



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2016 – 06:00 PM EDT

PDB ID : 5HY7
Title : SF3B10-SF3B130 from Chaetomium thermophilum
Authors : Ponce-Salvatierra, A.; Schmitzova, J.; Pena, V.
Deposited on : 2016-02-01
Resolution : 2.90 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

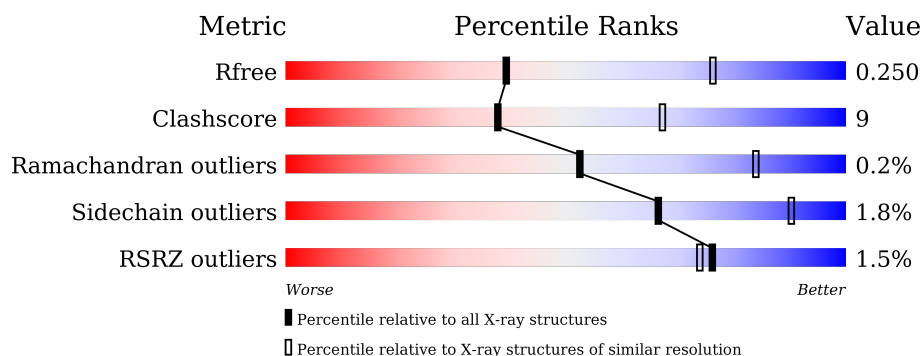
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	1213	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
1	B	1213	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div>
2	C	95	<div> <div></div> <div> <div>47%</div> <div>9%</div> <div>42%</div> </div> </div>
2	D	95	<div> <div>%</div> <div> <div></div> <div>45%</div> <div>13%</div> <div>42%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Putative pre-mRNA splicing protein.

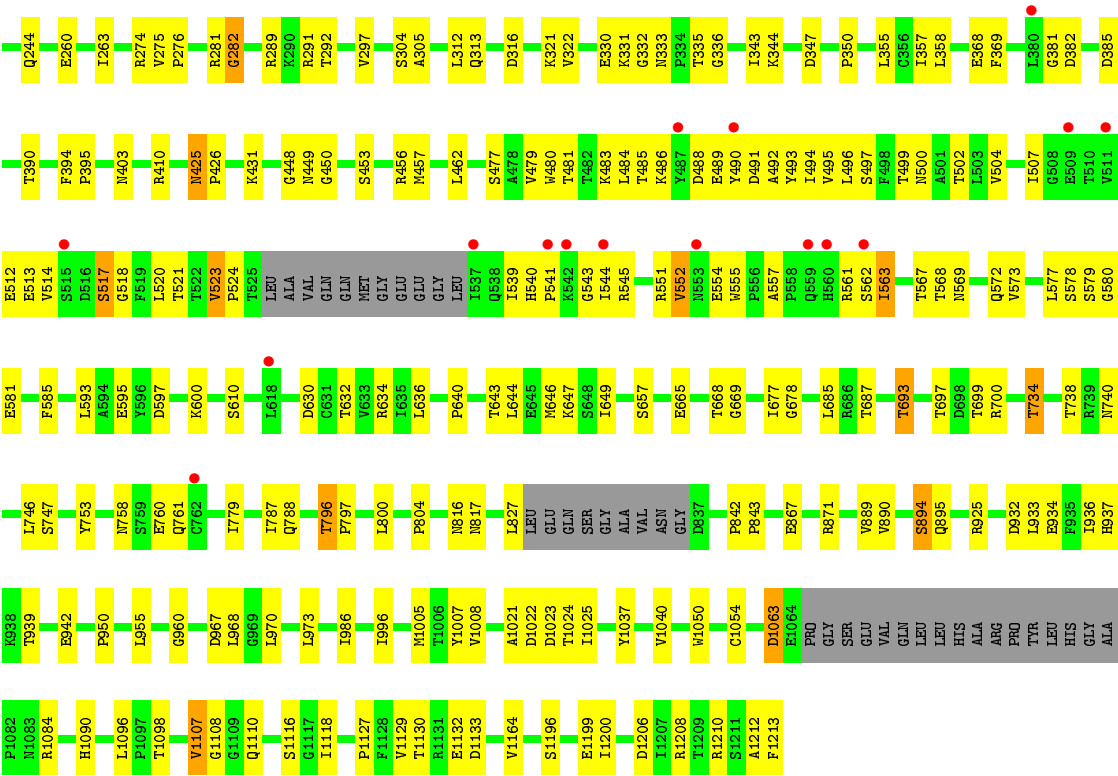
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1173	Total	C	N	O	S	0	0	0
			9164	5827	1556	1742	39			
1	B	1170	Total	C	N	O	S	0	0	0
			9149	5815	1555	1741	38			

- Molecule 2 is a protein called YSF3.

