	1:E:292:VAL:HG13	1.96	0.46
1:A:318:ALA:HB1	1:A:510:GLY:HA3	1.96	0.46
1:A:256:ILE:HA	1:A:377:VAL:HG12	1.97	0.46
1:C:351:TYR:O	1:C:370:THR:HG21	2.16	0.46
1:E:216:PRO:HD2	1:E:219:LEU:HD12	1.96	0.46
1:E:500:VAL:HG23	7:E:809:HOH:O	2.15	0.46
1:C:226:THR:HG21	1:C:268:ARG:HD3	1.98	0.46
1:B:281:VAL:HG12	1:B:332:PRO:O	2.16	0.45
1:B:201:ALA:HB3	1:B:329:LEU:HD11	1.98	0.45
1:B:374:GLY:O	1:B:377:VAL:HG22	2.15	0.45
1:A:465[B]:GLU:HA	1:A:465[B]:GLU:OE1	2.17	0.45
1:C:401:THR:CG2	1:C:500:VAL:HG21	2.47	0.45
1:C:91:LEU:HD23	1:C:92:ALA:N	2.31	0.45
1:E:66:PHE:HA	1:E:91:LEU:HD11	1.99	0.45
1:C:217:PRO:HB3	1:C:292:VAL:HG13	1.99	0.45
1:C:226:THR:HG21	1:C:268:ARG:CD	2.46	0.45
1:F:296:GLY:HA3	1:F:371:ASP:HB3	1.98	0.45
1:E:501:PHE:HA	1:E:507:THR:HG23	1.99	0.45
1:D:233:ALA:HB2	1:D:240:VAL:HG21	1.99	0.45
1:E:357:ILE:HD12	1:E:357:ILE:C	2.37	0.45
1:E:291:ILE:HB	1:E:294:ASP:HB3	1.99	0.44
1:E:353:ASN:HD22	1:E:370:THR:HG23	1.82	0.44
1:A:51:GLY:HA3	1:A:146:LEU:HD12	1.99	0.44
1:E:256:ILE:HA	1:E:377:VAL:HG12	2.00	0.44
1:D:91:LEU:HD23	1:D:92:ALA:N	2.32	0.44
1:A:216:PRO:HD2	1:A:219:LEU:HD12	1.99	0.44
1:A:442:VAL:HG13	1:A:473:SER:OG	2.17	0.44
1:C:151:LEU:HD13	1:C:516:GLU:OE1	2.17	0.44
1:C:291:ILE:HB	1:C:294:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:LEU:HD22	1:D:493:HIS:CE1	2.52	0.44
1:B:256:ILE:HA	1:B:377:VAL:HG12	2.00	0.43
1:B:291:ILE:HB	1:B:294:ASP:HB3	2.00	0.43
1:A:240:VAL:HG22	1:A:272:LEU:CD2	2.41	0.43
1:E:402:LEU:HD23	1:E:475:ALA:HB1	2.00	0.43
1:B:440:PHE:CD1	1:E:443:LEU:HD23	2.53	0.43
1:E:201:ALA:HB3	1:E:329:LEU:HD11	1.99	0.43
1:D:201:ALA:HB3	1:D:329:LEU:HD11	1.99	0.43
1:F:480:THR:HG22	1:F:491:HIS:ND1	2.33	0.43
1:B:240:VAL:HG22	1:B:272:LEU:CD2	2.48	0.43
1:A:374:GLY:HA2	1:A:377:VAL:HG22	2.01	0.43
1:F:291:ILE:HB	1:F:294:ASP:HB3	2.00	0.43
1:F:88:VAL:HG11	1:F:91:LEU:HD12	2.00	0.43
1:A:281:VAL:HG22	1:A:332:PRO:O	2.19	0.43
1:C:225:PHE:CE1	1:C:339:LEU:HD13	2.54	0.43
1:E:263:ALA:CB	1:E:343:GLU:HB3	2.49	0.43
1:D:291:ILE:HB	1:D:294:ASP:HB3	2.00	0.42
1:F:16:VAL:O	1:F:20:VAL:HG23	2.19	0.42
1:C:296:GLY:HA3	1:C:371:ASP:HB3	2.00	0.42
1:E:442:VAL:HG13	1:E:473:SER:OG	2.18	0.42
1:A:291:ILE:HB	1:A:294:ASP:HB3	2.00	0.42
1:F:255:GLY:HA2	1:F:357:ILE:HD12	2.01	0.42
1:F:43:SER:O	1:F:94:ALA:HB3	2.20	0.42
1:A:396:VAL:HG23	1:A:487:PHE:CE1	2.54	0.42
1:B:357:ILE:C	1:B:357:ILE:HD12	2.40	0.42
1:C:240:VAL:HG23	1:C:272:LEU:HD23	2.01	0.42
1:C:396:VAL:HG23	1:C:487:PHE:CE1	2.54	0.42
1:D:375:ARG:HD2	1:D:402:LEU:HD11	2.02	0.42
1:F:159:ARG:HG3	1:F:507:THR:O	2.20	0.42
1:D:375:ARG:N	1:D:375:ARG:HD3	2.35	0.42
1:D:402:LEU:HD22	1:D:493:HIS:HE1	1.84	0.42
