



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:00 PM UTC

PDB ID : 1L5J / pdb_00001l5j
Title : CRYSTAL STRUCTURE OF E. COLI ACONITASE B.
Authors : Williams, C.H.; Stillman, T.J.; Barynin, V.V.; Sedelnikova, S.E.; Tang, Y.;
Green, J.; Guest, J.R.; Artymiuk, P.J.
Deposited on : 2002-03-07
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

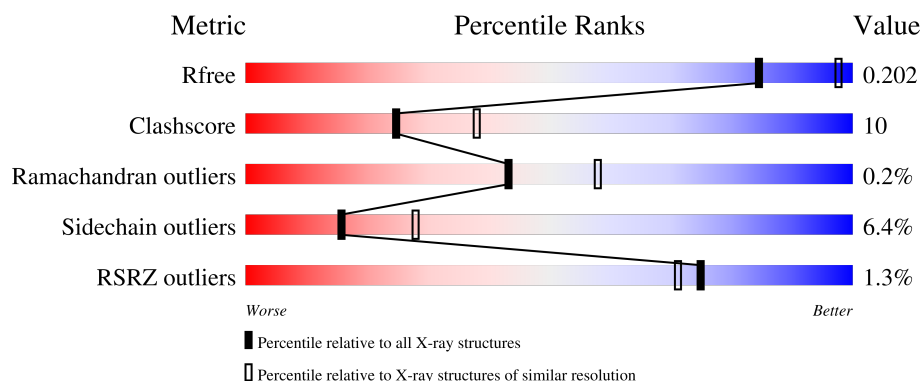
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	865	% 80% 17% .
1	B	865	% 81% 16% .

2 Entry composition [i](#)

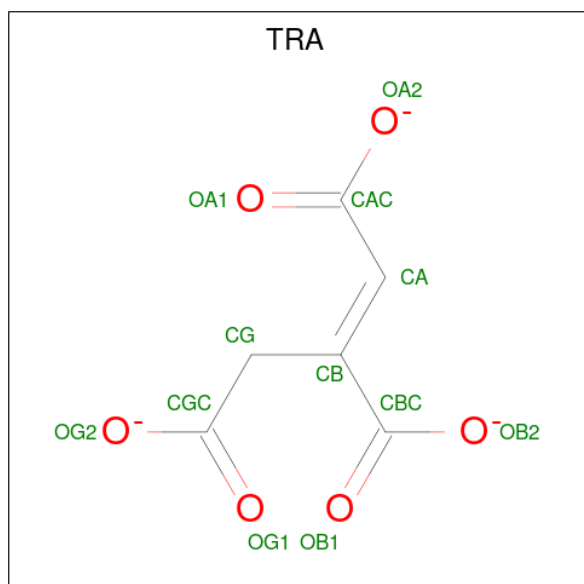
There are 4 unique types of molecules in this entry. The entry contains 13712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aconitate hydratase 2.

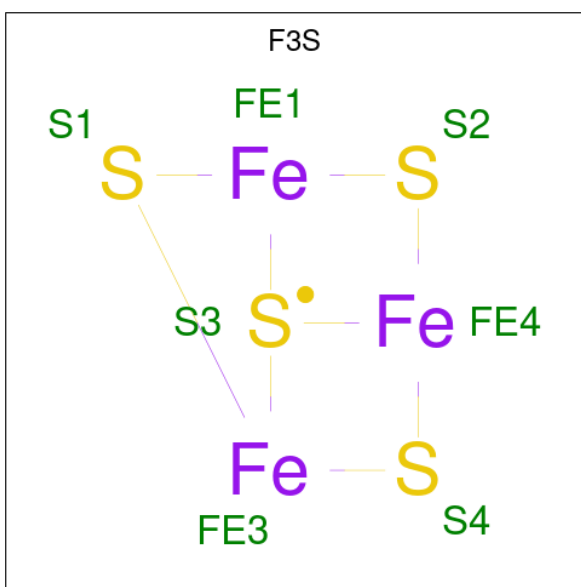
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	862	Total	C	N	O	S	0	0	0
			6552	4152	1122	1245	33			
1	B	862	Total	C	N	O	S	0	0	0
			6552	4152	1122	1245	33			

- Molecule 2 is ACONITATE ION (CCD ID: TRA) (formula: $C_6H_3O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			7	3	4		
3	B	1	Total	Fe	S	0	0
			7	3	4		

