



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:28 am GMT

PDB ID : 1U1J
Title : A. thaliana cobalamine independent methionine synthase
Authors : Ferrer, J.-L.; Ravanel, S.; Robert, M.; Dumas, R.
Deposited on : 2004-07-15
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

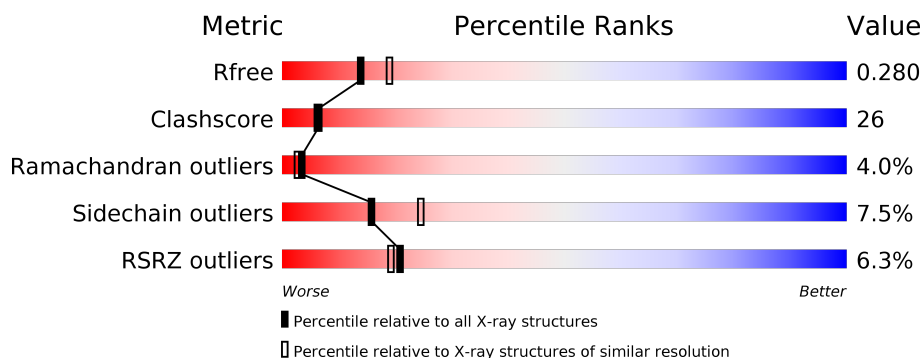
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	765	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	768	-	-	-	X
3	SO4	A	769	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	770	-	-	-	X
4	MET	A	772	-	-	-	X
5	C2F	A	773	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6130 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 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	746	Total	C	N	O	S	Se	0	0	0
			5783	3686	974	1099	6	18			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	11	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	49	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	74	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	97	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	107	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	109	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	212	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	351	MSE	LEU	MODIFIED RESIDUE	UNP O50008
A	496	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	538	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	545	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	549	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	554	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	557	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	648	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	663	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	718	MSE	MET	MODIFIED RESIDUE	UNP O50008