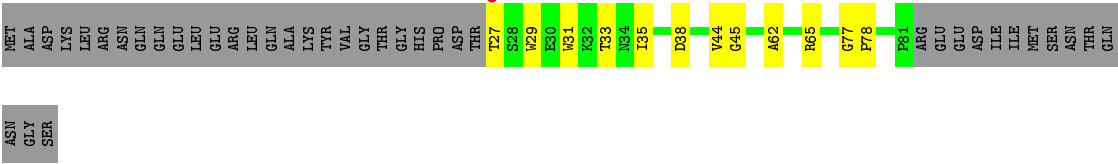
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	55	Total	C	N	O	S	0	0	0
			444	288	78	75	3			
2	C	55	Total	C	N	O	S	0	0	0
			444	288	78	75	3			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

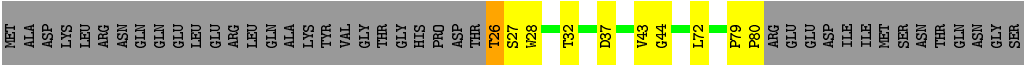
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total	Ca	0	0
			5	5		
3	A	4	Total	Ca	0	0
			4	4		



• Molecule 2: YSF3



• Molecule 2: YSF3



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	197.08Å 197.08Å 446.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.27 – 2.90 49.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-2.90) 99.7 (49.27-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.214 , 0.253 0.209 , 0.250	Depositor DCC
R_{free} test set	5675 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	97.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19210	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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:
CA

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	0.32	0/9363	0.50	0/12721
1	B	0.35	1/9347 (0.0%)	0.51	0/12698
2	C	0.34	0/460	0.42	0/629
2	D	0.30	0/460	0.39	0/629
All	All	0.33	1/19630 (0.0%)	0.50	0/26677

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	425	ASN	C-N	-5.55	1.23	1.34

There are no bond angle outliers.

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	9164	0	9131	180	0
1	B	9149	0	9110	170	0
2	C	444	0	448	7	0
2	D	444	0	448	8	0
3	A	4	0	0	0	0
3	B	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19210	0	19137	353	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 9.

