



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:52 AM UTC

PDB ID : 3B9B / pdb_00003b9b
Title : Structure of the E2 beryllium fluoride complex of the SERCA Ca²⁺-ATPase
Authors : Olesen, C.; Picard, M.; Winther, A.M.L.; Morth, J.P.; Moller, J.V.; Nissen, P.
Deposited on : 2007-11-04
Resolution : 2.65 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

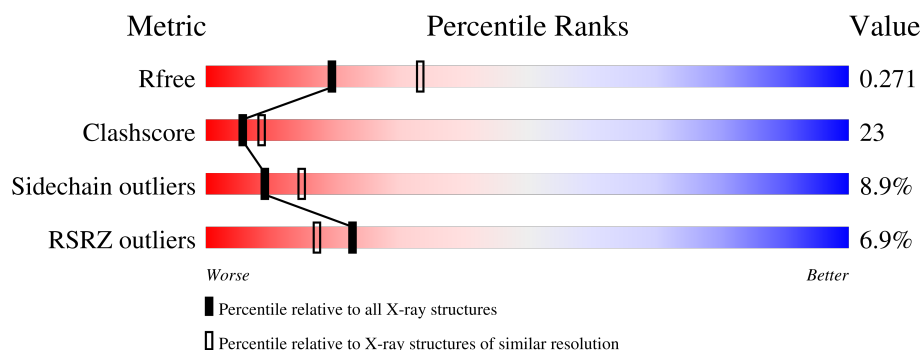
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	994	7% 58% 37% 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7743 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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	1	0	0
			7671	4876	1287	1451	57			

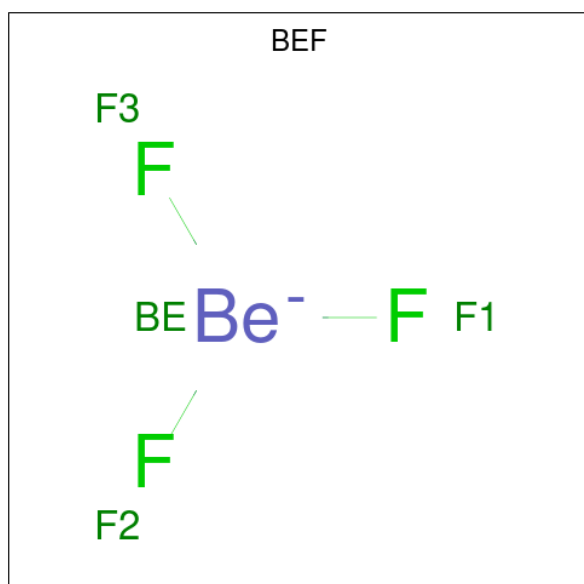
- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Be	F	0	0
			4	1	3		

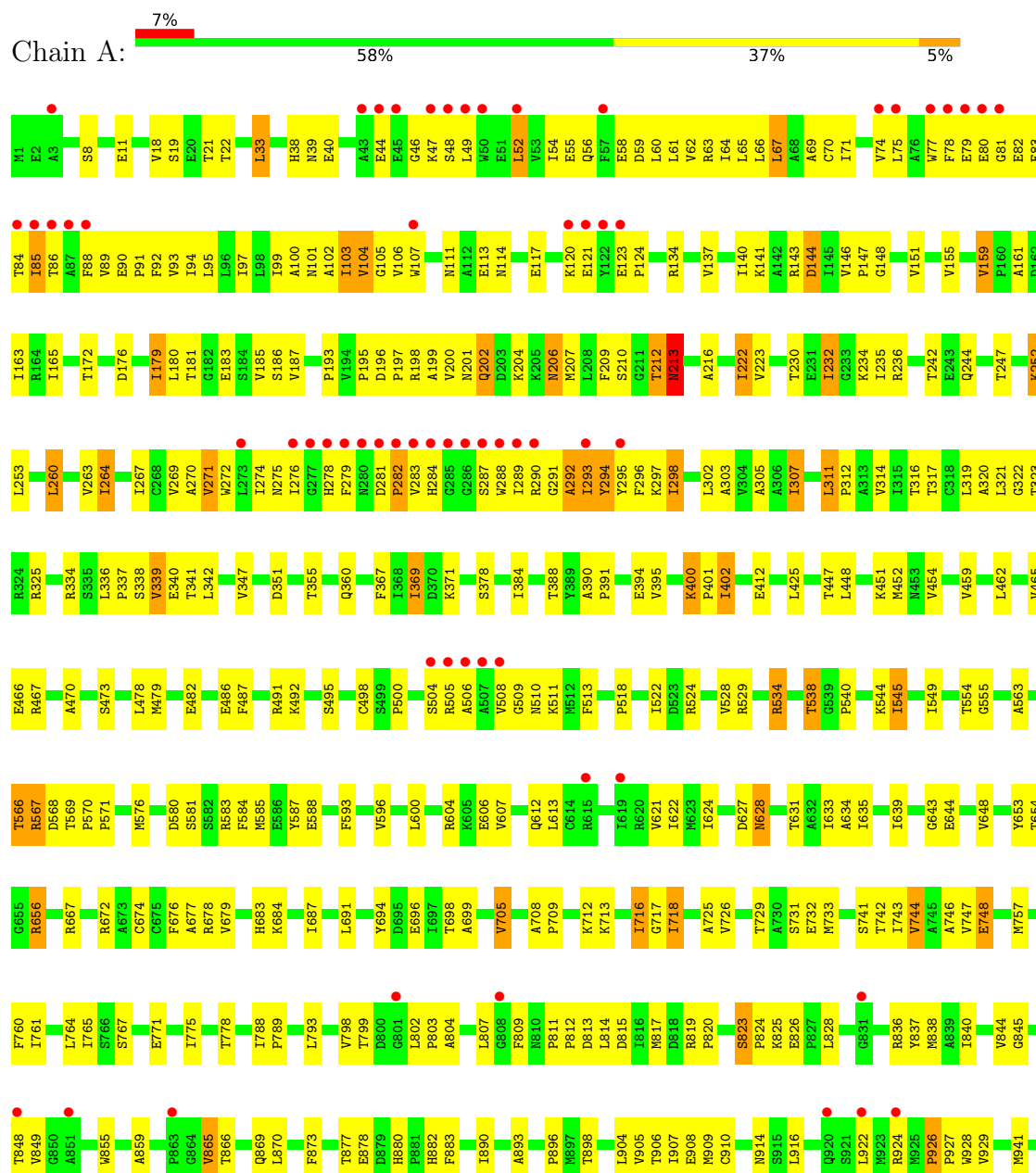
- Molecule 5 is water.