A	750	MSE	MET	MODIFIED RESIDUE	UNP O50008

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

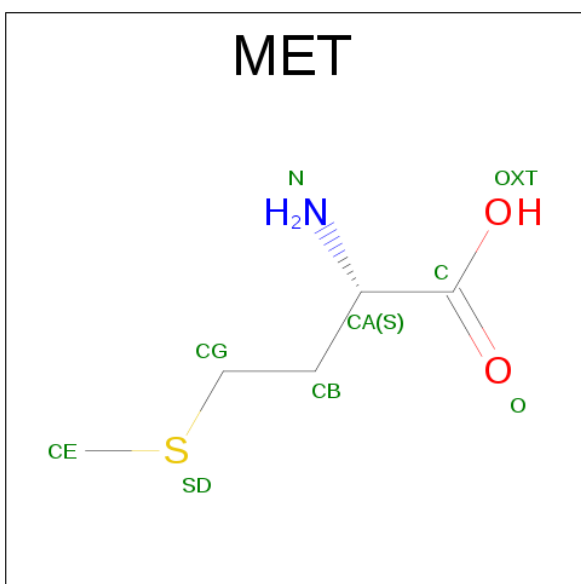
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



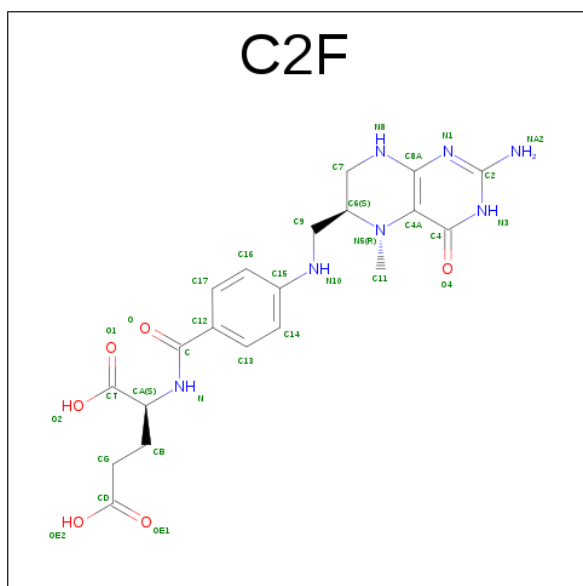
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 5 is 5-METHYL-5,6,7,8-TETRAHYDROFOLIC ACID (three-letter code: C2F) (formula: $C_{20}H_{25}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			33	20	7	6		

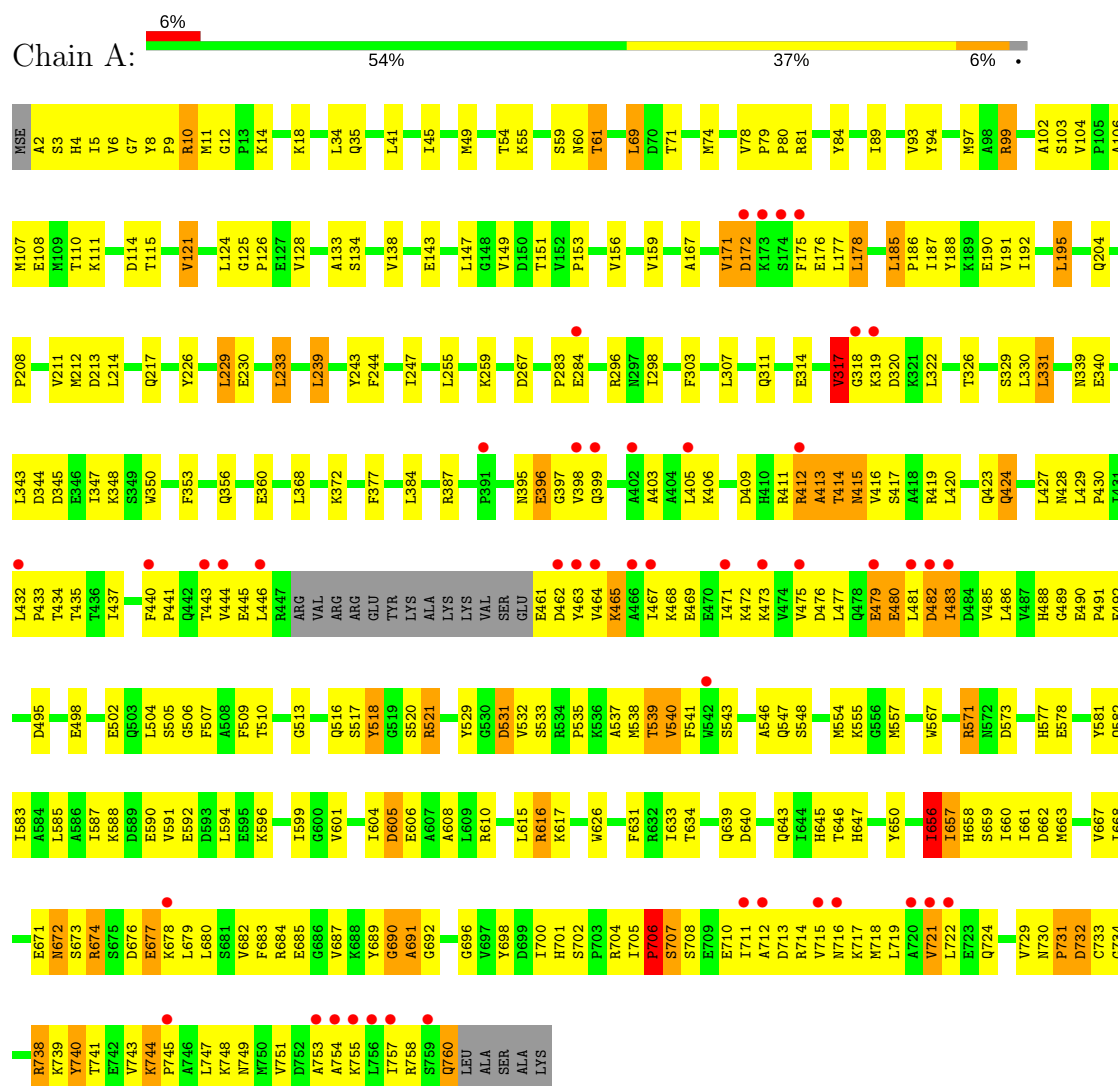
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	283	Total	O	0	0
			283	283		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	123.47Å 123.47Å 132.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.63 – 2.40 41.63 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.63-2.40) 99.4 (41.63-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.275 0.217 , 0.280	Depositor DCC
R_{free} test set	4120 reflections (9.25%)	DCC
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6130	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: ZN, C2F, SO4

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	0.37	0/5884	0.62	1/7949 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	GLY	N-CA-C	-5.19	100.13	113.10

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	5783	0	5793	309	0
2	A	2	0	0	0	0
3	A	20	0	0	0	0
4	A	9	0	8	0	0
5	A	33	0	22	2	0
6	A	283	0	0	6	0
All	All	6130	0	5823	309	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 26.