All (353) 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:A:535:GLY:HA2	1:A:547:ILE:O	1.67	0.93
1:A:319:LEU:HB2	1:A:347:ASP:O	1.69	0.92
1:A:527:ALA:HB2	1:A:536:LEU:HD23	1.53	0.90
1:A:506:SER:H	1:A:511:VAL:HG21	1.38	0.87
1:B:1007:TYR:HB2	1:B:1021:ALA:HB3	1.61	0.81
1:B:122:VAL:O	1:B:145:ASN:ND2	2.14	0.80
1:B:939:THR:HG21	1:B:973:LEU:H	1.48	0.78
1:B:108:ARG:HD2	1:B:111:LEU:HB2	1.66	0.78
1:A:1007:TYR:HB2	1:A:1021:ALA:HB3	1.65	0.77
1:B:448:GLY:HA3	1:B:453:SER:HA	1.66	0.76
1:A:233:ASP:OD2	1:A:266:ARG:NH2	2.13	0.75
1:A:717:GLN:NE2	1:A:780:GLU:O	2.20	0.75
1:B:554:GLU:HB3	1:B:555:TRP:HB2	1.67	0.74
1:B:551:ARG:HB3	1:B:552:VAL:HA	1.67	0.74
1:B:687:THR:HG22	1:B:699:THR:HG22	1.70	0.74
1:A:1106:VAL:HG12	1:A:1108:GLY:H	1.54	0.72
1:B:479:VAL:HG22	1:B:496:LEU:HG	1.71	0.71
1:B:1037:TYR:OH	1:B:1063:ASP:OD2	2.07	0.71
1:A:486:LYS:HG3	1:A:530:GLN:HA	1.73	0.71
1:B:368:GLU:O	1:B:425:ASN:ND2	2.24	0.70
1:A:206:GLN:HA	1:A:207:ALA:HB3	1.73	0.69
1:A:448:GLY:HA3	1:A:453:SER:HA	1.75	0.69
1:B:481:THR:HG22	1:B:494:ILE:HG13	1.74	0.69
1:B:291:ARG:NH1	1:B:316:ASP:OD2	2.23	0.69
1:A:206:GLN:HB2	1:A:208:ALA:N	2.08	0.68
1:A:572:GLN:NE2	1:A:584:TYR:OH	2.25	0.68
1:A:530:GLN:NE2	1:A:570:GLU:OE1	2.26	0.68
1:A:1129:VAL:HG21	1:A:1210:ARG:HH22	1.57	0.67
1:B:563:ILE:HA	1:B:577:LEU:HA	1.77	0.67
1:A:729:PRO:HG2	1:A:746:LEU:HB2	1.78	0.66
1:A:808:TYR:OH	1:A:931:ARG:NH1	2.27	0.66
1:A:524:PRO:HD2	1:A:539:ILE:HB	1.76	0.65
1:A:371:ASN:OD1	1:A:456:ARG:NH2	2.28	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PHE:O	1:A:255:VAL:HA	1.96	0.65
1:A:1035:VAL:O	1:A:1102:LYS:NZ	2.28	0.65
1:B:761:GLN:OE1	1:B:761:GLN:N	2.29	0.65
1:B:490:TYR:HB2	1:B:758:ASN:HB3	1.79	0.64
1:A:49:GLN:HB2	1:A:60:ILE:HD11	1.79	0.64
1:B:554:GLU:N	1:B:554:GLU:OE1	2.30	0.64
1:B:322:VAL:HG22	1:B:343:ILE:HG12	1.79	0.64
1:B:636:LEU:HD13	1:B:646:MET:HA	1.78	0.64
1:B:544:ILE:O	1:B:555:TRP:N	2.31	0.63
1:A:122:VAL:O	1:A:145:ASN:ND2	2.31	0.63
1:A:586:GLU:OE2	1:A:620:ARG:NE	2.26	0.63
1:A:506:SER:N	1:A:511:VAL:HG21	2.12	0.63
1:B:119:VAL:HG11	2:C:44:GLY:HA3	1.81	0.63
1:A:18:PRO:HG3	1:A:1121:THR:HG23	1.81	0.63
1:A:385:ASP:OD2	1:A:410:ARG:NH1	2.29	0.63
1:B:513:GLU:HG3	1:B:514:VAL:H	1.64	0.63
1:B:1110:GLN:HG2	1:B:1127:PRO:HG2	1.81	0.62
1:B:996:ILE:HB	1:B:1008:VAL:HG22	1.79	0.62
1:A:378:GLU:HB2	1:A:379:LYS:HA	1.81	0.62
1:B:942:GLU:N	1:B:942:GLU:OE1	2.31	0.62
1:B:517:SER:OG	1:B:545:ARG:NE	2.31	0.62
1:A:717:GLN:HE21	1:A:781:LYS:HA	1.64	0.62
1:B:804:PRO:HD3	1:B:889:VAL:HG11	1.81	0.62
1:B:49:GLN:HB2	1:B:60:ILE:HD11	1.82	0.62
1:A:410:ARG:NH1	1:A:413:GLU:OE2	2.28	0.62
1:B:1206:ASP:OD2	1:B:1210:ARG:NH1	2.33	0.61
1:B:456:ARG:NH1	1:B:788:GLN:OE1	2.33	0.61
1:A:890:VAL:HG21	1:A:955:LEU:HD13	1.82	0.61
1:A:97:ILE:HA	1:A:108:ARG:HA	1.82	0.61
1:B:1096:LEU:HB3	1:B:1118:ILE:HG13	1.82	0.61
1:A:942:GLU:OE1	1:A:942:GLU:N	2.30	0.61
1:B:523:VAL:HG12	1:B:524:PRO:HD3	1.83	0.61
1:B:263:ILE:HD12	1:B:343:ILE:HD11	1.82	0.61
1:A:556:PRO:HB2	1:A:558:PRO:HB3	1.83	0.60
1:B:202:ASP:OD1	1:B:204:THR:HG22	2.00	0.60
1:B:431:LYS:NZ	1:B:800:LEU:O	2.35	0.60
1:A:310:PHE:HB2	1:A:322:VAL:HB	1.84	0.60
1:B:450:GLY:H	1:B:796:THR:HG22	1.66	0.60
1:A:524:PRO:CD	1:A:539:ILE:HB	2.32	0.60
1:B:121:ARG:NH1	2:C:37:ASP:OD1	2.31	0.60
1:A:569:ASN:HD21	1:A:614:VAL:HG22	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1022:ASP:HB3	1:B:1084:ARG:HH11	1.67	0.59
1:B:1129:VAL:HG13	1:B:1130:THR:HG23	1.84	0.59
1:B:204:THR:HG23	1:B:206:GLN:H	1.67	0.59
1:B:894:SER:HB2	1:B:895:GLN:HE21	1.67	0.59
1:A:523:VAL:HB	1:A:524:PRO:HD3	1.85	0.59
1:B:211:LEU:HD23	2:C:72:LEU:HD22	1.85	0.59
1:B:1130:THR:OG1	1:B:1133:ASP:OD2	2.20	0.58
1:A:485:THR:HG22	1:A:487:TYR:H	1.68	0.58
1:A:331:LYS:HD2	1:A:331:LYS:H	1.68	0.57
1:B:313:GLN:NE2	1:B:350:PRO:O	2.36	0.57
1:B:665:GLU:HG3	1:B:734:THR:HG21	1.86	0.57
1:B:274:ARG:HD3	1:B:395:PRO:O	2.05	0.57
1:A:804:PRO:HD3	1:A:889:VAL:HG11	1.86	0.57
1:B:1096:LEU:HD22	1:B:1118:ILE:HD11	1.86	0.57