1:E:417:LEU:CD2	1:E:494:VAL:HG22	2.50	0.42
1:B:443:LEU:HD22	1:B:444:TYR:N	2.35	0.42
1:D:233:ALA:HB2	1:D:240:VAL:CG2	2.50	0.42
1:D:443:LEU:HD11	1:D:445:CYS:HB3	2.02	0.42
1:B:429:LEU:HD21	1:B:441:PRO:HD3	2.02	0.41
1:B:48:VAL:HG12	1:B:50:VAL:HG23	2.02	0.41
1:D:367:VAL:HG11	1:D:373:GLU:OE2	2.20	0.41
1:E:374:GLY:O	1:E:377:VAL:HG22	2.20	0.41
1:E:392:THR:HG22	1:E:486:LYS:CE	2.50	0.41
1:F:263:ALA:HB2	1:F:343:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ASP:OD2	1:B:493:HIS:ND1	2.50	0.41
1:C:35[B]:GLU:O	1:C:35[B]:GLU:OE1	2.38	0.41
1:A:42:LEU:HD22	1:A:100:VAL:HG11	2.02	0.41
1:C:88:VAL:CG1	1:C:91:LEU:HD12	2.47	0.41
1:F:217:PRO:HB3	1:F:292:VAL:HG13	2.02	0.41
1:D:308:LEU:HD21	1:D:498:TYR:CZ	2.56	0.41
1:F:401:THR:CG2	1:F:500:VAL:HG11	2.50	0.41
1:B:442:VAL:HG21	1:B:472:VAL:HG11	2.01	0.41
1:C:42:LEU:HD22	1:C:100:VAL:HG11	2.02	0.41
1:C:480:THR:HG22	1:C:491:HIS:CE1	2.56	0.41
1:E:296:GLY:HA3	1:E:371:ASP:HB3	2.02	0.41
1:A:335:LEU:HD11	1:A:518:PHE:CZ	2.56	0.41
1:A:432:GLY:HA2	1:A:513:LEU:HD13	2.02	0.41
1:A:480:THR:HG22	1:A:491:HIS:CD2	2.55	0.41
1:F:440:PHE:CD1	1:F:441:PRO:HD2	2.55	0.41
1:A:402:LEU:CD2	1:A:475:ALA:HB1	2.51	0.41
1:C:42:LEU:HD13	1:C:91:LEU:CD2	2.51	0.41
1:A:91:LEU:HD23	1:A:92:ALA:N	2.36	0.41
1:C:113[A]:ARG:NH2	4:C:607:GOL:O3	2.54	0.41
1:C:320:PHE:CE2	1:C:324:LEU:HD11	2.56	0.41
1:D:294:ASP:OD2	1:D:373:GLU:O	2.39	0.41
1:E:402:LEU:HD22	1:E:493:HIS:CE1	2.56	0.41
1:C:12:LEU:O	1:C:16:VAL:HG23	2.21	0.40
1:F:440:PHE:CG	1:F:441:PRO:HD2	2.56	0.40
1:F:449:HIS:CE1	1:F:473:SER:HB3	2.56	0.40
1:B:449:HIS:CE1	1:B:473:SER:HB3	2.56	0.40
1:C:417:LEU:CD2	1:C:494:VAL:HG22	2.51	0.40
1:F:212:LEU:O	1:F:220:LEU:HD22	2.21	0.40
1:A:375[A]:ARG:HG2	1:A:375[A]:ARG:H	1.44	0.40
1:C:480:THR:HG22	1:C:491:HIS:ND1	2.36	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	517/522 (99%)	505 (98%)	12 (2%)	0	100	100
1	B	520/522 (100%)	505 (97%)	15 (3%)	0	100	100
1	C	517/522 (99%)	498 (96%)	13 (2%)	6 (1%)	13	12
1	D	514/522 (98%)	501 (98%)	13 (2%)	0	100	100
1	E	514/522 (98%)	502 (98%)	12 (2%)	0	100	100
1	F	517/522 (99%)	498 (96%)	19 (4%)	0	100	100
All	All	3099/3132 (99%)	3009 (97%)	84 (3%)	6 (0%)	51	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	373[A]	GLU
1	C	373[B]	GLU
1	C	375[A]	ARG
1	C	375[B]	ARG
1	C	374[A]	GLY
1	C	374[B]	GLY

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	394/411 (96%)	386 (98%)	8 (2%)	55	67
1	B	393/411 (96%)	380 (97%)	13 (3%)	38	49
1	C	384/411 (93%)	375 (98%)	9 (2%)	50	63
1	D	386/411 (94%)	376 (97%)	10 (3%)	46	58
1	E	391/411 (95%)	384 (98%)	7 (2%)	59	71