All (309) 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:477:LEU:HB3	1:A:486:LEU:HD22	1.44	0.99
1:A:212:MSE:HE1	1:A:615:LEU:HB3	1.46	0.97
1:A:677:GLU:HG3	1:A:717:LYS:HB3	1.49	0.95
1:A:211:VAL:HG23	1:A:212:MSE:HE3	1.52	0.89
1:A:546:ALA:HB3	1:A:554:MSE:HE2	1.54	0.88
1:A:531:ASP:HA	1:A:582:GLN:HE22	1.43	0.84
1:A:481:LEU:HD22	1:A:751:VAL:HB	1.60	0.83
1:A:7:GLY:HA2	1:A:61:THR:HG21	1.59	0.83
1:A:477:LEU:HD13	1:A:486:LEU:HB3	1.60	0.82
1:A:738:ARG:NE	1:A:738:ARG:HA	1.94	0.81
1:A:111:LYS:HE2	1:A:115:THR:O	1.81	0.81
1:A:751:VAL:HG12	1:A:755:LYS:HE3	1.61	0.80
1:A:546:ALA:CB	1:A:554:MSE:HE2	2.12	0.80
1:A:124:LEU:O	1:A:167:ALA:HA	1.83	0.79
1:A:738:ARG:HE	1:A:738:ARG:HA	1.48	0.79
1:A:427:LEU:HB3	1:A:429:LEU:HD11	1.64	0.78
1:A:468:LYS:O	1:A:472:LYS:HG2	1.84	0.78
1:A:5:ILE:HB	1:A:49:MSE:HE1	1.66	0.77
1:A:444:VAL:HG23	1:A:445:GLU:H	1.48	0.77
1:A:473:LYS:HD3	1:A:489:GLY:HA3	1.65	0.77
1:A:677:GLU:HG3	1:A:717:LYS:CB	2.15	0.77
1:A:667:VAL:HG22	1:A:692:GLY:HA3	1.68	0.76
1:A:510:THR:CG2	1:A:513:GLY:H	2.00	0.75
1:A:748:LYS:NZ	1:A:748:LYS:HB2	2.00	0.75
1:A:510:THR:HG22	1:A:513:GLY:H	1.53	0.74
1:A:714:ARG:NH1	1:A:714:ARG:HB3	2.03	0.74
1:A:212:MSE:HE2	1:A:212:MSE:HA	1.68	0.74
1:A:557:MSE:HE1	1:A:605:ASP:OD2	1.87	0.74
1:A:702:SER:OG	1:A:704:ARG:HG2	1.89	0.73
1:A:398:VAL:HG22	1:A:531:ASP:OD2	1.88	0.73
1:A:498:GLU:O	1:A:502:GLU:HG3	1.89	0.72
1:A:533:SER:O	1:A:535:PRO:HD3	1.89	0.71
1:A:481:LEU:HD11	1:A:748:LYS:HG3	1.73	0.71
1:A:656:ILE:HG12	1:A:656:ILE:O	1.91	0.71
1:A:419:ARG:O	1:A:423:GLN:HG3	1.91	0.70
1:A:444:VAL:HG23	1:A:445:GLU:N	2.05	0.70
1:A:343:LEU:O	1:A:348:LYS:HD2	1.92	0.70
1:A:719:LEU:HD22	1:A:724:GLN:HB2	1.75	0.69
1:A:398:VAL:CG2	1:A:531:ASP:OD2	2.39	0.69
1:A:631:PHE:O	1:A:634:THR:HB	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLN:HE21	1:A:35:GLN:HA	1.56	0.69
1:A:495:ASP:HB3	1:A:498:GLU:HB2	1.75	0.69
1:A:714:ARG:HH11	1:A:714:ARG:HB3	1.59	0.68
1:A:504:LEU:HB3	1:A:532:VAL:HG13	1.76	0.68
1:A:744:LYS:HB3	1:A:745:PRO:HD3	1.75	0.68
1:A:307:LEU:O	1:A:311:GLN:HG3	1.95	0.67
1:A:81:ARG:HD2	1:A:104:VAL:HG13	1.77	0.67
1:A:340:GLU:O	1:A:348:LYS:HE3	1.96	0.66
1:A:538:MSE:HE3	1:A:590:GLU:HG3	1.78	0.66
1:A:395:ASN:O	1:A:398:VAL:HG23	1.96	0.66
1:A:143:GLU:O	1:A:147:LEU:HD13	1.95	0.66
1:A:208:PRO:O	1:A:211:VAL:HG22	1.96	0.66
1:A:713:ASP:OD2	1:A:717:LYS:HE3	1.95	0.65
1:A:213:ASP:HB2	1:A:617:LYS:NZ	2.10	0.65
1:A:464:VAL:O	1:A:468:LYS:HG3	1.97	0.65
1:A:604:ILE:HD13	1:A:634:THR:HG21	1.78	0.65
1:A:188:TYR:O	1:A:192:ILE:HG13	1.97	0.65
1:A:684:ARG:HG2	1:A:684:ARG:HH11	1.61	0.64
1:A:672:ASN:O	1:A:674:ARG:N	2.31	0.64
1:A:59:SER:HB2	1:A:151:THR:HB	1.79	0.64
1:A:708:SER:HA	1:A:749:ASN:HB3	1.80	0.63
1:A:661:ILE:CD1	1:A:687:VAL:HG13	2.28	0.63
1:A:41:LEU:O	1:A:45:ILE:HG12	1.99	0.63
1:A:211:VAL:HG23	1:A:212:MSE:CE	2.27	0.63
1:A:398:VAL:HG12	1:A:398:VAL:O	1.99	0.62
1:A:14:LYS:HE2	1:A:339:ASN:ND2	2.14	0.62
1:A:744:LYS:HB3	1:A:745:PRO:CD	2.29	0.62
1:A:698:TYR:O	1:A:732:ASP:HB2	2.01	0.61