1:B:449:ASN:HA	1:B:796:THR:HB	1.86	0.57
1:A:540:HIS:ND1	1:A:541:PRO:O	2.38	0.57
1:B:126:GLN:HG2	1:B:142:VAL:HG22	1.86	0.57
1:A:738:THR:OG1	1:A:740:ASN:OD1	2.21	0.57
1:A:524:PRO:HG3	1:A:566:ALA:HB3	1.87	0.56
1:A:544:ILE:HB	1:A:555:TRP:HB3	1.86	0.56
1:A:816:ASN:OD1	1:A:817:ASN:ND2	2.37	0.56
1:B:179:ALA:O	1:B:244:GLN:NE2	2.29	0.56
1:B:569:ASN:OD1	1:B:572:GLN:N	2.37	0.56
1:A:119:VAL:HG11	2:D:45:GLY:HA3	1.87	0.56
1:A:281:ARG:HB3	1:A:408:LYS:HD2	1.87	0.55
1:B:562:SER:O	1:B:578:SER:N	2.38	0.55
1:B:491:ASP:OD1	1:B:758:ASN:HB2	2.06	0.55
1:B:925:ARG:HB3	1:B:936:ILE:HD11	1.87	0.55
1:A:143:GLU:HB2	1:A:173:ILE:HD13	1.87	0.55
1:A:1095:ASP:OD2	1:A:1121:THR:OG1	2.18	0.55
1:B:867:GLU:OE2	1:B:871:ARG:NH1	2.39	0.55
1:B:512:GLU:N	1:B:512:GLU:OE1	2.39	0.55
1:B:561:ARG:HH11	1:B:579:SER:HB3	1.70	0.55
1:B:144:LYS:HG3	1:B:170:PRO:HA	1.88	0.55
1:A:493:TYR:HA	1:A:506:SER:HA	1.88	0.55
1:A:483:LYS:HE2	1:A:491:ASP:HB3	1.88	0.54
1:A:816:ASN:OD1	1:A:817:ASN:N	2.40	0.54
1:A:528:VAL:HG13	1:A:570:GLU:O	2.08	0.54
1:B:297:VAL:HG11	1:B:357:ILE:HG13	1.90	0.54
1:B:289:ARG:NH2	1:B:316:ASP:OD1	2.39	0.54
1:B:483:LYS:HG3	1:B:492:ALA:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:ARG:HG2	1:B:554:GLU:O	2.08	0.54
1:A:542:LYS:HA	1:A:557:ALA:HB2	1.90	0.54
1:B:746:LEU:HD21	1:B:779:ILE:HD11	1.89	0.54
1:A:486:LYS:NZ	1:A:527:ALA:HB3	2.22	0.53
1:A:534:GLU:HB3	1:A:548:VAL:HG13	1.89	0.53
1:A:122:VAL:HA	1:A:143:GLU:O	2.09	0.53
1:B:483:LYS:HD2	1:B:490:TYR:C	2.29	0.53
1:A:539:ILE:HG23	1:A:544:ILE:HG12	1.91	0.53
1:B:457:MET:O	1:B:788:GLN:HA	2.09	0.52
1:A:522:THR:HB	1:A:538:GLN:HE21	1.74	0.52
1:B:816:ASN:OD1	1:B:817:ASN:N	2.43	0.52
1:B:643:THR:HG22	1:B:644:LEU:HD12	1.91	0.52
1:A:427:LEU:HD11	1:A:445:ALA:HB1	1.91	0.52
1:A:108:ARG:HD2	1:A:111:LEU:HB2	1.92	0.51
1:A:166:GLU:OE1	1:A:168:HIS:NE2	2.43	0.51
1:B:297:VAL:CG2	1:B:355:LEU:HB2	2.41	0.51
1:B:483:LYS:HB2	1:B:491:ASP:HA	1.92	0.51
2:D:29:TRP:NE1	2:D:77:GLY:O	2.41	0.51
1:A:524:PRO:HG2	1:A:539:ILE:HD12	1.92	0.51
1:A:685:LEU:HA	1:A:700:ARG:O	2.10	0.51
1:B:481:THR:HA	1:B:493:TYR:O	2.11	0.51
1:A:294:VAL:HG13	2:D:62:ALA:HB3	1.92	0.51
1:B:523:VAL:N	1:B:539:ILE:O	2.42	0.51
1:B:573:VAL:HB	1:B:585:PHE:HB2	1.91	0.51
1:B:120:ARG:HD2	1:B:123:ILE:HD12	1.93	0.51
1:A:569:ASN:OD1	1:A:570:GLU:N	2.43	0.51
1:B:69:ILE:HA	1:B:89:THR:HG22	1.92	0.51
1:A:1129:VAL:HG21	1:A:1210:ARG:NH2	2.25	0.50
1:A:668:THR:HB	1:A:1183:ASN:HD21	1.75	0.50
1:B:1024:THR:OG1	1:B:1025:ILE:N	2.44	0.50
1:B:552:VAL:HB	1:B:554:GLU:OE1	2.12	0.50
1:B:581:GLU:HA	1:B:600:LYS:O	2.11	0.50
1:A:486:LYS:CG	1:A:530:GLN:HA	2.41	0.50
1:A:481:THR:HG22	1:A:494:ILE:HG13	1.94	0.50
1:A:754:THR:HA	1:A:767:VAL:O	2.11	0.50
1:A:254:GLY:HA2	1:A:267:HIS:HD2	1.77	0.50
1:A:516:ASP:OD1	1:A:517:SER:N	2.45	0.50
1:B:344:LYS:NZ	1:B:382:ASP:O	2.31	0.49
1:A:895:GLN:NE2	1:B:970:LEU:HB2	2.27	0.49
1:B:156:GLN:OE1	1:B:156:GLN:N	2.45	0.49
1:B:121:ARG:NE	1:B:143:GLU:OE2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:NH2	1:A:185:SER:O	2.38	0.49
1:B:932:ASP:OD1	1:B:933:LEU:N	2.41	0.49
1:A:932:ASP:OD1	1:A:933:LEU:N	2.41	0.49
1:B:369:PHE:HA	1:B:425:ASN:HD22	1.78	0.49
1:A:700:ARG:HG2	1:A:1202:ARG:HG3	1.94	0.49
1:A:999:GLY:HA2	1:A:1005:MET:HE1	1.94	0.49
1:A:483:LYS:HG2	1:A:491:ASP:HB3	1.93	0.49
1:A:154:ASN:OD1	1:A:158:GLU:N	2.41	0.49
1:B:144:LYS:HD3	1:B:145:ASN:OD1	2.12	0.49
1:B:543:GLY:HA2	1:B:557:ALA:HB2	1.95	0.49
1:B:738:THR:OG1	1:B:740:ASN:OD1	2.26	0.49
1:A:472:LEU:H	1:A:473:PRO:HA	1.77	0.48
1:A:819:LEU:HD12	1:A:820:PRO:HD2	1.94	0.48
1:A:956:LEU:HD11	1:A:996:ILE:HD13	1.95	0.48
1:B:544:ILE:H	1:B:555:TRP:HE3	1.59	0.48
1:B:925:ARG:HG2	1:B:934:GLU:HB3	1.94	0.48
1:A:1008:VAL:HA	1:A:1019:PRO:HA	1.95	0.48
1:A:14:THR:O	1:A:1208:ARG:NH2	2.46	0.48
1:A:261:GLU:OE1	1:A:402:TYR:OH	2.19	0.48
1:A:487:TYR:HE2	1:A:533:GLU:HG2	1.77	0.48
1:A:883:ALA:O	1:A:905:THR:HA	2.13	0.48
1:B:634:ARG:HG2	1:B:649:ILE:HG13	1.94	0.48
1:A:559:GLN:CD	1:A:559:GLN:H	2.15	0.48