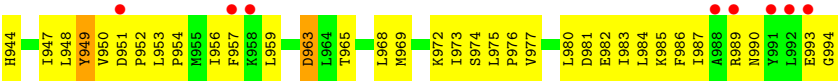
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		

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: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.60Å 114.60Å 229.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.35 – 2.65 29.35 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.35-2.65) 99.2 (29.35-2.65)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	0.27	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.64Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.271 0.215 , 0.271	Depositor DCC
R_{free} test set	1346 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7743	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, NA, MG

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	0/7812	0.89	19/10592 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLU	N-CA-C	-8.79	95.60	109.23
1	A	159	VAL	CA-C-N	8.56	128.27	119.19
1	A	159	VAL	C-N-CA	8.56	128.27	119.19
1	A	400	LYS	CA-C-N	8.11	128.11	119.76
1	A	400	LYS	C-N-CA	8.11	128.11	119.76
1	A	282	PRO	N-CA-C	7.66	124.42	113.47
1	A	292	ALA	N-CA-C	-7.42	103.81	112.86
1	A	213	ASN	N-CA-C	5.62	118.24	109.52
1	A	823	SER	CA-C-N	5.47	125.12	119.05
1	A	823	SER	C-N-CA	5.47	125.12	119.05
1	A	282	PRO	CA-C-O	-5.26	112.41	120.03
1	A	926	PRO	CA-C-N	5.20	125.50	119.47
1	A	926	PRO	C-N-CA	5.20	125.50	119.47
1	A	307	ILE	N-CA-C	5.19	113.00	107.76
1	A	294	TYR	N-CA-C	-5.18	107.50	113.88
1	A	121	GLU	CA-C-N	5.07	130.83	121.70
1	A	121	GLU	C-N-CA	5.07	130.83	121.70
1	A	569	THR	CA-C-N	5.05	125.59	120.38
1	A	569	THR	C-N-CA	5.05	125.59	120.38

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	7671	0	7764	359	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	4	0	0	0	0
5	A	65	0	0	4	0
All	All	7743	0	7764	359	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 23.