1:A:661:ILE:HD11	1:A:687:VAL:HG13	1.83	0.61
1:A:481:LEU:HD21	1:A:748:LYS:HG3	1.83	0.60
1:A:356:GLN:O	1:A:360:GLU:HG3	2.02	0.60
1:A:471:ILE:O	1:A:475:VAL:HB	2.02	0.60
1:A:657:ILE:HD11	1:A:683:PHE:CE1	2.37	0.60
1:A:350:TRP:CZ2	1:A:387:ARG:HA	2.37	0.59
1:A:318:GLY:C	1:A:320:ASP:H	2.06	0.59
1:A:340:GLU:CD	1:A:510:THR:HG23	2.22	0.59
1:A:498:GLU:HG2	1:A:509:PHE:HE2	1.68	0.59
1:A:708:SER:CA	1:A:749:ASN:HB3	2.32	0.59
1:A:479:GLU:O	1:A:481:LEU:N	2.36	0.58
1:A:405:LEU:N	1:A:405:LEU:HD22	2.18	0.58
1:A:226:TYR:O	1:A:259:LYS:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:LEU:O	1:A:751:VAL:HG23	2.03	0.58
1:A:740:TYR:HA	1:A:743:VAL:HG22	1.84	0.58
1:A:230:GLU:N	6:A:848:HOH:O	2.37	0.57
1:A:469:GLU:OE2	1:A:473:LYS:HE3	2.04	0.57
1:A:212:MSE:HE1	1:A:615:LEU:CB	2.29	0.57
1:A:212:MSE:HE1	1:A:615:LEU:HD13	1.86	0.57
1:A:6:VAL:HG13	1:A:326:THR:OG1	2.05	0.57
1:A:395:ASN:OD1	1:A:396:GLU:N	2.38	0.57
1:A:444:VAL:CG2	1:A:445:GLU:H	2.17	0.57
1:A:588:LYS:HD2	1:A:633:ILE:O	2.05	0.56
1:A:10:ARG:NE	1:A:516:GLN:HE22	2.03	0.56
1:A:751:VAL:O	1:A:755:LYS:HG3	2.04	0.56
1:A:395:ASN:O	1:A:398:VAL:CG2	2.53	0.56
1:A:59:SER:HB2	1:A:151:THR:CB	2.35	0.56
1:A:468:LYS:NZ	1:A:468:LYS:HB3	2.20	0.56
1:A:8:TYR:CE2	1:A:45:ILE:HD12	2.40	0.56
1:A:571:ARG:HG3	1:A:573:ASP:OD1	2.05	0.56
1:A:110:THR:HG22	1:A:121:VAL:HG12	1.87	0.56
1:A:99:ARG:C	1:A:106:ALA:HB2	2.26	0.56
1:A:413:ALA:O	1:A:414:THR:C	2.45	0.55
1:A:659:SER:O	1:A:663:MSE:HG3	2.06	0.55
1:A:35:GLN:NE2	1:A:35:GLN:HA	2.22	0.55
1:A:677:GLU:N	1:A:677:GLU:OE1	2.40	0.55
1:A:729:VAL:HA	6:A:782:HOH:O	2.06	0.55
1:A:10:ARG:HE	1:A:516:GLN:HE22	1.55	0.55
1:A:440:PHE:HB2	1:A:473:LYS:HE2	1.89	0.54
1:A:748:LYS:HB2	1:A:748:LYS:HZ3	1.71	0.54
1:A:18:LYS:NZ	1:A:521:ARG:HH21	2.04	0.54
1:A:477:LEU:CD1	1:A:486:LEU:HB3	2.35	0.54
1:A:606:GLU:HA	1:A:606:GLU:OE1	2.07	0.54
1:A:481:LEU:CD2	1:A:751:VAL:HB	2.36	0.53
1:A:430:PRO:HG2	1:A:758:ARG:NH2	2.24	0.53
1:A:114:ASP:OD1	1:A:296:ARG:NH2	2.41	0.53
1:A:138:VAL:HG12	6:A:970:HOH:O	2.09	0.53
1:A:605:ASP:HB3	1:A:647:HIS:HB3	1.90	0.53
1:A:684:ARG:HG2	1:A:684:ARG:NH1	2.23	0.53
1:A:684:ARG:HD2	1:A:721:VAL:HG12	1.91	0.53
1:A:424:GLN:OE1	1:A:429:LEU:N	2.35	0.53
1:A:661:ILE:HG12	1:A:689:TYR:HD1	1.74	0.53
1:A:186:PRO:O	1:A:190:GLU:HG3	2.09	0.52
1:A:424:GLN:OE1	1:A:428:ASN:HA	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:PHE:O	1:A:529:TYR:HE2	1.92	0.52
1:A:340:GLU:OE1	1:A:510:THR:HG23	2.09	0.52
1:A:537:ALA:HB1	1:A:540:VAL:HG21	1.91	0.52
1:A:69:LEU:HD13	1:A:94:TYR:CE1	2.45	0.52
1:A:661:ILE:HD11	1:A:687:VAL:CG1	2.39	0.52
1:A:477:LEU:HD13	1:A:486:LEU:CB	2.37	0.52
1:A:646:THR:HG22	1:A:668:ILE:HG22	1.91	0.52
1:A:187:ILE:O	1:A:191:VAL:HG23	2.10	0.52
1:A:476:ASP:O	1:A:480:GLU:N	2.42	0.52
1:A:211:VAL:CG2	1:A:212:MSE:HE3	2.35	0.52
1:A:521:ARG:NH2	5:A:773:C2F:HB1	2.24	0.52
1:A:3:SER:OG	1:A:54:THR:HA	2.11	0.51
1:A:243:TYR:HA	1:A:267:ASP:HB2	1.91	0.51
1:A:243:TYR:O	1:A:244:PHE:HB2	2.10	0.51