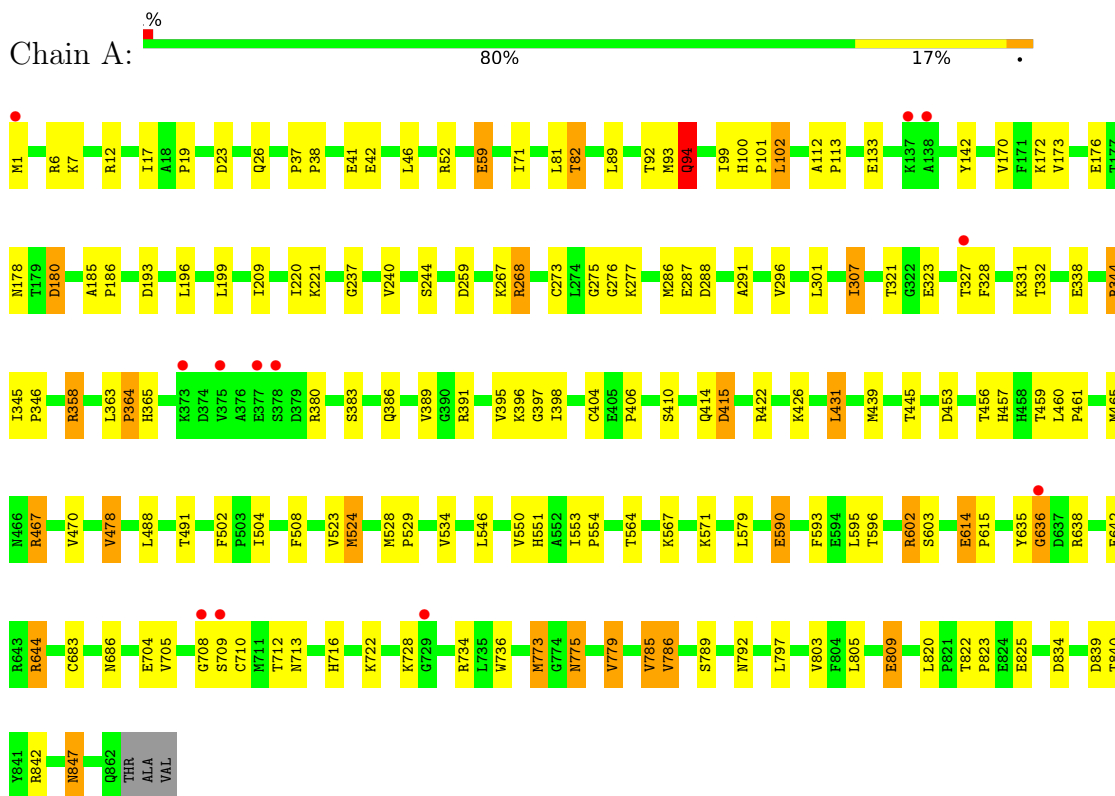
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	294	Total	O	0	0
			294	294		
4	B	276	Total	O	0	0
			276	276		

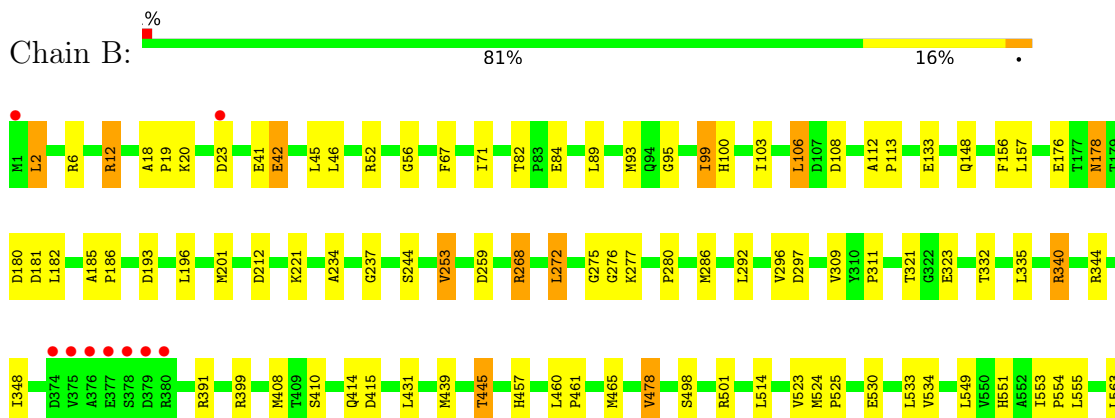
3 Residue-property plots

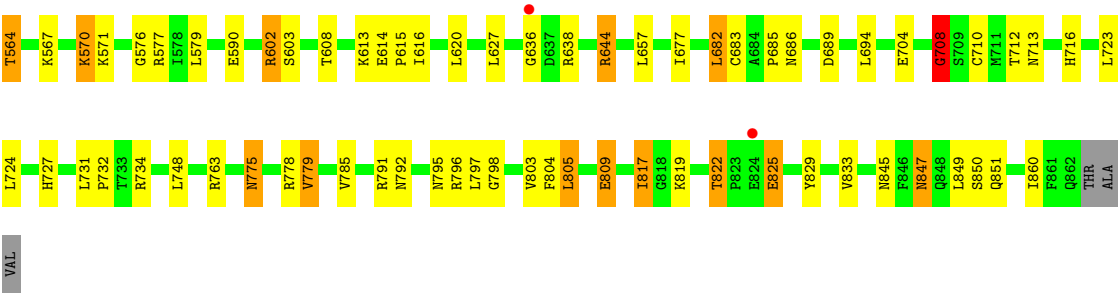
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Aconitate hydratase 2



• Molecule 1: Aconitate hydratase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	138.97Å 169.63Å 113.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.40) 95.8 (20.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.151 , 0.203 0.155 , 0.202	Depositor DCC
R_{free} test set	5019 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13712	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: F3S, TRA