All (359) 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:123:GLU:HG3	1:A:124:PRO:HD3	1.14	1.08
1:A:33:LEU:HD11	1:A:38:HIS:CD2	1.91	1.04
1:A:282:PRO:HG2	1:A:284:HIS:HD2	1.19	1.03
1:A:123:GLU:CG	1:A:124:PRO:HD3	1.88	1.03
1:A:282:PRO:HG2	1:A:284:HIS:CD2	1.96	0.99
1:A:33:LEU:HD11	1:A:38:HIS:HD2	1.22	0.98
1:A:264:ILE:HD11	1:A:307:ILE:HD11	1.45	0.96
1:A:342:LEU:HB3	1:A:747:VAL:HG22	1.50	0.93
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.52	0.92
1:A:504:SER:O	1:A:505:ARG:HG2	1.72	0.90
1:A:866:THR:H	1:A:869:GLN:HE21	1.21	0.89
1:A:276:ILE:HG13	1:A:292:ALA:HB1	1.53	0.89
1:A:718:ILE:HD12	1:A:733:MET:HE2	1.55	0.87
1:A:123:GLU:HG3	1:A:124:PRO:CD	2.03	0.87
1:A:44:GLU:HG2	1:A:46:GLY:H	1.40	0.87
1:A:282:PRO:CG	1:A:284:HIS:HD2	1.89	0.86
1:A:510:ASN:O	1:A:570:PRO:HG2	1.78	0.84
1:A:80:GLU:O	1:A:83:GLU:HG2	1.77	0.84
1:A:198:ARG:HD2	1:A:656:ARG:HH21	1.42	0.83
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.61	0.83
1:A:699:ALA:HB2	1:A:716:ILE:HD13	1.61	0.81
1:A:48:SER:HB3	1:A:52:LEU:HD12	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:PHE:O	1:A:282:PRO:HG3	1.81	0.81
1:A:212:THR:HG21	5:A:1004:HOH:O	1.81	0.80
1:A:176:ASP:OD1	1:A:186:SER:HB3	1.82	0.79
1:A:448:LEU:HG	1:A:452:MET:HE2	1.64	0.79
1:A:580:ASP:O	1:A:583:ARG:HG2	1.82	0.78
1:A:264:ILE:HD11	1:A:307:ILE:CD1	2.12	0.78
1:A:271:VAL:O	1:A:274:ILE:HG22	1.83	0.78
1:A:82:GLU:O	1:A:82:GLU:HG2	1.82	0.78
1:A:198:ARG:HD2	1:A:656:ARG:NH2	1.99	0.77
1:A:279:PHE:CE2	1:A:291:GLY:HA3	2.22	0.75
1:A:264:ILE:CD1	1:A:307:ILE:HD11	2.15	0.75
1:A:196:ASP:HB3	1:A:199:ALA:HB2	1.68	0.75
1:A:279:PHE:CZ	1:A:291:GLY:HA3	2.22	0.75
1:A:628:ASN:ND2	1:A:631:THR:H	1.85	0.74
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.68	0.74
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.70	0.73
1:A:253:LEU:HD21	1:A:757:MET:HE1	1.71	0.73
1:A:951:ASP:HB3	1:A:952:PRO:HD3	1.69	0.73
1:A:628:ASN:HD21	1:A:631:THR:H	1.37	0.72
1:A:67:LEU:HD22	1:A:71:ILE:HG12	1.70	0.72
1:A:85:ILE:HD13	1:A:85:ILE:H	1.53	0.72
1:A:518:PRO:O	1:A:522:ILE:HG13	1.89	0.71
1:A:893:ALA:O	1:A:896:PRO:HD2	1.92	0.70
1:A:244:GLN:HE21	1:A:712:LYS:HE2	1.56	0.70
1:A:395:VAL:HG12	1:A:402:ILE:CD1	2.21	0.69
1:A:77:TRP:HD1	1:A:78:PHE:CD2	2.11	0.69
1:A:819:ARG:HG2	1:A:820:PRO:HD2	1.74	0.69
1:A:90:GLU:HG3	1:A:793:LEU:HD12	1.75	0.69
1:A:341:THR:CG2	1:A:716:ILE:HG13	2.22	0.68
1:A:342:LEU:HB3	1:A:747:VAL:CG2	2.24	0.67
1:A:554:THR:HG22	1:A:555:GLY:N	2.09	0.67
1:A:206:ASN:HD22	1:A:206:ASN:H	1.41	0.67
1:A:338:SER:OG	1:A:732:GLU:HG2	1.95	0.67
1:A:914:ASN:HB3	1:A:981:ASP:OD2	1.94	0.67
1:A:983:ILE:O	1:A:987:ILE:HG12	1.95	0.67
1:A:866:THR:H	1:A:869:GLN:NE2	1.91	0.66
1:A:924:ARG:O	1:A:926:PRO:HD3	1.95	0.66
1:A:341:THR:HG21	1:A:716:ILE:HG13	1.76	0.66
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.78	0.66
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.79	0.65
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:THR:O	1:A:910:CYS:HB2	1.97	0.65
1:A:155:VAL:HG22	1:A:216:ALA:HA	1.77	0.64
1:A:276:ILE:CG1	1:A:292:ALA:HB1	2.27	0.64
1:A:77:TRP:CD1	1:A:78:PHE:CD2	2.85	0.64
1:A:528:VAL:HG12	1:A:593:PHE:HB3	1.80	0.64
1:A:88:PHE:O	1:A:91:PRO:HD2	1.96	0.64
1:A:70:CYS:O	1:A:74:VAL:HG13	1.98	0.63
1:A:529:ARG:HH22	1:A:568:ASP:CG	2.06	0.63
1:A:77:TRP:CD1	1:A:78:PHE:HD2	2.16	0.63
1:A:202:GLN:H	1:A:202:GLN:HE21	1.47	0.63
1:A:114:ASN:HA	1:A:117:GLU:HB2	1.79	0.63
1:A:56:GLN:HG3	1:A:102:ALA:O	1.99	0.63
1:A:908:GLU:OE2	1:A:908:GLU:HA	1.97	0.63
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.81	0.62
1:A:334:ARG:NH2	1:A:729:THR:HA	2.14	0.61
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.82	0.61
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.83	0.61
1:A:44:GLU:HG2	1:A:46:GLY:N	2.13	0.61
1:A:855:TRP:CE3	1:A:896:PRO:HG3	2.36	0.61
1:A:281:ASP:N	1:A:282:PRO:HD3	2.15	0.60
1:A:369:ILE:HD11	1:A:545:ILE:HD11	1.81	0.60
1:A:283:VAL:O	1:A:283:VAL:HG23	2.01	0.60
1:A:148:GLY:HA2	1:A:222:ILE:HD11	1.83	0.60