1:A:298:ILE:HG13	1:A:353:PHE:CE1	2.45	0.51
1:A:427:LEU:O	1:A:428:ASN:HB3	2.09	0.51
1:A:2:ALA:HB1	1:A:55:LYS:CB	2.40	0.51
1:A:464:VAL:HG13	1:A:465:LYS:HE3	1.92	0.51
1:A:463:TYR:O	1:A:467:ILE:HG13	2.10	0.51
1:A:480:GLU:O	1:A:482:ASP:N	2.42	0.51
1:A:504:LEU:HB3	1:A:532:VAL:CG1	2.41	0.51
1:A:577:HIS:HB3	1:A:626:TRP:CD2	2.46	0.51
1:A:661:ILE:HG12	1:A:689:TYR:CD1	2.44	0.51
1:A:212:MSE:CE	1:A:615:LEU:HD13	2.41	0.51
1:A:395:ASN:O	1:A:398:VAL:HB	2.11	0.50
1:A:444:VAL:CG2	1:A:445:GLU:N	2.73	0.50
1:A:610:ARG:HB3	1:A:650:TYR:CZ	2.46	0.50
1:A:461:GLU:CD	1:A:462:ASP:H	2.14	0.50
1:A:696:GLY:HA2	1:A:731:PRO:O	2.11	0.50
1:A:445:GLU:C	1:A:446:LEU:HD22	2.32	0.50
1:A:471:ILE:CD1	1:A:475:VAL:HG23	2.42	0.49
1:A:690:GLY:O	1:A:691:ALA:HB2	2.12	0.49
1:A:585:LEU:HD12	1:A:633:ILE:HG21	1.95	0.49
1:A:412:ARG:O	1:A:413:ALA:C	2.51	0.49
1:A:517:SER:O	1:A:518:TYR:HB3	2.12	0.49
1:A:446:LEU:N	1:A:446:LEU:HD22	2.27	0.49
1:A:591:VAL:HG21	1:A:634:THR:HG23	1.95	0.49
1:A:740:TYR:O	1:A:744:LYS:HB2	2.12	0.49
1:A:372:LYS:HE3	1:A:377:PHE:CD2	2.48	0.49
1:A:539:THR:O	1:A:541:PHE:N	2.46	0.49
1:A:748:LYS:HB2	1:A:748:LYS:HZ2	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:TYR:CZ	1:A:521:ARG:HG3	2.48	0.49
1:A:590:GLU:O	1:A:594:LEU:HD13	2.13	0.49
1:A:481:LEU:HD13	1:A:748:LYS:HA	1.94	0.49
1:A:78:VAL:HG21	1:A:84:TYR:CB	2.43	0.48
1:A:8:TYR:CD2	1:A:9:PRO:HD2	2.48	0.48
1:A:247:ILE:HD12	1:A:247:ILE:N	2.28	0.48
1:A:398:VAL:CG1	1:A:398:VAL:O	2.61	0.48
1:A:229:LEU:HB3	1:A:233:LEU:CD2	2.44	0.48
1:A:204:GLN:HG3	1:A:239:LEU:HD13	1.96	0.48
1:A:567:TRP:CE2	1:A:608:ALA:HB2	2.49	0.48
1:A:656:ILE:HG12	1:A:660:ILE:CD1	2.43	0.48
1:A:672:ASN:C	1:A:674:ARG:H	2.17	0.48
1:A:71:THR:HG21	1:A:156:VAL:HB	1.94	0.48
1:A:577:HIS:CD2	1:A:578:GLU:N	2.83	0.47
1:A:18:LYS:HZ1	1:A:521:ARG:NH2	2.12	0.47
1:A:403:ALA:C	1:A:405:LEU:H	2.16	0.47
1:A:706:PRO:O	1:A:707:SER:O	2.31	0.47
1:A:710:GLU:O	1:A:714:ARG:HG3	2.14	0.47
1:A:594:LEU:O	1:A:599:ILE:HB	2.15	0.47
1:A:416:VAL:O	1:A:420:LEU:HG	2.14	0.47
1:A:74:MSE:HA	1:A:134:SER:HB3	1.97	0.47
1:A:468:LYS:O	1:A:471:ILE:HG22	2.15	0.47
1:A:555:LYS:HA	1:A:601:VAL:O	2.15	0.47
1:A:344:ASP:O	1:A:347:ILE:HG22	2.15	0.46
1:A:318:GLY:O	1:A:320:ASP:N	2.37	0.46
1:A:510:THR:HG21	1:A:513:GLY:HA3	1.96	0.46
1:A:481:LEU:HD12	1:A:481:LEU:N	2.30	0.46
1:A:434:THR:OG1	1:A:483:ILE:HA	2.15	0.46
1:A:539:THR:HB	1:A:594:LEU:HD11	1.98	0.46
1:A:676:ASP:HB2	1:A:679:LEU:HG	1.96	0.46
1:A:78:VAL:HG21	1:A:84:TYR:HB2	1.96	0.46
1:A:437:ILE:HG22	1:A:437:ILE:O	2.15	0.46
1:A:35:GLN:HE21	1:A:35:GLN:CA	2.22	0.46
1:A:481:LEU:HB3	1:A:751:VAL:HG11	1.98	0.46
1:A:229:LEU:O	1:A:233:LEU:HD22	2.16	0.46
1:A:395:ASN:O	1:A:398:VAL:CB	2.63	0.46
1:A:416:VAL:HG13	1:A:417:SER:N	2.30	0.46
1:A:716:ASN:HD21	1:A:757:ILE:CD1	2.29	0.46
1:A:84:TYR:HA	6:A:1008:HOH:O	2.16	0.46
1:A:167:ALA:HB1	1:A:171:VAL:HB	1.96	0.45
1:A:213:ASP:HB2	1:A:617:LYS:HZ3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLU:O	1:A:348:LYS:CE	2.63	0.45
1:A:4:HIS:C	1:A:5:ILE:HD12	2.36	0.45