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	0.46	1/6686 (0.0%)	0.91	12/9076 (0.1%)
1	B	0.49	1/6686 (0.0%)	0.91	8/9076 (0.1%)
All	All	0.48	2/13372 (0.0%)	0.91	20/18152 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	286	MET	SD-CE	-10.70	1.52	1.79
1	A	524	MET	SD-CE	-5.12	1.66	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	635	TYR	N-CA-C	6.88	119.62	110.53
1	A	478	VAL	N-CA-C	6.79	118.53	109.37
1	B	99	ILE	N-CA-C	6.74	116.86	110.53
1	A	99	ILE	N-CA-C	6.56	116.69	110.53
1	B	478	VAL	N-CA-C	5.99	117.45	109.37
1	A	7	LYS	N-CA-C	-5.92	104.82	111.28
1	A	803	VAL	N-CA-C	5.86	116.30	107.75
1	B	708	GLY	N-CA-C	5.76	126.83	113.18
1	A	276	GLY	N-CA-C	-5.54	106.09	112.73
1	B	276	GLY	N-CA-C	-5.43	106.22	112.73
1	B	803	VAL	N-CA-C	5.42	115.66	107.75
1	A	380	ARG	N-CA-C	5.30	116.93	110.41
1	A	240	VAL	N-CA-C	5.29	115.75	108.12
1	B	23	ASP	CB-CA-C	-5.25	99.53	110.40
1	A	94	GLN	N-CA-C	5.13	121.72	110.80
1	A	636	GLY	N-CA-C	5.07	125.21	113.18
1	A	728	LYS	N-CA-C	5.07	116.83	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	822	THR	N-CA-C	-5.05	103.59	110.36
1	B	785	VAL	N-CA-C	5.02	115.94	108.46
1	A	415	ASP	N-CA-C	5.02	119.38	113.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6552	0	6569	131	0
1	B	6552	0	6569	127	0
2	A	12	0	3	2	0
2	B	12	0	3	3	0
3	A	7	0	0	0	0
3	B	7	0	0	0	0
4	A	294	0	0	14	0
4	B	276	0	0	11	0
All	All	13712	0	13144	258	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 10.