1	F	393/411 (96%)	388 (99%)	5 (1%)	69	79
All	All	2341/2466 (95%)	2289 (98%)	52 (2%)	53	64

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	225	PHE
1	A	244	CYS
1	A	375[A]	ARG
1	A	375[B]	ARG
1	A	388	GLU
1	A	442	VAL
1	A	496	LEU
1	B	35	GLU
1	B	91	LEU
1	B	225	PHE
1	B	250	GLU
1	B	312[A]	ASP
1	B	312[B]	ASP
1	B	388	GLU
1	B	398	ASP
1	B	419	VAL
1	B	442	VAL
1	B	467	ARG
1	B	496	LEU
1	B	500	VAL
1	C	250	GLU
1	C	282	LYS
1	C	353	ASN
1	C	388	GLU
1	C	398	ASP
1	C	419	VAL
1	C	465	GLU
1	C	496	LEU
1	C	500	VAL
1	D	190[A]	GLU
1	D	190[B]	GLU
1	D	225	PHE
1	D	346	ILE
1	D	375	ARG
1	D	388	GLU
1	D	398	ASP
1	D	464	MET
1	D	496	LEU
1	D	500	VAL
1	E	91	LEU
1	E	225	PHE

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Mol	Chain	Res	Type
1	E	375[A]	ARG
1	E	375[B]	ARG
1	E	398	ASP
1	E	419	VAL
1	E	496	LEU
1	F	35	GLU
1	F	225	PHE
1	F	250	GLU
1	F	388	GLU
1	F	496	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	148	ASN
1	A	311	HIS
1	A	334	GLN
1	A	353	ASN
1	A	491	HIS
1	B	334	GLN
1	B	504	ASN
1	C	62	GLN
1	C	148	ASN
1	C	230	GLN
1	C	334	GLN
1	D	230	GLN
1	D	334	GLN
1	D	491	HIS
1	E	334	GLN
1	E	353	ASN
1	E	449	HIS
1	F	207	GLN
1	F	334	GLN
1	F	504	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 6 are unknown and 10 are monoatomic - leaving 20 for Mogul analysis.

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	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	B	601	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	B	607	-	5,5,5	0.41	0	5,5,5	0.07	0
2	SO4	E	601	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	F	601	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	602	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	A	606	-	5,5,5	0.39	0	5,5,5	0.21	0
2	SO4	D	602	-	4,4,4	0.14	0	6,6,6	0.04	0
4	GOL	C	606	-	5,5,5	0.38	0	5,5,5	0.13	0
2	SO4	F	602	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	A	605	-	5,5,5	0.41	0	5,5,5	0.20	0
4	GOL	B	605	-	5,5,5	0.37	0	5,5,5	0.27	0
2	SO4	C	602	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	601	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	B	606	-	5,5,5	0.38	0	5,5,5	0.19	0
2	SO4	A	602	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	A	604	-	5,5,5	0.37	0	5,5,5	0.28	0
2	SO4	E	602	-	4,4,4	0.13	0	6,6,6	0.06	0
4	GOL	C	607	-	5,5,5	0.35	0	5,5,5	0.28	0
2	SO4	D	601	-	4,4,4	0.14	0	6,6,6	0.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	607	-	-	0/4/4/4	-
4	GOL	B	607	-	-	4/4/4/4	-
4	GOL	A	606	-	-	0/4/4/4	-
4	GOL	C	606	-	-	2/4/4/4	-
4	GOL	A	605	-	-	0/4/4/4	-
4	GOL	B	605	-	-	0/4/4/4	-
4	GOL	B	606	-	-	0/4/4/4	-