1:B:330:GLU:N	1:B:330:GLU:OE1	2.41	0.48
1:A:936:ILE:HG21	1:B:970:LEU:HD21	1.95	0.48
1:A:207:ALA:N	1:A:210:GLN:OE1	2.47	0.48
1:A:208:ALA:C	1:A:210:GLN:H	2.16	0.48
1:A:475:THR:HG22	1:A:772:ASN:OD1	2.14	0.48
1:B:630:ASP:OD1	1:B:632:THR:OG1	2.21	0.48
1:B:281:ARG:HA	1:B:282:GLY:HA2	1.71	0.47
1:B:967:ASP:OD1	1:B:968:LEU:N	2.47	0.47
2:D:29:TRP:O	2:D:33:THR:OG1	2.26	0.47
1:B:502:THR:HB	1:B:518:GLY:O	2.14	0.47
1:B:499:THR:HA	1:B:500:ASN:HA	1.40	0.47
1:A:245:VAL:HG21	1:A:265:TYR:HE1	1.78	0.47
1:B:1063:ASP:N	1:B:1063:ASP:OD1	2.46	0.47
1:B:210:GLN:N	1:B:210:GLN:OE1	2.48	0.47
1:B:263:ILE:HD13	1:B:312:LEU:HD12	1.96	0.47
1:A:267:HIS:CG	1:A:268:SER:H	2.33	0.47
1:B:520:LEU:HG	1:B:521:THR:H	1.79	0.47
1:A:318:ASP:OD1	1:A:348:THR:OG1	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LYS:HG2	1:A:390:THR:HG22	1.96	0.46
1:A:478:ALA:HB3	1:A:497:SER:HB3	1.97	0.46
1:A:630:ASP:OD1	1:A:632:THR:OG1	2.24	0.46
1:A:494:ILE:HD11	1:A:757:PHE:HE2	1.80	0.46
1:A:28:GLN:NE2	1:A:76:ARG:HH12	2.13	0.46
2:D:31:TRP:O	2:D:35:ILE:HG12	2.15	0.46
1:A:66:PHE:HB2	1:A:1150:PRO:HB3	1.98	0.46
1:B:489:GLU:HA	1:B:490:TYR:HA	1.59	0.46
1:B:520:LEU:HG	1:B:521:THR:N	2.30	0.46
1:B:490:TYR:CB	1:B:758:ASN:HB3	2.45	0.46
1:A:180:LEU:HD11	1:A:217:TYR:CZ	2.50	0.46
1:A:477:SER:N	1:A:497:SER:O	2.35	0.46
1:A:496:LEU:HD21	1:A:774:LEU:HD12	1.98	0.46
1:A:339:LYS:HG3	1:A:340:ARG:HG3	1.98	0.46
1:B:331:LYS:O	1:B:333:ASN:N	2.44	0.46
1:B:685:LEU:HA	1:B:700:ARG:O	2.15	0.46
1:A:320:PHE:CD1	1:A:345:TYR:HA	2.51	0.46
1:A:666:ASP:OD2	1:A:668:THR:OG1	2.34	0.45
1:B:1212:ALA:O	1:B:1213:PHE:HB2	2.15	0.45
1:B:585:PHE:HD2	1:B:593:LEU:HB3	1.80	0.45
1:A:297:VAL:CG2	1:A:355:LEU:HB2	2.46	0.45
1:A:486:LYS:HZ1	1:A:527:ALA:HB3	1.79	0.45
1:A:502:THR:OG1	1:A:520:LEU:O	2.23	0.45
1:A:264:THR:HG22	1:A:266:ARG:HB2	1.97	0.45
1:B:567:THR:HG21	1:B:610:SER:HA	1.99	0.45
1:A:181:ASP:O	1:A:247:GLY:HA3	2.16	0.45
1:A:487:TYR:CE2	1:A:533:GLU:HG2	2.52	0.45
1:A:905:THR:OG1	1:A:920:ALA:HB3	2.16	0.45
1:B:1090:HIS:CD2	1:B:1164:VAL:HB	2.52	0.45
1:A:967:ASP:OD1	1:A:968:LEU:N	2.50	0.45
1:A:592:SER:OG	1:A:592:SER:O	2.32	0.45
1:B:960:GLY:O	1:B:986:ILE:HG12	2.17	0.45
1:A:723:LEU:HD23	1:A:754:THR:HG21	1.98	0.44
1:B:747:SER:HB2	1:B:787:ILE:HD12	1.98	0.44
1:B:477:SER:OG	1:B:497:SER:O	2.25	0.44
1:B:890:VAL:HG22	1:B:950:PRO:HG3	1.99	0.44
1:A:527:ALA:HA	1:A:536:LEU:HA	1.99	0.44
1:A:748:TYR:OH	1:A:775:ARG:HD3	2.18	0.44
1:B:385:ASP:OD2	1:B:410:ARG:NH2	2.50	0.44
1:A:16:GLN:HB2	1:A:1122:VAL:HB	1.98	0.44
1:B:1107:VAL:HG23	1:B:1108:GLY:H	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:ARG:HD2	1:B:551:ARG:HA	1.89	0.44
2:C:26:THR:HG22	2:C:27:SER:H	1.82	0.44
1:B:275:VAL:HG11	1:B:343:ILE:HG13	2.00	0.44
2:D:44:VAL:HG13	2:D:65:ARG:HG3	1.98	0.44
1:A:484:LEU:HD11	1:A:493:TYR:HE1	1.83	0.44
1:B:1196:SER:OG	1:B:1199:GLU:HB2	2.18	0.44
1:B:500:ASN:O	1:B:521:THR:N	2.51	0.44
1:B:541:PRO:HD2	1:B:543:GLY:O	2.18	0.43
1:A:25:LEU:HB3	1:A:38:ILE:HG22	2.00	0.43
1:A:483:LYS:HG2	1:A:491:ASP:CB	2.48	0.43
1:A:652:LEU:HD13	1:A:679:LEU:HD21	2.00	0.43
1:B:151:LEU:HD23	1:B:161:ILE:CD1	2.48	0.43
1:B:321:LYS:HZ1	1:B:381:GLY:H	1.64	0.43
1:B:585:PHE:HB3	1:B:593:LEU:HG	2.00	0.43
1:B:936:ILE:HG22	1:B:937:HIS:ND1	2.33	0.43
1:A:690:ASP:O	1:A:691:GLU:HB2	2.18	0.43
1:A:1103:THR:OG1	1:A:1104:ASN:N	2.52	0.43
1:A:327:VAL:O	1:A:335:THR:HG22	2.19	0.43
1:A:475:THR:OG1	1:A:475:THR:O	2.32	0.43
1:A:798:LYS:HB2	1:A:812:ILE:HG13	2.01	0.43
1:A:882:GLU:HG2	1:A:905:THR:HB	2.01	0.43
1:B:577:LEU:HD11	1:B:581:GLU:N	2.34	0.43
1:A:546:HIS:HB3	1:A:553:ASN:O	2.19	0.43
1:A:558:PRO:HD2	1:A:559:GLN:NE2	2.33	0.43
1:A:572:GLN:NE2	1:A:620:ARG:HB2	2.33	0.43
1:B:540:HIS:ND1	1:B:543:GLY:O	2.51	0.43
1:A:1179:THR:HG22	1:A:1201:GLU:OE1	2.19	0.43
1:A:171:GLY:HA2	1:A:196:TYR:CE2	2.53	0.43
1:B:894:SER:OG	1:B:967:ASP:OD1	2.27	0.43
1:A:642:SER:HB2	1:A:645:GLU:OE1	2.19	0.43
1:A:960:GLY:O	1:A:986:ILE:HG12	2.19	0.43
1:B:304:SER:HA	1:B:305:ALA:HA	1.84	0.43