1:A:479:MET:HE3	1:A:498:CYS:HB3	1.84	0.60
1:A:200:VAL:HG12	1:A:201:ASN:N	2.17	0.60
1:A:93:VAL:O	1:A:97:ILE:HG12	2.01	0.60
1:A:491:ARG:NH1	1:A:588:GLU:OE1	2.34	0.59
1:A:276:ILE:HG13	1:A:292:ALA:CB	2.29	0.59
1:A:232:ILE:HD13	1:A:705:VAL:HG21	1.84	0.59
1:A:264:ILE:HG23	1:A:303:ALA:HB1	1.84	0.59
1:A:18:VAL:HG12	1:A:19:SER:N	2.17	0.59
1:A:64:ILE:HG21	1:A:260:LEU:HD21	1.85	0.59
1:A:371:LYS:HB2	1:A:378:SER:OG	2.03	0.58
1:A:691:LEU:O	1:A:696:GLU:HB2	2.03	0.58
1:A:60:LEU:O	1:A:64:ILE:HG12	2.04	0.57
1:A:206:ASN:ND2	1:A:207:MET:HG2	2.18	0.57
1:A:491:ARG:NH1	1:A:588:GLU:CD	2.62	0.57
1:A:906:THR:HG22	1:A:974:SER:CB	2.34	0.57
1:A:486:GLU:O	1:A:491:ARG:NH2	2.37	0.57
1:A:305:ALA:HA	5:A:1062:HOH:O	2.03	0.57
1:A:448:LEU:CG	1:A:452:MET:HE2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:ASP:O	1:A:954:PRO:HD2	2.05	0.57
1:A:33:LEU:CD1	1:A:38:HIS:HD2	2.07	0.57
1:A:757:MET:HA	1:A:760:PHE:CE2	2.40	0.56
1:A:836:ARG:HH22	1:A:985:LYS:CG	2.18	0.56
1:A:336:LEU:O	1:A:339:VAL:HG13	2.05	0.56
1:A:412:GLU:OE2	1:A:566:THR:HG21	2.04	0.56
1:A:209:PHE:O	1:A:212:THR:HB	2.06	0.56
1:A:44:GLU:C	1:A:46:GLY:H	2.14	0.56
1:A:201:ASN:HA	1:A:204:LYS:HD2	1.86	0.56
1:A:814:LEU:HD12	1:A:814:LEU:H	1.70	0.56
1:A:33:LEU:HD12	1:A:33:LEU:O	2.05	0.56
1:A:653:TYR:OH	1:A:672:ARG:NH1	2.38	0.56
1:A:95:LEU:O	1:A:99:ILE:HG12	2.07	0.55
1:A:54:ILE:O	1:A:54:ILE:HG22	2.06	0.55
1:A:200:VAL:CG1	1:A:201:ASN:N	2.70	0.55
1:A:840:ILE:O	1:A:844:VAL:HG23	2.05	0.55
1:A:311:LEU:O	1:A:314:VAL:HG12	2.07	0.55
1:A:764:LEU:O	1:A:767:SER:HB3	2.07	0.55
1:A:86:THR:HG22	1:A:86:THR:O	2.07	0.55
1:A:914:ASN:HD22	1:A:914:ASN:H	1.54	0.55
1:A:222:ILE:HD13	1:A:223:VAL:N	2.22	0.54
1:A:718:ILE:HG21	1:A:743:ILE:HD11	1.89	0.54
1:A:282:PRO:CB	1:A:284:HIS:HD2	2.21	0.54
1:A:287:SER:C	1:A:288:TRP:CD1	2.86	0.54
1:A:487:PHE:CE2	1:A:492:LYS:HA	2.43	0.54
1:A:287:SER:O	1:A:288:TRP:CD1	2.61	0.54
1:A:788:ILE:HB	1:A:789:PRO:HD2	1.90	0.54
1:A:143:ARG:HG3	1:A:144:ASP:N	2.23	0.54
1:A:159:VAL:O	1:A:210:SER:HA	2.08	0.54
1:A:576:MET:HG2	1:A:587:TYR:CE1	2.43	0.54
1:A:113:GLU:O	1:A:117:GLU:HG2	2.08	0.54
1:A:699:ALA:CB	1:A:716:ILE:HD13	2.33	0.53
1:A:837:TYR:CD1	1:A:837:TYR:C	2.86	0.53
1:A:725:ALA:O	1:A:729:THR:HG23	2.07	0.53
1:A:969:MET:HE3	1:A:973:ILE:HD11	1.91	0.53
1:A:289:ILE:HG22	1:A:290:ARG:N	2.24	0.53
1:A:321:LEU:HD21	1:A:809:PHE:HE1	1.72	0.53
1:A:165:ILE:HD12	1:A:206:ASN:C	2.33	0.53
1:A:836:ARG:HH22	1:A:985:LYS:HG3	1.73	0.53
1:A:950:VAL:HB	1:A:953:LEU:HD12	1.91	0.53
1:A:80:GLU:HB2	1:A:83:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:O	1:A:267:ILE:HG13	2.09	0.52
1:A:141:LYS:HB2	1:A:141:LYS:NZ	2.24	0.52
1:A:486:GLU:CD	1:A:486:GLU:H	2.16	0.52
1:A:80:GLU:O	1:A:82:GLU:N	2.42	0.52
1:A:59:ASP:O	1:A:62:VAL:HG22	2.10	0.52
1:A:951:ASP:CB	1:A:952:PRO:HD3	2.38	0.52
1:A:269:VAL:O	1:A:270:ALA:C	2.51	0.52
1:A:554:THR:HG22	1:A:555:GLY:H	1.74	0.52
1:A:880:HIS:HB3	1:A:883:PHE:HD2	1.75	0.52
1:A:718:ILE:HG23	1:A:733:MET:HE2	1.92	0.52
1:A:491:ARG:HH11	1:A:588:GLU:CD	2.17	0.51
1:A:683:HIS:O	1:A:687:ILE:HG13	2.10	0.51
1:A:716:ILE:HD12	1:A:716:ILE:N	2.25	0.51
1:A:986:PHE:C	1:A:986:PHE:CD2	2.89	0.51
1:A:287:SER:O	1:A:288:TRP:CG	2.63	0.51
1:A:294:TYR:CE1	1:A:297:LYS:HD2	2.45	0.51
1:A:748:GLU:HB2	1:A:817:MET:SD	2.51	0.51
1:A:151:VAL:HG21	1:A:163:ILE:HD13	1.93	0.51
1:A:395:VAL:CG1	1:A:402:ILE:HD11	2.34	0.50
1:A:448:LEU:HG	1:A:452:MET:CE	2.39	0.50
1:A:877:THR:HG22	1:A:878:GLU:N	2.26	0.50
1:A:909:MET:N	1:A:909:MET:HE2	2.26	0.50
1:A:38:HIS:O	1:A:40:GLU:N	2.43	0.50
1:A:624:ILE:HG22	1:A:684:LYS:HE2	1.93	0.50
1:A:926:PRO:HG2	1:A:929:VAL:HG23	1.93	0.50
1:A:146:VAL:HG23	1:A:147:PRO:O	2.12	0.50
1:A:52:LEU:HD13	1:A:55:GLU:OE1	2.11	0.50
1:A:447:THR:HG22	1:A:451:LYS:HE3	1.93	0.49
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.94	0.49
1:A:880:HIS:HE1	1:A:882:HIS:HD2	1.60	0.49
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.94	0.49
1:A:321:LEU:CD2	1:A:809:PHE:HE1	2.25	0.49