All (258) 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:B:530:GLU:OE2	1:B:577:ARG:NH1	1.79	1.15
1:A:439:MET:HE2	4:A:1105:HOH:O	1.51	1.07
1:B:465:MET:SD	1:B:636:GLY:HA3	1.98	1.03
1:B:178:ASN:ND2	1:B:180:ASP:H	1.55	1.03
1:A:439:MET:HB3	4:A:1105:HOH:O	1.60	1.00
1:A:321:THR:CG2	1:A:323:GLU:HG3	1.91	0.99
1:A:301:LEU:HD22	1:A:307:ILE:HD11	1.45	0.99
1:A:296:VAL:HG12	1:A:328:PHE:HB3	1.44	0.98
1:B:590:GLU:HG3	4:B:931:HOH:O	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:ASN:HA	1:B:792:ASN:O	1.65	0.96
1:B:178:ASN:HD22	1:B:180:ASP:H	1.13	0.96
1:B:847:ASN:H	1:B:847:ASN:HD22	1.13	0.96
1:A:590:GLU:HG2	4:A:888:HOH:O	1.66	0.95
1:A:508:PHE:HB2	1:A:524:MET:HE1	1.47	0.94
1:A:564:THR:HG22	1:A:571:LYS:H	1.30	0.94
1:B:708:GLY:O	4:B:1117:HOH:O	1.87	0.93
1:A:296:VAL:CG1	1:A:328:PHE:HB3	2.00	0.90
1:A:686:ASN:HA	1:A:792:ASN:O	1.70	0.90
1:A:847:ASN:HD22	1:A:847:ASN:H	1.19	0.89
1:A:286:MET:HG3	1:A:291:ALA:HB3	1.53	0.88
1:A:321:THR:HG22	1:A:323:GLU:HG3	1.55	0.88
1:A:775:ASN:HD22	1:A:775:ASN:H	1.23	0.87
1:B:52:ARG:HD3	4:B:878:HOH:O	1.72	0.87
1:A:301:LEU:HD22	1:A:307:ILE:CD1	2.08	0.83
1:B:410:SER:OG	1:B:644:ARG:NH2	2.12	0.83
1:B:778:ARG:CZ	4:B:1052:HOH:O	2.25	0.83
1:A:89:LEU:O	1:A:92:THR:HG22	1.80	0.82
1:B:478:VAL:HG11	1:B:710:CYS:HB3	1.63	0.81
1:A:52:ARG:HD3	4:A:957:HOH:O	1.80	0.80
1:A:331:LYS:HG3	1:A:332:THR:HG23	1.62	0.80
1:A:288:ASP:OD1	1:A:344:ARG:HD2	1.80	0.80
1:A:564:THR:CG2	1:A:571:LYS:H	1.95	0.80
1:B:178:ASN:HD22	1:B:180:ASP:N	1.79	0.79
1:B:775:ASN:HD22	1:B:775:ASN:H	1.30	0.79
1:B:465:MET:SD	1:B:636:GLY:CA	2.73	0.77
1:B:100:HIS:HB3	4:B:1130:HOH:O	1.84	0.77
1:A:321:THR:HG21	1:A:323:GLU:HG3	1.67	0.75
1:A:488:LEU:O	1:A:491:THR:HG22	1.85	0.75
1:A:773:MET:HG2	1:A:775:ASN:ND2	2.02	0.75
1:B:817:ILE:HG22	1:B:819:LYS:HG2	1.69	0.74
1:A:259:ASP:O	1:A:268:ARG:HG3	1.86	0.74
1:A:267:LYS:HE2	4:A:1090:HOH:O	1.87	0.74
1:A:713:ASN:H	1:A:716:HIS:CD2	2.08	0.72
1:A:12:ARG:NH2	1:A:193:ASP:OD2	2.18	0.72
1:B:704:GLU:CD	1:B:779:VAL:HG22	2.15	0.72
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.53	0.71
1:B:259:ASP:O	1:B:268:ARG:HG3	1.89	0.71
1:A:713:ASN:H	1:A:716:HIS:HD2	1.38	0.71
1:A:410:SER:OG	1:A:644:ARG:NH2	2.23	0.71
1:A:704:GLU:CD	1:A:779:VAL:HG22	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:PRO:HG3	1:B:602:ARG:CZ	2.22	0.70
1:A:465:MET:SD	1:A:636:GLY:HA2	2.31	0.70
1:B:822:THR:H	1:B:825:GLU:HG3	1.57	0.70
1:A:259:ASP:C	1:A:268:ARG:HG3	2.16	0.70
1:A:773:MET:HE1	2:A:866:TRA:HG2	1.72	0.70
1:B:817:ILE:CG2	1:B:819:LYS:HG2	2.23	0.69
1:B:415:ASP:OD2	1:B:445:THR:HG22	1.93	0.69
1:A:71:ILE:HG21	1:A:81:LEU:HD13	1.73	0.68
1:B:178:ASN:ND2	1:B:180:ASP:N	2.37	0.67
1:A:636:GLY:N	4:A:905:HOH:O	2.22	0.67
1:B:234:ALA:HB1	1:B:272:LEU:CD1	2.24	0.67
1:B:201:MET:HE1	1:B:253:VAL:HB	1.78	0.66
1:A:173:VAL:HG22	1:A:209:ILE:HD11	1.77	0.66
1:A:590:GLU:CG	4:A:888:HOH:O	2.35	0.65
1:B:234:ALA:HB2	1:B:272:LEU:HD11	1.78	0.65
1:B:280:PRO:HG3	1:B:576:GLY:HA2	1.79	0.65
1:B:234:ALA:CB	1:B:272:LEU:HD11	2.27	0.64
1:A:638:ARG:HD3	1:A:642:GLU:OE1	1.97	0.63
1:B:234:ALA:CB	1:B:272:LEU:CD1	2.76	0.63
1:B:833:VAL:HG12	1:B:833:VAL:O	1.99	0.62
1:B:713:ASN:H	1:B:716:HIS:HD2	1.46	0.61
1:B:259:ASP:C	1:B:268:ARG:HG3	2.25	0.61
1:A:847:ASN:HD22	1:A:847:ASN:N	1.95	0.61
1:B:182:LEU:HD22	1:B:201:MET:HE2	1.82	0.61
1:B:321:THR:HG21	1:B:323:GLU:HG3	1.83	0.60
1:B:514:LEU:HD11	1:B:525:PRO:HD2	1.82	0.60
1:B:683:CYS:HB2	1:B:805:LEU:HB2	1.82	0.60
1:A:775:ASN:HD22	1:A:775:ASN:N	1.94	0.60
1:B:445:THR:HG23	1:B:457:HIS:NE2	2.17	0.60
1:A:244:SER:HB2	2:A:866:TRA:OG1	2.02	0.60
1:B:713:ASN:H	1:B:716:HIS:CD2	2.20	0.60
1:B:685:PRO:HD3	1:B:804:PHE:CE2	2.36	0.60
1:B:847:ASN:HD22	1:B:847:ASN:N	1.92	0.59
1:A:383:SER:H	1:A:386:GLN:NE2	2.01	0.59
1:B:847:ASN:H	1:B:847:ASN:ND2	1.92	0.59
1:A:296:VAL:CG1	1:A:328:PHE:CB	2.78	0.59
1:A:395:VAL:HG12	1:A:397:GLY:H	1.68	0.59
1:A:273:CYS:HB2	1:A:286:MET:HE2	1.84	0.59