1:B:1005:MET:HE3	1:B:1050:TRP:HH2	1.83	0.43
1:B:13:LEU:HD22	1:B:1208:ARG:NH1	2.33	0.43
1:B:26:LEU:HD11	1:B:358:LEU:HD12	2.00	0.43
1:B:485:THR:HG22	1:B:486:LYS:HG3	2.00	0.43
1:B:677:ILE:HB	1:B:685:LEU:HB2	2.00	0.43
1:A:949:CYS:O	1:A:956:LEU:HB2	2.19	0.42
1:A:203:PRO:O	2:D:78:PRO:HB2	2.19	0.42
1:A:206:GLN:HB2	1:A:207:ALA:C	2.40	0.42
1:A:491:ASP:N	1:A:491:ASP:OD1	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ILE:HD11	1:A:277:ILE:HD11	2.02	0.42
1:B:1132:GLU:N	1:B:1132:GLU:OE1	2.39	0.42
1:B:369:PHE:HB3	1:B:426:PRO:HG3	2.02	0.42
1:B:595:GLU:HB3	1:B:597:ASP:OD1	2.20	0.42
1:A:1184:ASP:OD1	1:A:1185:LYS:N	2.52	0.42
1:A:144:LYS:HG2	1:A:170:PRO:HA	2.01	0.42
1:A:241:LEU:HA	1:A:241:LEU:HD23	1.87	0.42
1:B:480:TRP:HE3	1:B:495:VAL:HG23	1.85	0.42
1:A:1132:GLU:N	1:A:1132:GLU:OE1	2.47	0.42
1:A:93:ARG:HG2	1:A:113:THR:HA	2.01	0.42
1:A:322:VAL:HA	1:A:342:LYS:O	2.20	0.42
1:B:453:SER:HB3	1:B:797:PRO:HD3	2.02	0.42
1:B:480:TRP:HB2	1:B:495:VAL:HG22	2.01	0.42
1:B:462:LEU:N	1:B:787:ILE:HD11	2.35	0.42
1:B:335:THR:OG1	1:B:336:GLY:N	2.52	0.42
1:A:279:ARG:HE	1:A:404:PRO:HB3	1.84	0.42
1:A:275:VAL:HG11	1:A:343:ILE:HG13	2.02	0.42
1:A:341:VAL:O	1:A:390:THR:HA	2.18	0.42
1:A:970:LEU:HB2	1:B:895:GLN:OE1	2.19	0.42
1:B:260:GLU:HA	1:B:292:THR:HG22	2.02	0.42
1:B:126:GLN:NE2	2:C:43:VAL:HG12	2.34	0.42
1:A:861:ILE:HD11	1:A:933:LEU:HG	2.01	0.42
1:B:31:GLY:O	1:B:81:HIS:ND1	2.46	0.42
1:B:483:LYS:HG2	1:B:484:LEU:H	1.85	0.42
1:B:539:ILE:HG22	1:B:540:HIS:HB2	2.02	0.42
1:B:541:PRO:HG3	1:B:545:ARG:HG3	2.01	0.42
1:B:640:PRO:O	1:B:643:THR:OG1	2.38	0.42
1:A:179:ALA:O	1:A:244:GLN:NE2	2.49	0.41
1:B:657:SER:N	1:B:678:GLY:O	2.49	0.41
1:B:842:PRO:HA	1:B:843:PRO:HD3	1.91	0.41
1:A:446:ILE:HD13	1:A:800:LEU:HB2	2.01	0.41
1:A:818:THR:HG22	1:A:850:LYS:HD3	2.02	0.41
2:C:28:TRP:O	2:C:32:THR:OG1	2.27	0.41
1:A:585:PHE:CE2	1:A:595:GLU:HB2	2.55	0.41
1:A:378:GLU:CB	1:A:379:LYS:HA	2.49	0.41
1:B:1098:THR:HG1	1:B:1116:SER:HG	1.68	0.41
1:B:25:LEU:HD12	1:B:25:LEU:HA	1.91	0.41
1:A:254:GLY:HA2	1:A:267:HIS:CD2	2.54	0.41
1:A:297:VAL:HG11	1:A:357:ILE:HG13	2.03	0.41
1:A:374:PHE:O	1:A:418:VAL:HG22	2.20	0.41
1:B:577:LEU:HD12	1:B:580:GLY:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:THR:OG1	1:B:669:GLY:N	2.53	0.41
1:A:21:ILE:HG23	1:A:39:THR:HB	2.02	0.41
1:B:276:PRO:HG3	1:B:394:PHE:CE1	2.56	0.41
1:B:483:LYS:NZ	1:B:491:ASP:O	2.53	0.41
1:A:970:LEU:HD21	1:B:936:ILE:HG21	2.01	0.41
1:A:1081:ALA:N	1:A:1082:PRO:HD3	2.35	0.41
1:A:486:LYS:HG3	1:A:529:GLN:O	2.21	0.41
1:B:1196:SER:O	1:B:1200:ILE:HG12	2.20	0.41
1:A:143:GLU:HA	1:A:144:LYS:HA	1.83	0.41
1:A:173:ILE:O	1:A:193:GLU:HA	2.21	0.41
1:A:526:LEU:HD23	1:A:527:ALA:N	2.36	0.41
1:B:1022:ASP:OD1	1:B:1023:ASP:N	2.51	0.41
1:B:492:ALA:HA	1:B:507:ILE:HG13	2.02	0.41
1:A:1138:GLN:HA	1:A:1170:ILE:HD12	2.03	0.41
1:A:154:ASN:HB3	1:A:160:THR:CG2	2.51	0.41
1:A:274:ARG:HG2	1:A:395:PRO:O	2.21	0.41
1:A:299:HIS:HB2	1:A:357:ILE:HD12	2.03	0.41
1:B:540:HIS:CE1	1:B:563:ILE:HG12	2.55	0.41
1:B:939:THR:HG21	1:B:973:LEU:N	2.26	0.41
1:A:121:ARG:HD3	2:D:38:ASP:OD1	2.22	0.40
1:A:679:LEU:HD12	1:A:683:VAL:HB	2.04	0.40
1:B:1007:TYR:CE2	1:B:1054:CYS:HB2	2.56	0.40
1:A:400:ALA:HA	1:A:401:PRO:HD3	1.98	0.40
1:A:620:ARG:NH1	1:A:640:PRO:HD3	2.37	0.40
1:B:1007:TYR:OH	1:B:1040:VAL:HG12	2.21	0.40
1:B:647:LYS:HE3	1:B:693:THR:O	2.21	0.40
1:B:760:GLU:O	1:B:760:GLU:HG3	2.21	0.40
1:A:539:ILE:HG12	1:A:544:ILE:HG12	2.01	0.40
1:B:504:VAL:O	1:B:512:GLU:HB3	2.22	0.40
1:B:540:HIS:CG	1:B:563:ILE:HG12	2.56	0.40
1:A:561:ARG:HG2	1:A:579:SER:HB3	2.04	0.40
1:B:890:VAL:HG21	1:B:955:LEU:HD13	2.03	0.40
2:C:79:PRO:HA	2:C:80:PRO:HD3	1.93	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	1167/1213 (96%)	1101 (94%)	63 (5%)	3 (0%)	46	79
1	B	1162/1213 (96%)	1082 (93%)	77 (7%)	3 (0%)	46	79
2	C	53/95 (56%)	53 (100%)	0	0	100	100
2	D	53/95 (56%)	52 (98%)	1 (2%)	0	100	100
All	All	2435/2616 (93%)	2288 (94%)	141 (6%)	6 (0%)	52	84