1:A:77:TRP:HD1	1:A:78:PHE:HD2	1.51	0.49
1:A:643:GLY:O	1:A:644:GLU:C	2.56	0.49
1:A:462:LEU:HD22	1:A:466:GLU:HB3	1.95	0.49
1:A:717:GLY:O	1:A:731:SER:HB3	2.13	0.49
1:A:107:TRP:O	1:A:111:ASN:HB2	2.13	0.49
1:A:272:TRP:HD1	1:A:296:PHE:HA	1.77	0.49
1:A:508:VAL:HG12	1:A:508:VAL:O	2.12	0.49
1:A:633:ILE:HD13	1:A:648:VAL:HG21	1.94	0.49
1:A:922:LEU:O	1:A:926:PRO:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ASN:C	1:A:570:PRO:HG2	2.37	0.49
1:A:741:SER:O	1:A:744:VAL:HG12	2.13	0.49
1:A:103:ILE:O	1:A:106:VAL:HG22	2.13	0.48
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.94	0.48
1:A:269:VAL:O	1:A:272:TRP:N	2.46	0.48
1:A:288:TRP:CZ3	1:A:289:ILE:HD11	2.48	0.48
1:A:79:GLU:O	1:A:80:GLU:HG2	2.13	0.48
1:A:926:PRO:HB2	1:A:928:TRP:CD2	2.49	0.48
1:A:321:LEU:HD21	1:A:809:PHE:CE1	2.47	0.48
1:A:581:SER:HA	1:A:584:PHE:CE1	2.48	0.48
1:A:980:LEU:O	1:A:984:LEU:HD13	2.14	0.48
1:A:317:THR:O	1:A:321:LEU:HB2	2.14	0.48
1:A:478:LEU:C	1:A:479:MET:HG2	2.38	0.48
1:A:117:GLU:O	1:A:120:LYS:HG2	2.14	0.47
1:A:462:LEU:HD22	1:A:466:GLU:CB	2.44	0.47
1:A:319:LEU:O	1:A:322:GLY:N	2.47	0.47
1:A:947:ILE:HA	1:A:953:LEU:CD1	2.43	0.47
1:A:621:VAL:C	1:A:622:ILE:HD12	2.40	0.47
1:A:624:ILE:CG2	1:A:679:VAL:HG21	2.43	0.47
1:A:679:VAL:HB	1:A:683:HIS:HB2	1.95	0.47
1:A:635:ILE:O	1:A:639:ILE:HG12	2.14	0.47
1:A:267:ILE:HD11	1:A:303:ALA:N	2.30	0.47
1:A:648:VAL:O	1:A:648:VAL:HG23	2.14	0.47
1:A:159:VAL:HG13	1:A:163:ILE:HD12	1.96	0.47
1:A:898:THR:HA	1:A:959:LEU:HD22	1.96	0.47
1:A:267:ILE:HD13	1:A:302:LEU:HB3	1.96	0.47
1:A:278:HIS:CG	1:A:278:HIS:O	2.68	0.47
1:A:948:LEU:O	1:A:954:PRO:HG3	2.15	0.47
1:A:123:GLU:CB	1:A:124:PRO:HD3	2.45	0.47
1:A:949:TYR:N	1:A:949:TYR:CD1	2.82	0.47
1:A:500:PRO:HD3	1:A:509:GLY:O	2.15	0.47
1:A:89:VAL:O	1:A:93:VAL:HG22	2.14	0.46
1:A:230:THR:O	1:A:234:LYS:HG3	2.14	0.46
1:A:269:VAL:O	1:A:271:VAL:N	2.47	0.46
1:A:870:LEU:O	1:A:873:PHE:HD2	1.98	0.46
1:A:771:GLU:O	1:A:775:ILE:HG12	2.15	0.46
1:A:179:ILE:HG23	5:A:1010:HOH:O	2.14	0.46
1:A:334:ARG:HH21	1:A:729:THR:HA	1.80	0.46
1:A:195:PRO:O	1:A:196:ASP:C	2.58	0.46
1:A:798:VAL:O	1:A:799:THR:C	2.59	0.46
1:A:974:SER:O	1:A:977:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:VAL:C	1:A:147:PRO:O	2.57	0.46
1:A:295:TYR:O	1:A:298:ILE:HG12	2.15	0.46
1:A:470:ALA:O	1:A:473:SER:HB2	2.16	0.46
1:A:176:ASP:HB2	1:A:213:ASN:OD1	2.16	0.46
1:A:206:ASN:H	1:A:206:ASN:ND2	2.10	0.46
1:A:963:ASP:OD2	1:A:963:ASP:C	2.57	0.46
1:A:78:PHE:CD1	1:A:78:PHE:C	2.94	0.45
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.38	0.45
1:A:554:THR:CG2	1:A:555:GLY:N	2.78	0.45
1:A:49:LEU:O	1:A:52:LEU:HB2	2.16	0.45
1:A:206:ASN:HD22	1:A:206:ASN:N	2.04	0.45
1:A:367:PHE:CD2	1:A:367:PHE:C	2.94	0.45
1:A:18:VAL:HG12	1:A:19:SER:H	1.81	0.45
1:A:222:ILE:HD13	1:A:222:ILE:C	2.42	0.45
1:A:44:GLU:C	1:A:46:GLY:N	2.74	0.45
1:A:743:ILE:O	1:A:747:VAL:HG23	2.17	0.45
1:A:916:LEU:HD23	1:A:916:LEU:HA	1.73	0.45
1:A:989:ARG:NH1	1:A:990:ASN:HD21	2.15	0.45
1:A:319:LEU:O	1:A:320:ALA:C	2.58	0.45
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.99	0.45
1:A:59:ASP:O	1:A:63:ARG:HG2	2.17	0.45
1:A:59:ASP:HB3	1:A:62:VAL:HG22	1.99	0.45
1:A:718:ILE:CG2	1:A:733:MET:HE2	2.47	0.45
1:A:193:PRO:O	1:A:195:PRO:HD3	2.17	0.44
1:A:613:LEU:HB2	1:A:744:VAL:HG21	1.98	0.44
1:A:823:SER:HA	1:A:824:PRO:HD3	1.83	0.44
1:A:845:GLY:O	1:A:849:VAL:HG23	2.17	0.44
1:A:904:LEU:O	1:A:905:VAL:C	2.60	0.44
1:A:340:GLU:O	1:A:341:THR:C	2.59	0.44
1:A:90:GLU:O	1:A:94:ILE:HG12	2.17	0.44
1:A:287:SER:C	1:A:288:TRP:CG	2.96	0.44
1:A:55:GLU:HG2	1:A:58:GLU:OE2	2.17	0.44
1:A:244:GLN:HE21	1:A:712:LYS:CE	2.28	0.44
1:A:811:PRO:HA	1:A:812:PRO:HD3	1.87	0.44
1:A:100:ALA:O	1:A:104:VAL:HG12	2.18	0.43
1:A:347:VAL:CG1	1:A:622:ILE:HD13	2.48	0.43
1:A:947:ILE:HD13	1:A:957:PHE:CE1	2.53	0.43
1:A:291:GLY:C	1:A:293:ILE:N	2.73	0.43
1:A:927:PRO:HG2	1:A:928:TRP:CE3	2.53	0.43
1:A:103:ILE:C	1:A:105:GLY:N	2.74	0.43
1:A:235:ILE:HG21	1:A:705:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ILE:HD13	1:A:545:ILE:HG21	1.99	0.43