1:A:406:PRO:HD2	1:A:524:MET:O	2.02	0.59
1:A:478:VAL:HG11	1:A:710:CYS:HB3	1.85	0.58
1:A:593:PHE:HA	1:A:596:THR:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE3	1:A:26:GLN:HB3	1.85	0.58
1:B:833:VAL:O	1:B:833:VAL:CG1	2.51	0.58
1:B:67:PHE:CZ	1:B:71:ILE:HD11	2.39	0.58
1:A:459:THR:HG23	4:A:971:HOH:O	2.02	0.58
1:B:778:ARG:NE	4:B:1052:HOH:O	2.34	0.58
1:B:822:THR:OG1	1:B:825:GLU:HG2	2.05	0.57
1:A:185:ALA:HB3	1:A:186:PRO:HD3	1.86	0.57
1:A:395:VAL:HG12	1:A:396:LYS:N	2.18	0.57
1:B:614:GLU:HB2	1:B:615:PRO:HD3	1.86	0.57
1:B:182:LEU:HD22	1:B:201:MET:CE	2.35	0.57
1:B:20:LYS:HE2	1:B:193:ASP:OD2	2.06	0.56
1:A:112:ALA:HB3	1:A:113:PRO:HD3	1.87	0.56
1:A:237:GLY:O	1:A:275:GLY:HA2	2.05	0.56
1:A:321:THR:HG21	1:A:323:GLU:CG	2.34	0.56
1:A:554:PRO:HG3	1:A:602:ARG:CZ	2.37	0.55
1:A:358:ARG:HH11	1:A:358:ARG:CG	2.20	0.55
1:A:602:ARG:O	1:A:603:SER:HB2	2.06	0.55
1:B:704:GLU:HG2	1:B:734:ARG:HB3	1.87	0.55
1:B:553:ILE:HB	1:B:554:PRO:HD3	1.89	0.54
1:B:682:LEU:N	1:B:682:LEU:HD23	2.22	0.54
1:B:851:GLN:H	1:B:851:GLN:CD	2.12	0.54
1:A:170:VAL:HG21	1:A:307:ILE:HD12	1.89	0.54
1:A:389:VAL:HG12	1:A:398:ILE:HD12	1.88	0.54
1:B:12:ARG:HD2	1:B:19:PRO:HA	1.90	0.54
1:A:508:PHE:CB	1:A:524:MET:HE1	2.31	0.54
1:A:12:ARG:HD3	1:A:17:ILE:HG13	1.89	0.54
1:A:712:THR:HA	1:A:716:HIS:CD2	2.43	0.54
1:B:817:ILE:HD11	1:B:829:TYR:OH	2.07	0.54
1:B:704:GLU:OE2	1:B:779:VAL:HG22	2.08	0.53
1:A:773:MET:O	1:A:773:MET:HG3	2.08	0.53
1:B:613:LYS:HD3	4:B:961:HOH:O	2.09	0.53
1:A:395:VAL:CG1	1:A:396:LYS:N	2.72	0.53
1:B:344:ARG:O	1:B:348:ILE:HG12	2.08	0.53
1:A:100:HIS:HB2	1:A:101:PRO:HD3	1.90	0.53
1:B:112:ALA:HB3	1:B:113:PRO:HD3	1.91	0.53
1:B:685:PRO:HD3	1:B:804:PHE:CD2	2.44	0.53
1:A:705:VAL:HG22	1:A:786:VAL:CG1	2.39	0.52
1:A:465:MET:SD	1:A:636:GLY:CA	2.96	0.52
1:A:553:ILE:HB	1:A:554:PRO:HD3	1.91	0.52
1:B:212:ASP:OD1	1:B:221:LYS:HD3	2.10	0.52
1:A:705:VAL:HG22	1:A:786:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ARG:HG3	1:A:363:LEU:HB2	1.92	0.52
1:A:683:CYS:HB2	1:A:805:LEU:HB2	1.93	0.51
1:A:92:THR:HG21	4:A:877:HOH:O	2.11	0.51
1:B:551:HIS:O	1:B:554:PRO:HD2	2.10	0.51
1:A:199:LEU:HD22	1:A:220:ILE:CD1	2.40	0.51
1:A:345:ILE:HB	1:A:346:PRO:HD3	1.93	0.51
1:A:422:ARG:HD3	1:A:426:LYS:HE2	1.92	0.51
1:B:792:ASN:HB3	1:B:805:LEU:HD13	1.93	0.50
1:B:445:THR:CG2	1:B:457:HIS:NE2	2.74	0.50
1:A:286:MET:HG3	1:A:291:ALA:CB	2.35	0.50
1:B:176:GLU:HB2	1:B:567:LYS:HG2	1.93	0.50
1:B:178:ASN:HD22	1:B:178:ASN:C	2.20	0.50
1:B:845:ASN:ND2	4:B:976:HOH:O	2.44	0.50
1:A:445:THR:OG1	1:A:457:HIS:HE1	1.94	0.49
1:B:727:HIS:NE2	1:B:829:TYR:HE2	2.09	0.49
1:B:778:ARG:NH2	4:B:1052:HOH:O	2.39	0.49
1:A:734:ARG:HD3	1:A:736:TRP:HE1	1.78	0.49
1:B:234:ALA:HB1	1:B:272:LEU:HD12	1.93	0.49
1:B:551:HIS:C	1:B:554:PRO:HD2	2.38	0.48
1:A:178:ASN:OD1	1:A:180:ASP:HB2	2.12	0.48
1:B:712:THR:HA	1:B:716:HIS:CD2	2.48	0.48
1:A:470:VAL:HA	1:A:636:GLY:O	2.14	0.48
1:B:82:THR:HB	1:B:84:GLU:OE2	2.14	0.48
1:A:534:VAL:CG2	1:A:579:LEU:HD11	2.44	0.48
1:A:551:HIS:O	1:A:554:PRO:HD2	2.12	0.48
1:B:602:ARG:NH1	1:B:689:ASP:OD2	2.47	0.48
1:A:712:THR:HA	1:A:716:HIS:HD2	1.79	0.47
1:A:709:SER:HB2	1:A:789:SER:HA	1.95	0.47
1:B:244:SER:HB2	2:B:867:TRA:OG1	2.15	0.47
1:A:398:ILE:HD13	1:A:404:CYS:SG	2.55	0.47
1:B:234:ALA:CB	1:B:272:LEU:HD12	2.44	0.47
1:B:712:THR:HA	1:B:716:HIS:HD2	1.80	0.47
1:B:851:GLN:OE1	1:B:851:GLN:N	2.32	0.47
1:A:358:ARG:CG	1:A:358:ARG:NH1	2.78	0.47
1:B:795:ASN:HA	1:B:798:GLY:O	2.15	0.47
1:B:296:VAL:HG22	1:B:297:ASP:N	2.29	0.46
1:B:564:THR:HG22	1:B:571:LYS:H	1.80	0.46
1:A:809:GLU:H	1:A:809:GLU:CD	2.21	0.46
1:A:460:LEU:N	1:A:461:PRO:CD	2.79	0.46
1:A:713:ASN:N	1:A:716:HIS:HD2	2.09	0.46
1:B:12:ARG:HD3	1:B:18:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ALA:N	1:B:186:PRO:CD	2.78	0.46
1:B:727:HIS:NE2	1:B:829:TYR:CE2	2.83	0.46
1:B:332:THR:HG23	1:B:335:LEU:H	1.81	0.46
1:B:564:THR:HG22	1:B:570:LYS:HG2	1.96	0.46
1:A:822:THR:CG2	1:A:825:GLU:H	2.29	0.45