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	PRO
1	A	570	GLU
1	B	332	GLY
1	B	144	LYS
1	A	472	LEU
1	B	282	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	1010/1041 (97%)	991 (98%)	19 (2%)	65	89
1	B	1009/1041 (97%)	991 (98%)	18 (2%)	66	90
2	C	50/85 (59%)	49 (98%)	1 (2%)	63	88
2	D	50/85 (59%)	49 (98%)	1 (2%)	63	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2119/2252 (94%)	2080 (98%)	39 (2%)	66 90

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LYS
1	A	206	GLN
1	A	210	GLN
1	A	393	ASP
1	A	475	THR
1	A	479	VAL
1	A	587	MET
1	A	653	THR
1	A	692	ILE
1	A	718	ASN
1	A	753	TYR
1	A	782	LEU
1	A	784	GLN
1	A	866	SER
1	A	939	THR
1	A	986	ILE
1	A	1039	SER
1	A	1121	THR
1	A	1135	ASP
2	D	27	THR
1	B	347	ASP
1	B	390	THR
1	B	403	ASN
1	B	488	ASP
1	B	517	SER
1	B	523	VAL
1	B	552	VAL
1	B	563	ILE
1	B	568	THR
1	B	693	THR
1	B	697	THR
1	B	734	THR
1	B	753	TYR
1	B	796	THR
1	B	827	LEU
1	B	894	SER
1	B	1063	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1107	VAL
2	C	26	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	530	GLN
1	A	572	GLN
1	A	717	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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 ⓘ