1:A:968:LEU:O	1:A:972:LYS:HG3	2.17	0.43
1:A:71:ILE:HA	1:A:74:VAL:HG22	1.99	0.43
1:A:804:ALA:O	1:A:807:LEU:HB2	2.18	0.43
1:A:819:ARG:HG2	1:A:820:PRO:CD	2.46	0.43
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.84	0.43
1:A:495:SER:HA	1:A:513:PHE:O	2.17	0.43
1:A:950:VAL:O	1:A:951:ASP:C	2.62	0.43
1:A:247:THR:OG1	1:A:337:PRO:HB2	2.18	0.43
1:A:282:PRO:CG	1:A:284:HIS:CD2	2.77	0.43
1:A:518:PRO:HA	1:A:563:ALA:HB2	2.01	0.43
1:A:571:PRO:HB2	1:A:576:MET:SD	2.59	0.43
1:A:742:THR:O	1:A:746:ALA:N	2.45	0.43
1:A:865:VAL:HB	1:A:869:GLN:NE2	2.33	0.43
1:A:274:ILE:HG23	1:A:275:ASN:OD1	2.19	0.43
1:A:290:ARG:NH1	1:A:291:GLY:O	2.52	0.43
1:A:39:ASN:O	1:A:143:ARG:HA	2.18	0.43
1:A:180:LEU:HD23	1:A:181:THR:HG23	2.01	0.43
1:A:287:SER:O	1:A:289:ILE:HG12	2.19	0.43
1:A:412:GLU:OE1	1:A:529:ARG:HD2	2.19	0.42
1:A:538:THR:OG1	1:A:540:PRO:HD2	2.19	0.42
1:A:183:GLU:HA	1:A:627:ASP:OD1	2.19	0.42
1:A:667:ARG:NH1	1:A:694:TYR:CE2	2.88	0.42
1:A:993:GLU:O	1:A:994:GLY:C	2.62	0.42
1:A:80:GLU:O	1:A:81:GLY:C	2.62	0.42
1:A:288:TRP:CH2	1:A:289:ILE:HD11	2.54	0.42
1:A:289:ILE:HG21	1:A:294:TYR:CD1	2.54	0.42
1:A:613:LEU:CB	1:A:744:VAL:HG21	2.49	0.42
1:A:351:ASP:HA	1:A:624:ILE:O	2.19	0.42
1:A:760:PHE:CD1	1:A:760:PHE:C	2.98	0.42
1:A:953:LEU:HD23	1:A:956:ILE:HD11	2.01	0.42
1:A:196:ASP:HA	1:A:197:PRO:HD3	1.69	0.42
1:A:653:TYR:O	1:A:676:PHE:HA	2.20	0.42
1:A:232:ILE:HD13	1:A:232:ILE:HA	1.87	0.42
1:A:716:ILE:HD12	1:A:716:ILE:H	1.85	0.42
1:A:269:VAL:HG12	1:A:270:ALA:N	2.34	0.42
1:A:316:THR:O	1:A:316:THR:HG22	2.20	0.42
1:A:19:SER:C	1:A:21:THR:H	2.27	0.42
1:A:252:LYS:NZ	1:A:826:GLU:O	2.50	0.42
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.85	0.42
1:A:92:PHE:HA	1:A:95:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HG22	1:A:104:VAL:N	2.34	0.42
1:A:877:THR:CG2	1:A:878:GLU:N	2.83	0.42
1:A:336:LEU:N	1:A:337:PRO:HD2	2.35	0.41
1:A:390:ALA:HA	1:A:391:PRO:HD3	1.72	0.41
1:A:412:GLU:OE1	1:A:529:ARG:CD	2.68	0.41
1:A:500:PRO:HB2	1:A:506:ALA:HB2	2.02	0.41
1:A:683:HIS:O	1:A:684:LYS:C	2.61	0.41
1:A:906:THR:HG22	1:A:974:SER:HB2	2.01	0.41
1:A:8:SER:H	1:A:11:GLU:HB2	1.85	0.41
1:A:159:VAL:HG12	1:A:161:ALA:O	2.21	0.41
1:A:289:ILE:CG2	1:A:290:ARG:N	2.84	0.41
1:A:148:GLY:CA	1:A:222:ILE:HD11	2.50	0.41
1:A:291:GLY:O	1:A:292:ALA:HB3	2.21	0.41
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.92	0.41
1:A:654:THR:HA	1:A:677:ALA:O	2.21	0.41
1:A:975:LEU:HB2	1:A:976:PRO:HD3	2.03	0.41
1:A:33:LEU:HD12	1:A:33:LEU:C	2.45	0.41
1:A:48:SER:CB	1:A:52:LEU:HD12	2.42	0.41
1:A:75:LEU:HD23	1:A:75:LEU:O	2.20	0.41
1:A:360:GLN:OE1	1:A:388:THR:HB	2.21	0.41
1:A:400:LYS:HA	1:A:401:PRO:HD3	1.83	0.41
1:A:922:LEU:HD13	1:A:982:GLU:OE1	2.20	0.41
1:A:529:ARG:NH2	1:A:568:ASP:OD1	2.50	0.41
1:A:947:ILE:HA	1:A:953:LEU:HD13	2.01	0.41
1:A:140:ILE:HG22	1:A:141:LYS:O	2.20	0.41
1:A:146:VAL:O	1:A:147:PRO:C	2.61	0.41
1:A:518:PRO:HA	1:A:563:ALA:CB	2.51	0.41
1:A:633:ILE:O	1:A:634:ALA:C	2.62	0.41
1:A:242:THR:HG23	1:A:713:LYS:HD2	2.02	0.41
1:A:511:LYS:HE2	5:A:1039:HOH:O	2.21	0.41
1:A:926:PRO:HD2	1:A:929:VAL:HG23	2.03	0.41
1:A:69:ALA:HB2	1:A:94:ILE:HG21	2.03	0.40
1:A:302:LEU:O	1:A:305:ALA:HB3	2.21	0.40
1:A:534:ARG:HH21	1:A:568:ASP:HB2	1.86	0.40
1:A:92:PHE:O	1:A:95:LEU:HB2	2.21	0.40
1:A:275:ASN:HB3	1:A:295:TYR:CE2	2.56	0.40
1:A:500:PRO:HB2	1:A:506:ALA:CB	2.51	0.40
1:A:628:ASN:ND2	1:A:628:ASN:C	2.79	0.40
1:A:761:ILE:O	1:A:765:ILE:HG22	2.21	0.40
1:A:948:LEU:HB2	1:A:949:TYR:HD1	1.87	0.40
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:THR:O	1:A:86:THR:N	2.48	0.40
1:A:200:VAL:CG1	1:A:201:ASN:H	2.33	0.40
1:A:844:VAL:O	1:A:848:THR:HG23	2.21	0.40
1:A:941:MET:O	1:A:944:HIS:HB3	2.21	0.40
1:A:47:LYS:HG3	1:A:47:LYS:O	2.21	0.40
1:A:319:LEU:O	1:A:321:LEU:N	2.55	0.40
1:A:19:SER:C	1:A:21:THR:N	2.79	0.40
1:A:252:LYS:HD2	1:A:252:LYS:HA	1.70	0.40
1:A:351:ASP:O	1:A:355:THR:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	840/840 (100%)	765 (91%)	75 (9%)	9 15