1:A:125:GLY:O	1:A:128:VAL:HG12	2.17	0.45
1:A:175:PHE:HE2	1:A:177:LEU:HD23	1.81	0.45
1:A:171:VAL:O	1:A:172:ASP:O	2.34	0.45
1:A:671:GLU:O	1:A:672:ASN:CB	2.64	0.45
1:A:716:ASN:HD21	1:A:757:ILE:HD11	1.80	0.45
1:A:517:SER:OG	5:A:773:C2F:H16	2.17	0.45
1:A:739:LYS:HD2	1:A:741:THR:H	1.82	0.45
1:A:212:MSE:HE2	1:A:212:MSE:CA	2.44	0.45
1:A:437:ILE:HD11	1:A:730:ASN:ND2	2.31	0.45
1:A:567:TRP:CZ2	1:A:608:ALA:HB2	2.51	0.45
1:A:480:GLU:HG3	1:A:480:GLU:O	2.17	0.44
1:A:510:THR:HG21	1:A:513:GLY:N	2.33	0.44
1:A:711:ILE:O	1:A:715:VAL:HG23	2.17	0.44
1:A:754:ALA:O	1:A:758:ARG:HG3	2.17	0.44
1:A:443:THR:OG1	1:A:444:VAL:N	2.50	0.44
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.84	0.44
1:A:317:VAL:HB	1:A:318:GLY:H	1.64	0.44
1:A:411:ARG:HD3	1:A:419:ARG:NH1	2.33	0.44
1:A:700:ILE:HD12	1:A:701:HIS:CD2	2.53	0.44
1:A:481:LEU:CB	1:A:751:VAL:HG11	2.48	0.44
1:A:414:THR:O	1:A:415:ASN:C	2.56	0.44
1:A:521:ARG:HA	1:A:521:ARG:HE	1.82	0.44
1:A:12:GLY:HA2	1:A:41:LEU:HD11	1.99	0.43
1:A:314:GLU:OE1	1:A:368:LEU:HD22	2.18	0.43
1:A:213:ASP:HB2	1:A:617:LYS:HZ1	1.83	0.43
1:A:303:PHE:N	1:A:303:PHE:CD1	2.85	0.43
1:A:93:VAL:O	1:A:97:MSE:HG3	2.18	0.43
1:A:490:GLU:OE1	1:A:557:MSE:HE2	2.17	0.43
1:A:712:ALA:CA	1:A:753:ALA:HB1	2.49	0.43
1:A:571:ARG:NH1	1:A:573:ASP:OD1	2.52	0.43
1:A:599:ILE:N	1:A:599:ILE:HD12	2.33	0.43
1:A:733:CYS:SG	1:A:734:GLY:N	2.90	0.43
1:A:429:LEU:N	1:A:429:LEU:HD12	2.34	0.43
1:A:464:VAL:HG13	1:A:465:LYS:CE	2.48	0.43
1:A:676:ASP:HB3	1:A:678:LYS:HG3	1.99	0.43
1:A:691:ALA:O	1:A:692:GLY:C	2.57	0.43
1:A:755:LYS:O	1:A:758:ARG:HB2	2.19	0.43
1:A:396:GLU:C	1:A:398:VAL:N	2.69	0.43
1:A:477:LEU:HD22	1:A:483:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:GLY:H	1:A:532:VAL:HA	1.83	0.43
1:A:706:PRO:O	1:A:707:SER:C	2.57	0.43
1:A:318:GLY:C	1:A:320:ASP:N	2.71	0.42
1:A:347:ILE:CG2	1:A:348:LYS:N	2.82	0.42
1:A:571:ARG:NH1	1:A:573:ASP:OD2	2.52	0.42
1:A:592:GLU:O	1:A:596:LYS:HG3	2.19	0.42
1:A:490:GLU:N	1:A:491:PRO:CD	2.82	0.42
1:A:18:LYS:HG3	1:A:520:SER:O	2.20	0.42
1:A:583:ILE:O	1:A:587:ILE:HG12	2.20	0.42
1:A:435:THR:HB	1:A:485:VAL:HB	1.99	0.42
1:A:464:VAL:HG13	1:A:465:LYS:NZ	2.34	0.42
1:A:657:ILE:CG2	1:A:658:HIS:N	2.83	0.42
1:A:657:ILE:HD11	1:A:683:PHE:CD1	2.54	0.42
1:A:547:GLN:O	1:A:547:GLN:HG3	2.19	0.42
1:A:581:TYR:O	1:A:585:LEU:HD13	2.19	0.42
1:A:59:SER:O	1:A:60:ASN:CB	2.68	0.42
1:A:671:GLU:O	1:A:696:GLY:N	2.45	0.42
1:A:414:THR:O	1:A:419:ARG:HB2	2.20	0.42
1:A:18:LYS:HZ3	1:A:521:ARG:HH21	1.67	0.42
1:A:126:PRO:HG3	1:A:175:PHE:CE1	2.55	0.42
1:A:464:VAL:HA	1:A:467:ILE:HD12	2.01	0.42
1:A:481:LEU:HD22	1:A:748:LYS:O	2.20	0.42
1:A:89:ILE:HG23	1:A:93:VAL:HB	2.02	0.42
1:A:226:TYR:C	6:A:848:HOH:O	2.57	0.41
1:A:423:GLN:NE2	1:A:643:GLN:HA	2.35	0.41
1:A:204:GLN:HG3	1:A:239:LEU:CD1	2.50	0.41
1:A:714:ARG:HA	1:A:717:LYS:HD2	2.02	0.41
1:A:79:PRO:HA	1:A:80:PRO:HD3	1.86	0.41
1:A:384:LEU:HD12	6:A:793:HOH:O	2.19	0.41
1:A:398:VAL:HG23	1:A:531:ASP:OD2	2.20	0.41