1:B:244:SER:HG	2:B:867:TRA:CA	2.29	0.45
1:B:775:ASN:H	1:B:775:ASN:ND2	2.06	0.45
1:A:564:THR:HG22	1:A:571:LYS:N	2.14	0.45
1:A:23:ASP:C	1:A:23:ASP:OD1	2.59	0.45
1:B:682:LEU:N	1:B:682:LEU:CD2	2.79	0.45
1:A:321:THR:HG21	1:A:323:GLU:CD	2.41	0.45
1:B:103:ILE:O	1:B:106:LEU:HB2	2.16	0.45
1:B:93:MET:C	1:B:95:GLY:H	2.23	0.45
1:B:616:ILE:HD12	1:B:657:LEU:HD11	1.97	0.45
1:B:108:ASP:C	1:B:108:ASP:OD1	2.60	0.45
1:B:638:ARG:NH2	1:B:860:ILE:O	2.50	0.45
1:A:288:ASP:OD1	1:A:344:ARG:CD	2.60	0.44
1:A:59:GLU:OE2	1:A:426:LYS:NZ	2.51	0.44
1:B:272:LEU:HD12	1:B:272:LEU:O	2.17	0.44
1:B:602:ARG:HA	1:B:602:ARG:HD3	1.83	0.44
1:B:93:MET:O	1:B:95:GLY:N	2.49	0.44
1:B:498:SER:OG	1:B:791:ARG:NH2	2.45	0.44
1:A:93:MET:C	1:A:94:GLN:HG2	2.42	0.44
1:A:364:PRO:HB2	1:A:365:HIS:H	1.55	0.44
1:A:602:ARG:NH2	4:A:1018:HOH:O	2.21	0.44
1:A:102:LEU:HD12	1:A:102:LEU:HA	1.86	0.43
1:A:112:ALA:HB1	1:A:142:TYR:CD2	2.53	0.43
1:A:467:ARG:NH1	4:A:1007:HOH:O	2.51	0.43
1:B:234:ALA:HB2	1:B:272:LEU:CD1	2.46	0.43
1:B:602:ARG:O	1:B:603:SER:HB2	2.17	0.43
1:B:796:ARG:NH1	2:B:867:TRA:OG2	2.46	0.43
1:B:847:ASN:N	1:B:847:ASN:ND2	2.60	0.43
1:A:734:ARG:HD3	1:A:736:TRP:NE1	2.33	0.43
1:A:199:LEU:HD22	1:A:220:ILE:HD11	2.01	0.43
1:A:439:MET:CB	4:A:1105:HOH:O	2.40	0.43
1:B:272:LEU:HD12	1:B:272:LEU:C	2.44	0.43
1:B:809:GLU:CD	1:B:809:GLU:H	2.27	0.43
1:A:363:LEU:HB3	1:A:364:PRO:CD	2.49	0.43
1:A:785:VAL:HG23	1:A:786:VAL:N	2.33	0.43
1:A:822:THR:OG1	1:A:823:PRO:HD2	2.19	0.43
1:B:156:PHE:CE2	1:B:340:ARG:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:ARG:HA	1:A:602:ARG:HD3	1.87	0.42
1:B:608:THR:HG23	4:B:898:HOH:O	2.18	0.42
1:B:2:LEU:HD12	1:B:2:LEU:HA	1.79	0.42
1:B:178:ASN:HB3	1:B:181:ASP:OD2	2.19	0.42
1:B:534:VAL:CG2	1:B:579:LEU:HD11	2.49	0.42
1:B:822:THR:N	1:B:825:GLU:HG3	2.29	0.42
1:B:178:ASN:ND2	1:B:178:ASN:C	2.77	0.42
1:B:309:VAL:O	1:B:311:PRO:HD3	2.19	0.42
1:A:839:ASP:O	1:A:842:ARG:HD3	2.19	0.42
1:A:704:GLU:OE2	1:A:779:VAL:HG22	2.19	0.42
1:B:498:SER:O	1:B:501:ARG:HD3	2.20	0.42
1:A:564:THR:HG21	4:A:919:HOH:O	2.20	0.42
1:B:602:ARG:NH2	4:B:990:HOH:O	2.46	0.42
1:A:12:ARG:HD2	1:A:19:PRO:HA	2.01	0.42
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.91	0.42
1:A:722:LYS:NZ	1:A:840:THR:OG1	2.31	0.42
1:A:176:GLU:HB2	1:A:567:LYS:HD2	2.02	0.42
1:A:820:LEU:HD23	1:A:820:LEU:HA	1.85	0.42
1:A:37:PRO:HA	1:A:38:PRO:HD3	1.91	0.41
1:A:100:HIS:N	1:A:101:PRO:CD	2.83	0.41
1:B:534:VAL:HG21	1:B:579:LEU:HD11	2.02	0.41
1:B:723:LEU:HG	1:B:833:VAL:HG21	2.02	0.41
1:B:731:LEU:HA	1:B:732:PRO:HD3	1.82	0.41
1:B:41:GLU:O	1:B:45:LEU:HG	2.20	0.41
1:B:56:GLY:HA2	1:B:95:GLY:O	2.20	0.41
1:B:321:THR:CG2	1:B:323:GLU:HG3	2.50	0.41
1:A:42:GLU:CD	1:A:42:GLU:H	2.27	0.41
1:B:408:MET:HA	1:B:408:MET:HE2	2.03	0.41
1:A:453:ASP:O	1:A:456:THR:HB	2.20	0.41
1:B:237:GLY:O	1:B:275:GLY:HA2	2.20	0.41
1:A:363:LEU:HB3	1:A:364:PRO:HD2	2.02	0.41
1:A:415:ASP:OD1	1:A:415:ASP:N	2.52	0.41
1:A:502:PHE:HB3	1:A:504:ILE:O	2.21	0.41
1:A:550:VAL:HG22	1:A:595:LEU:HD23	2.02	0.41
1:B:460:LEU:N	1:B:461:PRO:CD	2.84	0.41
1:B:439:MET:HE2	1:B:439:MET:HB3	1.87	0.41
1:B:524:MET:HA	1:B:525:PRO:HD3	1.98	0.41
1:A:287:GLU:OE2	1:A:338:GLU:OE1	2.40	0.40
1:A:82:THR:HG22	4:A:1033:HOH:O	2.21	0.40
1:A:534:VAL:HG23	1:A:579:LEU:HD11	2.03	0.40
1:A:528:MET:HA	1:A:529:PRO:HD3	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:GLU:N	1:A:615:PRO:HD2	2.37	0.40
1:B:42:GLU:H	1:B:42:GLU:HG2	1.26	0.40
1:B:727:HIS:CE1	1:B:829:TYR:HE2	2.39	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	860/865 (99%)	831 (97%)	26 (3%)	3 (0%)	36	50
1	B	860/865 (99%)	828 (96%)	31 (4%)	1 (0%)	48	64
All	All	1720/1730 (99%)	1659 (96%)	57 (3%)	4 (0%)	43	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	PRO
1	A	94	GLN
1	A	708	GLY
1	B	708	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	690/692 (100%)	653 (95%)	37 (5%)	20	35
1	B	690/692 (100%)	639 (93%)	51 (7%)	13	22
All	All	1380/1384 (100%)	1292 (94%)	88 (6%)	16	28