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	33	LEU
1	A	52	LEU
1	A	65	LEU
1	A	66	LEU
1	A	67	LEU
1	A	85	ILE

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Mol	Chain	Res	Type
1	A	101	ASN
1	A	103	ILE
1	A	104	VAL
1	A	137	VAL
1	A	144	ASP
1	A	172	THR
1	A	179	ILE
1	A	185	VAL
1	A	187	VAL
1	A	202	GLN
1	A	206	ASN
1	A	212	THR
1	A	213	ASN
1	A	222	ILE
1	A	232	ILE
1	A	236	ARG
1	A	252	LYS
1	A	260	LEU
1	A	263	VAL
1	A	264	ILE
1	A	271	VAL
1	A	293	ILE
1	A	298	ILE
1	A	311	LEU
1	A	323	THR
1	A	339	VAL
1	A	369	ILE
1	A	384	ILE
1	A	394	GLU
1	A	402	ILE
1	A	454	VAL
1	A	459	VAL
1	A	465	VAL
1	A	467	ARG
1	A	482	GLU
1	A	524	ARG
1	A	534	ARG
1	A	538	THR
1	A	544	LYS
1	A	545	ILE
1	A	566	THR
1	A	567	ARG

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Mol	Chain	Res	Type
1	A	585	MET
1	A	600	LEU
1	A	606	GLU
1	A	612	GLN
1	A	628	ASN
1	A	656	ARG
1	A	674	CYS
1	A	678	ARG
1	A	698	THR
1	A	705	VAL
1	A	716	ILE
1	A	718	ILE
1	A	726	VAL
1	A	744	VAL
1	A	748	GLU
1	A	778	THR
1	A	813	ASP
1	A	815	ASP
1	A	825	LYS
1	A	828	LEU
1	A	838	MET
1	A	865	VAL
1	A	890	ILE
1	A	949	TYR
1	A	963	ASP
1	A	965	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	206	ASN
1	A	244	GLN
1	A	250	GLN
1	A	284	HIS
1	A	398	ASN
1	A	428	ASN
1	A	469	ASN
1	A	472	ASN
1	A	628	ASN
1	A	756	ASN
1	A	868	HIS