1:A:6:VAL:HG22	1:A:329:SER:HA	2.03	0.41
1:A:705:ILE:HD12	1:A:745:PRO:HG2	2.03	0.41
1:A:481:LEU:HD11	1:A:748:LYS:CG	2.47	0.41
1:A:660:ILE:N	1:A:660:ILE:HD12	2.35	0.41
1:A:443:THR:O	1:A:445:GLU:HG2	2.20	0.41
1:A:679:LEU:O	1:A:682:VAL:HG22	2.20	0.41
1:A:714:ARG:NH1	1:A:718:MSE:HE2	2.35	0.41
1:A:432:LEU:HD13	1:A:719:LEU:HD21	2.02	0.41
1:A:671:GLU:O	1:A:672:ASN:HB3	2.20	0.41
1:A:757:ILE:O	1:A:760:GLN:HB2	2.21	0.41
1:A:79:PRO:CG	1:A:107:MSE:HE3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HG13	1:A:133:ALA:HB1	2.02	0.41
1:A:185:LEU:N	1:A:186:PRO:CD	2.84	0.41
1:A:406:LYS:NZ	1:A:406:LYS:HB3	2.34	0.41
1:A:434:THR:O	1:A:435:THR:HB	2.21	0.41
1:A:121:VAL:O	1:A:121:VAL:CG2	2.69	0.41
1:A:195:LEU:HA	1:A:195:LEU:HD12	1.90	0.41
1:A:243:TYR:O	1:A:244:PHE:CB	2.69	0.41
1:A:432:LEU:N	1:A:433:PRO:CD	2.83	0.41
1:A:700:ILE:C	1:A:700:ILE:HD12	2.41	0.41
1:A:59:SER:HB3	1:A:153:PRO:HA	2.04	0.40
1:A:298:ILE:O	1:A:298:ILE:HG23	2.20	0.40
1:A:303:PHE:N	1:A:303:PHE:HD1	2.19	0.40
1:A:429:LEU:HB3	1:A:430:PRO:HD2	2.03	0.40
1:A:488:HIS:HB3	1:A:554:MSE:HE1	2.02	0.40
1:A:645:HIS:HA	1:A:667:VAL:O	2.20	0.40
1:A:680:LEU:HD22	1:A:722:LEU:HD11	2.03	0.40
1:A:329:SER:C	1:A:331:LEU:H	2.24	0.40
1:A:9:PRO:HG3	1:A:330:LEU:O	2.22	0.40
1:A:539:THR:HG22	1:A:543:SER:OG	2.20	0.40
1:A:639:GLN:HE21	1:A:640:ASP:H	1.70	0.40
1:A:211:VAL:O	1:A:616:ARG:NH2	2.48	0.40
1:A:676:ASP:C	1:A:678:LYS:H	2.24	0.40
1:A:441:PRO:HB2	1:A:740:TYR:CD2	2.57	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	742/765 (97%)	636 (86%)	76 (10%)	30 (4%)	3 3

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	ASP
1	A	284	GLU
1	A	412	ARG
1	A	540	VAL
1	A	548	SER
1	A	673	SER
1	A	707	SER
1	A	171	VAL
1	A	317	VAL
1	A	319	LYS
1	A	413	ALA
1	A	415	ASN
1	A	539	THR
1	A	656	ILE
1	A	672	ASN
1	A	690	GLY
1	A	706	PRO
1	A	731	PRO
1	A	103	SER
1	A	482	ASP
1	A	691	ALA
1	A	102	ALA
1	A	414	THR
1	A	740	TYR
1	A	283	PRO
1	A	483	ILE
1	A	518	TYR
1	A	674	ARG
1	A	480	GLU
1	A	721	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	622/619 (100%)	575 (92%)	47 (8%)	15	24

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	11	MSE
1	A	34	LEU
1	A	61	THR
1	A	69	LEU
1	A	99	ARG
1	A	108	GLU
1	A	121	VAL
1	A	149	VAL
1	A	159	VAL
1	A	176	GLU
1	A	178	LEU
1	A	185	LEU
1	A	195	LEU
1	A	214	LEU
1	A	217	GLN
1	A	229	LEU
1	A	233	LEU
1	A	239	LEU
1	A	255	LEU
1	A	317	VAL
1	A	322	LEU
1	A	331	LEU
1	A	345	ASP
1	A	396	GLU
1	A	399	GLN
1	A	409	ASP
1	A	424	GLN
1	A	465	LYS
1	A	479	GLU
1	A	492	GLU
1	A	505	SER
1	A	521	ARG
1	A	531	ASP
1	A	571	ARG
1	A	605	ASP
1	A	616	ARG
1	A	656	ILE
1	A	657	ILE
1	A	662	ASP
1	A	677	GLU
1	A	685	GLU

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Mol	Chain	Res	Type
1	A	706	PRO
1	A	732	ASP
1	A	738	ARG
1	A	744	LYS
1	A	760	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	116	ASN
1	A	217	GLN
1	A	220	GLN
1	A	478	GLN
1	A	494	ASN
1	A	516	GLN
1	A	547	GLN
1	A	582	GLN
1	A	635	ASN
1	A	639	GLN
1	A	701	HIS
1	A	730	ASN
1	A	749	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