4	GOL	A	604	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	607	GOL	C1-C2-C3-O3
4	C	606	GOL	O1-C1-C2-C3
4	B	607	GOL	O1-C1-C2-C3
4	A	604	GOL	C1-C2-C3-O3
4	B	607	GOL	O2-C2-C3-O3
4	A	604	GOL	O2-C2-C3-O3
4	C	606	GOL	O1-C1-C2-O2
4	B	607	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	GOL	1	0
4	C	607	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	517/522 (99%)	0.16	15 (2%) 51 47	35, 48, 59, 65	0
1	B	515/522 (98%)	0.20	33 (6%) 19 16	31, 43, 54, 65	0
1	C	514/522 (98%)	0.32	37 (7%) 15 11	34, 53, 62, 66	0
1	D	516/522 (98%)	0.15	27 (5%) 27 24	35, 47, 58, 65	0
1	E	515/522 (98%)	0.12	24 (4%) 31 29	30, 42, 53, 65	0
1	F	516/522 (98%)	0.01	23 (4%) 33 30	26, 37, 49, 65	0
All	All	3093/3132 (98%)	0.16	159 (5%) 28 25	26, 44, 58, 66	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	LEU	7.2
1	A	302	PRO	5.3
1	B	302	PRO	5.2
1	C	296	GLY	5.1
1	E	302	PRO	4.6
1	D	300	LEU	4.5
1	E	137	PRO	4.5
1	F	346	ILE	4.4
1	A	348	PRO	4.2
1	D	298	LEU	4.2
1	D	302	PRO	4.2
1	B	297	GLY	4.0
1	D	351	TYR	4.0
1	C	295	CYS	3.9
1	B	351	TYR	3.9
1	B	303	ALA	3.8
1	E	278	GLY	3.8
1	E	279	THR	3.8
1	D	307	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	315	GLY	3.7
1	F	288	GLY	3.5
1	E	288	GLY	3.4
1	C	316	ALA	3.4
1	B	312[A]	ASP	3.4
1	F	287	VAL	3.3
1	F	290	GLY	3.3
1	B	318	ALA	3.2
1	C	278	GLY	3.2
1	E	287	VAL	3.2
1	A	351	TYR	3.2
1	E	375[A]	ARG	3.2
1	C	288	GLY	3.1
1	C	375[A]	ARG	3.1
1	D	295	CYS	3.1
1	C	4	LEU	3.1
1	A	290	GLY	3.1
1	D	346	ILE	3.1
1	C	488	THR	3.1
1	B	319	VAL	3.1
1	C	319	VAL	3.1
1	D	246	ASP	3.1
1	C	297	GLY	3.1
1	D	297	GLY	3.0
1	E	298	LEU	3.0
1	C	305	TYR	3.0
1	E	295	CYS	3.0
1	E	315	GLY	3.0
1	E	306	MET	3.0
1	B	137	PRO	3.0
1	C	137	PRO	2.9
1	E	289	LYS	2.9
1	C	300	LEU	2.9
1	B	304	ASP	2.8
1	A	4	LEU	2.8
1	D	279	THR	2.8
1	B	143	VAL	2.8
1	F	302	PRO	2.8
1	B	316	ALA	2.8
1	B	288	GLY	2.7
1	C	279	THR	2.7
1	F	345	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	4	LEU	2.7
1	B	299	ALA	2.7
1	C	299	ALA	2.7
1	E	290	GLY	2.7
1	D	377	VAL	2.7
1	E	299	ALA	2.7
1	B	236	LEU	2.7
1	F	278	GLY	2.7
1	C	346	ILE	2.6
1	B	250	GLU	2.6
1	C	304	ASP	2.6
1	B	279	THR	2.6
1	C	290	GLY	2.6
1	D	374	GLY	2.6
1	F	298	LEU	2.6
1	A	297	GLY	2.6
1	D	315	GLY	2.6
1	F	400	ALA	2.6
1	F	378	LEU	2.6
1	C	312[A]	ASP	2.5
1	F	289	LYS	2.5
1	C	302	PRO	2.5
1	D	137	PRO	2.5
1	F	375[A]	ARG	2.5
1	C	289	LYS	2.5
1	C	246	ASP	2.5
1	F	494	VAL	2.5
1	B	296	GLY	2.5
1	E	377	VAL	2.5
1	D	278	GLY	2.5
1	B	48	VAL	2.4
1	D	36	SER	2.4
1	C	244	CYS	2.4
1	C	307	LYS	2.4
1	D	138	ASN	2.4
1	D	136	GLU	2.4
1	C	318	ALA	2.4
1	D	349	LYS	2.4
1	E	95	ALA	2.4
1	A	306	MET	2.4
1	C	351	TYR	2.4