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Mol	Chain	Res	Type
1	A	869	GLN
1	A	875	GLN
1	A	882	HIS
1	A	920	GLN
1	A	990	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](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
4	BEF	A	998	1	0,3,3	-	-	-		

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 [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	994/994 (100%)	0.10	69 (6%)	23 17	8, 49, 133, 318	1 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	VAL	8.7
1	A	50	TRP	6.5
1	A	281	ASP	5.7
1	A	78	PHE	5.5
1	A	505	ARG	5.0
1	A	122	TYR	4.9
1	A	507	ALA	4.9
1	A	506	ALA	4.7
1	A	74	VAL	4.7
1	A	282	PRO	4.6
1	A	48	SER	4.5
1	A	279	PHE	4.4
1	A	508	VAL	4.3
1	A	80	GLU	4.2
1	A	863	PRO	4.2
1	A	287	SER	4.1
1	A	87	ALA	4.1
1	A	992	LEU	4.0
1	A	288	TRP	3.9
1	A	957	PHE	3.9
1	A	121	GLU	3.8
1	A	52	LEU	3.8
1	A	295	TYR	3.7
1	A	278	HIS	3.5
1	A	43	ALA	3.5
1	A	289	ILE	3.4
1	A	286	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	86	THR	3.2
1	A	85	ILE	3.2
1	A	290	ARG	3.2
1	A	808	GLY	3.2
1	A	951	ASP	3.1
1	A	49	LEU	3.1
1	A	79	GLU	3.1
1	A	84	THR	3.1
1	A	75	LEU	3.1
1	A	280	ASN	3.0
1	A	285	GLY	3.0
1	A	284	HIS	3.0
1	A	991	TYR	3.0
1	A	47	LYS	2.9
1	A	851	ALA	2.9
1	A	293	ILE	2.8
1	A	88	PHE	2.8
1	A	120	LYS	2.8
1	A	45	GLU	2.7
1	A	920	GLN	2.6
1	A	77	TRP	2.6
1	A	848	THR	2.5
1	A	619	ILE	2.5
1	A	922	LEU	2.4
1	A	107	TRP	2.4
1	A	988	ALA	2.4
1	A	276	ILE	2.4
1	A	924	ARG	2.4
1	A	801	GLY	2.3
1	A	831	GLY	2.3
1	A	277	GLY	2.3
1	A	57	PHE	2.3
1	A	273	LEU	2.2
1	A	44	GLU	2.2
1	A	504	SER	2.2
1	A	81	GLY	2.2
1	A	3	ALA	2.1
1	A	989	ARG	2.1
1	A	123	GLU	2.1
1	A	615	ARG	2.0
1	A	993	GLU	2.0
1	A	958	LYS	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 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
3	MG	A	997	1/1	0.85	0.20	98,98,98,98	0
2	NA	A	995	1/1	0.88	0.36	69,69,69,69	0
4	BEF	A	998	4/4	0.98	0.05	30,35,37,45	0
3	MG	A	996	1/1	0.99	0.03	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.