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	41	GLU
1	A	46	LEU
1	A	59	GLU
1	A	82	THR
1	A	94	GLN
1	A	102	LEU
1	A	133	GLU
1	A	172	LYS
1	A	180	ASP
1	A	196	LEU
1	A	221	LYS
1	A	268	ARG
1	A	277	LYS
1	A	307	ILE
1	A	327	THR
1	A	344	ARG
1	A	358	ARG
1	A	391	ARG
1	A	414	GLN
1	A	431	LEU
1	A	467	ARG
1	A	523	VAL
1	A	546	LEU
1	A	590	GLU
1	A	602	ARG
1	A	614	GLU
1	A	644	ARG
1	A	773	MET
1	A	775	ASN
1	A	779	VAL
1	A	785	VAL
1	A	786	VAL
1	A	797	LEU
1	A	809	GLU

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Mol	Chain	Res	Type
1	A	834	ASP
1	A	847	ASN
1	B	2	LEU
1	B	6	ARG
1	B	12	ARG
1	B	42	GLU
1	B	46	LEU
1	B	89	LEU
1	B	99	ILE
1	B	106	LEU
1	B	133	GLU
1	B	148	GLN
1	B	157	LEU
1	B	178	ASN
1	B	196	LEU
1	B	253	VAL
1	B	268	ARG
1	B	272	LEU
1	B	277	LYS
1	B	292	LEU
1	B	340	ARG
1	B	391	ARG
1	B	399	ARG
1	B	414	GLN
1	B	431	LEU
1	B	445	THR
1	B	523	VAL
1	B	533	LEU
1	B	549	LEU
1	B	555	LEU
1	B	563	LEU
1	B	564	THR
1	B	570	LYS
1	B	602	ARG
1	B	620	LEU
1	B	627	LEU
1	B	644	ARG
1	B	677	ILE
1	B	682	LEU
1	B	694	LEU
1	B	724	LEU
1	B	748	LEU