1	D	306	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	295	CYS	2.4
1	A	378	LEU	2.4
1	B	295	CYS	2.4
1	F	300	LEU	2.4
1	D	316	ALA	2.3
1	B	350	SER	2.3
1	E	297	GLY	2.3
1	E	314	GLY	2.3
1	C	298	LEU	2.3
1	B	289	LYS	2.3
1	C	378	LEU	2.3
1	D	486	LYS	2.3
1	E	494	VAL	2.3
1	B	340	CYS	2.3
1	C	309	MET	2.3
1	A	288	GLY	2.3
1	E	340	CYS	2.3
1	E	316	ALA	2.3
1	B	136	GLU	2.3
1	B	246	ASP	2.2
1	D	345	ALA	2.2
1	F	286	LEU	2.2
1	B	399	MET	2.2
1	F	399	MET	2.2
1	C	234	LYS	2.2
1	A	374	GLY	2.2
1	D	32	ALA	2.2
1	A	279	THR	2.2
1	E	488	THR	2.2
1	B	5	PRO	2.2
1	D	296	GLY	2.2
1	F	307	LYS	2.2
1	B	467	ARG	2.2
1	F	279	THR	2.2
1	F	377	VAL	2.2
1	C	139	THR	2.2
1	B	300	LEU	2.2
1	C	37	ASN	2.1
1	F	351	TYR	2.1
1	A	287	VAL	2.1
1	F	315	GLY	2.1
1	D	247	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	278	GLY	2.1
1	B	290	GLY	2.1
1	E	378	LEU	2.1
1	A	301	LYS	2.1
1	C	337	CYS	2.1
1	B	430	ARG	2.1
1	C	486	LYS	2.1
1	B	286	LEU	2.1
1	C	247	ASP	2.0
1	B	278	GLY	2.0
1	C	317	ALA	2.0
1	F	316	ALA	2.0
1	F	305	TYR	2.0
1	D	299	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
5	UNX	B	608	1/1	0.36	0.70	30,30,30,30	0
5	UNX	C	608	1/1	0.45	0.39	30,30,30,30	0
5	UNX	F	606	1/1	0.62	0.56	30,30,30,30	0
5	UNX	D	604	1/1	0.70	0.57	30,30,30,30	0
4	GOL	B	607	6/6	0.70	0.32	73,73,73,73	0
4	GOL	A	606	6/6	0.70	0.39	59,59,59,59	0
4	GOL	A	604	6/6	0.71	0.28	72,72,72,72	0
5	UNX	E	603	1/1	0.75	0.49	30,30,30,30	0
4	GOL	C	606	6/6	0.80	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	605	6/6	0.81	0.19	82,82,82,82	0
4	GOL	A	605	6/6	0.83	0.22	68,68,68,68	0
5	UNX	A	607	1/1	0.84	0.86	30,30,30,30	0
4	GOL	C	607	6/6	0.84	0.20	61,61,62,62	0
6	NA	F	605	1/1	0.84	0.14	47,47,47,47	0
2	SO4	E	602	5/5	0.84	0.31	98,98,98,98	0
3	MN	B	603	1/1	0.85	0.06	92,92,92,92	0
3	MN	A	603	1/1	0.85	0.07	95,95,95,95	0
3	MN	F	604	1/1	0.87	0.09	99,99,99,99	0
6	NA	C	603	1/1	0.88	0.18	67,67,67,67	0
2	SO4	C	602	5/5	0.89	0.22	103,103,103,103	0
2	SO4	D	601	5/5	0.90	0.15	104,104,104,104	0
2	SO4	B	601	5/5	0.90	0.18	92,92,92,92	0
3	MN	D	603	1/1	0.91	0.04	94,94,94,94	0
4	GOL	B	606	6/6	0.92	0.24	52,52,52,52	0
2	SO4	F	602	5/5	0.92	0.23	76,76,76,76	0
2	SO4	A	602	5/5	0.93	0.22	93,93,94,94	0
2	SO4	F	601	5/5	0.94	0.15	64,64,64,64	0
3	MN	B	604	1/1	0.94	0.10	80,80,80,80	0
3	MN	C	604	1/1	0.95	0.07	82,82,82,82	0
2	SO4	D	602	5/5	0.95	0.10	68,68,68,68	0
3	MN	C	605	1/1	0.95	0.16	100,100,100,100	0
2	SO4	C	601	5/5	0.96	0.09	70,70,70,70	0
2	SO4	A	601	5/5	0.96	0.14	66,66,66,66	0
2	SO4	B	602	5/5	0.96	0.10	74,74,74,74	0
3	MN	F	603	1/1	0.98	0.26	85,85,85,85	0
2	SO4	E	601	5/5	0.98	0.08	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.