3	SO4	A	768	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	A	769	-	4,4,4	0.36	0	6,6,6	0.06	0
3	SO4	A	770	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	A	771	-	4,4,4	0.39	0	6,6,6	0.10	0
4	MET	A	772	-	3,8,8	0.19	0	3,9,9	0.37	0
5	C2F	A	773	-	25,35,35	3.55	11 (44%)	30,49,49	2.69	9 (30%)

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
3	SO4	A	768	-	-	0/0/0/0	0/0/0/0
3	SO4	A	769	-	-	0/0/0/0	0/0/0/0
3	SO4	A	770	-	-	0/0/0/0	0/0/0/0
3	SO4	A	771	-	-	0/0/0/0	0/0/0/0
4	MET	A	772	-	-	0/4/8/8	0/0/0/0
5	C2F	A	773	-	-	0/16/35/35	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	773	C2F	C2-N3	-7.65	1.21	1.35
5	A	773	C2F	C14-C13	2.10	1.42	1.38
5	A	773	C2F	C11-N5	2.14	1.52	1.46
5	A	773	C2F	C13-C12	2.22	1.43	1.39
5	A	773	C2F	C14-C15	2.37	1.43	1.39
5	A	773	C2F	C4A-C8A	3.57	1.48	1.41
5	A	773	C2F	C4-C4A	3.93	1.45	1.41
5	A	773	C2F	C4-N3	4.06	1.40	1.33
5	A	773	C2F	O4-C4	6.36	1.40	1.24
5	A	773	C2F	C2-NA2	6.68	1.47	1.34
5	A	773	C2F	C6-N5	9.42	1.56	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	773	C2F	C16-C15-N10	-6.49	107.96	121.03
5	A	773	C2F	NA2-C2-N3	-4.13	110.64	117.24
5	A	773	C2F	C4A-C4-N3	-2.39	119.62	123.37
5	A	773	C2F	CB-CA-N	3.21	115.10	110.22
5	A	773	C2F	C7-C6-N5	3.31	112.45	108.79
5	A	773	C2F	CA-N-C	3.62	127.11	122.15
5	A	773	C2F	N3-C2-N1	5.05	133.64	125.45
5	A	773	C2F	C14-C15-N10	5.63	132.38	121.03
5	A	773	C2F	C11-N5-C4A	6.82	122.93	113.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	773	C2F	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	728/765 (95%)	0.01	46 (6%) 21 19	31, 58, 103, 120	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	TYR	5.7
1	A	712	ALA	4.9
1	A	402	ALA	4.8
1	A	481	LEU	4.6
1	A	440	PHE	4.4
1	A	432	LEU	4.3
1	A	711	ILE	4.2
1	A	174	SER	3.5
1	A	467	ILE	3.5
1	A	542	TRP	3.5
1	A	398	VAL	3.5
1	A	443	THR	3.4
1	A	464	VAL	3.4
1	A	471	ILE	3.2
1	A	756	LEU	3.2
1	A	475	VAL	3.1
1	A	399	GLN	3.1
1	A	483	ILE	2.9
1	A	754	ALA	2.9
1	A	678	LYS	2.9
1	A	319	LYS	2.9
1	A	405	LEU	2.7
1	A	175	PHE	2.7
1	A	391	PRO	2.7
1	A	715	VAL	2.5
1	A	444	VAL	2.5
1	A	721	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	745	PRO	2.4
1	A	753	ALA	2.4
1	A	446	LEU	2.4
1	A	482	ASP	2.4
1	A	759	SER	2.4
1	A	173	LYS	2.3
1	A	412	ARG	2.3
1	A	473	LYS	2.3
1	A	755	LYS	2.3
1	A	466	ALA	2.2
1	A	479	GLU	2.2
1	A	757	ILE	2.2
1	A	462	ASP	2.2
1	A	172	ASP	2.1
1	A	284	GLU	2.1
1	A	318	GLY	2.1
1	A	720	ALA	2.0
1	A	716	ASN	2.0
1	A	722	LEU	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	SO4	A	768	5/5	0.76	0.40	8.70	153,153,153,153	0
3	SO4	A	770	5/5	0.75	0.24	5.14	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	C2F	A	773	33/33	0.68	0.34	5.08	111,113,120,121	0
4	MET	A	772	9/9	0.93	0.19	2.20	67,68,69,69	0
3	SO4	A	769	5/5	0.88	0.21	2.04	136,136,137,137	0
3	SO4	A	771	5/5	0.88	0.15	0.69	94,94,94,94	0
2	ZN	A	766	1/1	0.97	0.15	-	64,64,64,64	0
2	ZN	A	767	1/1	0.98	0.15	-	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.