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Mol	Chain	Res	Type
1	B	763	ARG
1	B	775	ASN
1	B	779	VAL
1	B	797	LEU
1	B	805	LEU
1	B	809	GLU
1	B	817	ILE
1	B	825	GLU
1	B	847	ASN
1	B	849	LEU
1	B	850	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	36	ASN
1	A	51	ASN
1	A	204	ASN
1	A	213	GLN
1	A	228	GLN
1	A	386	GLN
1	A	455	ASN
1	A	457	HIS
1	A	466	ASN
1	A	623	ASN
1	A	646	GLN
1	A	716	HIS
1	A	775	ASN
1	A	802	ASN
1	A	847	ASN
1	A	848	GLN
1	B	51	ASN
1	B	148	GLN
1	B	178	ASN
1	B	371	GLN
1	B	466	ASN
1	B	623	ASN
1	B	646	GLN
1	B	654	ASN
1	B	716	HIS
1	B	775	ASN

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Mol	Chain	Res	Type
1	B	832	GLN
1	B	845	ASN
1	B	847	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TRA	B	867	-	11,11,11	1.26	2 (18%)	13,14,14	1.92	6 (46%)
3	F3S	B	869	1	0,9,9	-	-	-		
3	F3S	A	868	1	0,9,9	-	-	-		
2	TRA	A	866	-	11,11,11	1.25	2 (18%)	13,14,14	2.16	6 (46%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRA	B	867	-	-	2/12/12/12	-
3	F3S	B	869	1	-	-	0/3/3/3
3	F3S	A	868	1	-	-	0/3/3/3
2	TRA	A	866	-	-	4/12/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	866	TRA	CA-CAC	2.77	1.54	1.47
2	B	867	TRA	CA-CAC	2.66	1.54	1.47
2	B	867	TRA	CBC-CB	2.54	1.55	1.49
2	A	866	TRA	CBC-CB	2.26	1.54	1.49

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	866	TRA	CGC-CG-CB	-3.54	107.06	113.25
2	A	866	TRA	OA2-CAC-CA	3.21	122.93	113.40
2	B	867	TRA	CGC-CG-CB	-3.00	108.00	113.25
2	B	867	TRA	OA2-CAC-CA	2.94	122.14	113.40
2	A	866	TRA	CAC-CA-CB	-2.88	116.68	126.33
2	A	866	TRA	OA1-CAC-CA	-2.63	115.96	124.02
2	A	866	TRA	CG-CB-CA	-2.61	118.95	125.59
2	A	866	TRA	OB2-CBC-CB	2.57	120.87	115.43
2	B	867	TRA	OA1-CAC-CA	-2.53	116.27	124.02
2	B	867	TRA	CG-CB-CA	-2.50	119.21	125.59
2	B	867	TRA	OB2-CBC-CB	2.24	120.17	115.43
2	B	867	TRA	CAC-CA-CB	-2.12	119.23	126.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	866	TRA	CB-CA-CAC-OA2
2	B	867	TRA	CB-CA-CAC-OA2
2	A	866	TRA	CB-CA-CAC-OA1
2	B	867	TRA	CB-CA-CAC-OA1
2	A	866	TRA	CB-CG-CGC-OG2
2	A	866	TRA	CB-CG-CGC-OG1

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	867	TRA	3	0
2	A	866	TRA	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	862/865 (99%)	-0.59	12 (1%) 73 69	17, 32, 71, 97	0
1	B	862/865 (99%)	-0.64	11 (1%) 75 71	18, 32, 66, 96	0
All	All	1724/1730 (99%)	-0.61	23 (1%) 75 71	17, 32, 68, 97	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	6.4
1	A	636	GLY	4.7
1	B	377	GLU	4.7
1	A	377	GLU	4.6
1	B	376	ALA	4.6
1	B	636	GLY	3.7
1	B	375	VAL	3.6
1	A	138	ALA	3.4
1	A	1	MET	3.3
1	B	378	SER	3.0
1	A	378	SER	2.7
1	B	379	ASP	2.7
1	A	375	VAL	2.6
1	A	373	LYS	2.6
1	B	380	ARG	2.4
1	A	327	THR	2.4
1	A	708	GLY	2.3
1	B	824	GLU	2.3
1	A	729	GLY	2.3
1	B	374	ASP	2.3
1	A	709	SER	2.3
1	A	137	LYS	2.2
1	B	23	ASP	2.2

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	TRA	B	867	12/12	0.95	0.08	25,31,40,65	0
2	TRA	A	866	12/12	0.97	0.06	18,26,31,37	0
3	F3S	A	868	7/7	0.99	0.05	19,26,30,30	0
3	F3S	B	869	7/7	0.99	0.05	21,26,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.