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	1173/1213 (96%)	-0.16	20 (1%) 73 70	50, 88, 145, 190	0
1	B	1170/1213 (96%)	-0.18	16 (1%) 78 76	48, 82, 155, 207	0
2	C	55/95 (57%)	-0.02	0 100 100	53, 68, 99, 124	0
2	D	55/95 (57%)	-0.09	1 (1%) 71 68	63, 85, 111, 125	0
All	All	2453/2616 (93%)	-0.16	37 (1%) 76 74	48, 84, 150, 207	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	487	TYR	6.8
1	A	531	MET	6.6
1	B	762	CYS	6.3
1	A	473	PRO	5.8
1	A	530	GLN	5.4
1	A	493	TYR	4.5
1	A	381	GLY	4.3
1	A	529	GLN	4.1
1	B	541	PRO	3.9
1	A	558	PRO	3.9
1	A	380	LEU	3.8
1	B	511	VAL	3.6
1	B	542	LYS	3.5
1	B	380	LEU	3.3
1	B	490	TYR	3.3
1	B	544	ILE	3.1
1	A	533	GLU	3.0
1	B	553	ASN	3.0
1	B	537	ILE	2.9
1	B	560	HIS	2.8
1	A	536	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	211	LEU	2.6
1	A	474	GLY	2.6
1	A	534	GLU	2.5
2	D	27	THR	2.4
1	A	303	GLY	2.4
1	B	515	SER	2.3
1	B	559	GLN	2.3
1	B	509	GLU	2.3
1	A	306	GLY	2.3
1	B	618	LEU	2.2
1	A	7	ASN	2.2
1	A	528	VAL	2.2
1	B	562	SER	2.2
1	A	22	THR	2.1
1	A	592	SER	2.1
1	A	354	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CA	A	1301	1/1	0.95	0.12	-	88,88,88,88	0
3	CA	A	1302	1/1	0.95	0.10	-	134,134,134,134	0
3	CA	B	1303	1/1	0.94	0.15	-	123,123,123,123	0
3	CA	B	1304	1/1	0.24	0.99	-	313,313,313,313	0
3	CA	A	1304	1/1	0.92	0.51	-	138,138,138,138	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	B	1302	1/1	0.77	0.34	-	124,124,124,124	0
3	CA	B	1305	1/1	0.92	0.55	-	140,140,140,140	0
3	CA	A	1303	1/1	0.70	0.50	-	191,191,191,191	0
3	CA	B	1301	1/1	0.97	0.13	-	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.