



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:33 AM GMT

PDB ID : 3B9B  
Title : Structure of the E2 beryllium fluoride complex of the SERCA Ca<sup>2+</sup>-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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

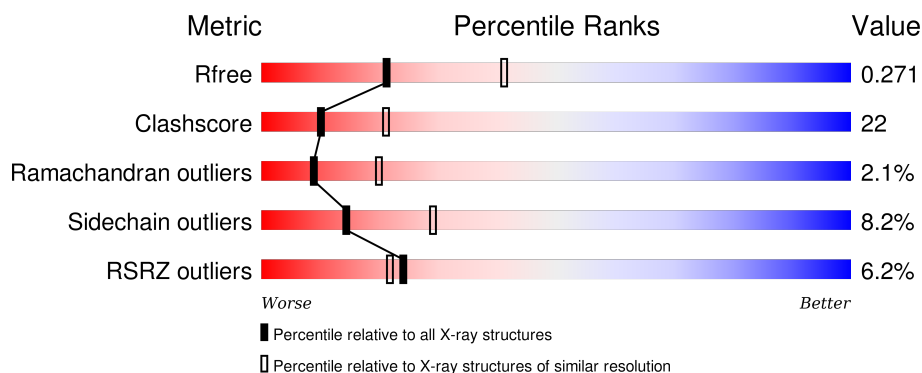
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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  $\geq 3$ , 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	994	

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
2	NA	A	995	-	-	-	X

## 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			

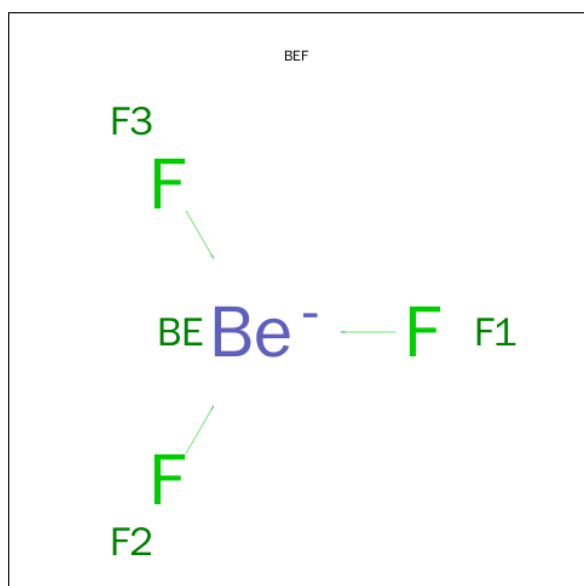
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



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

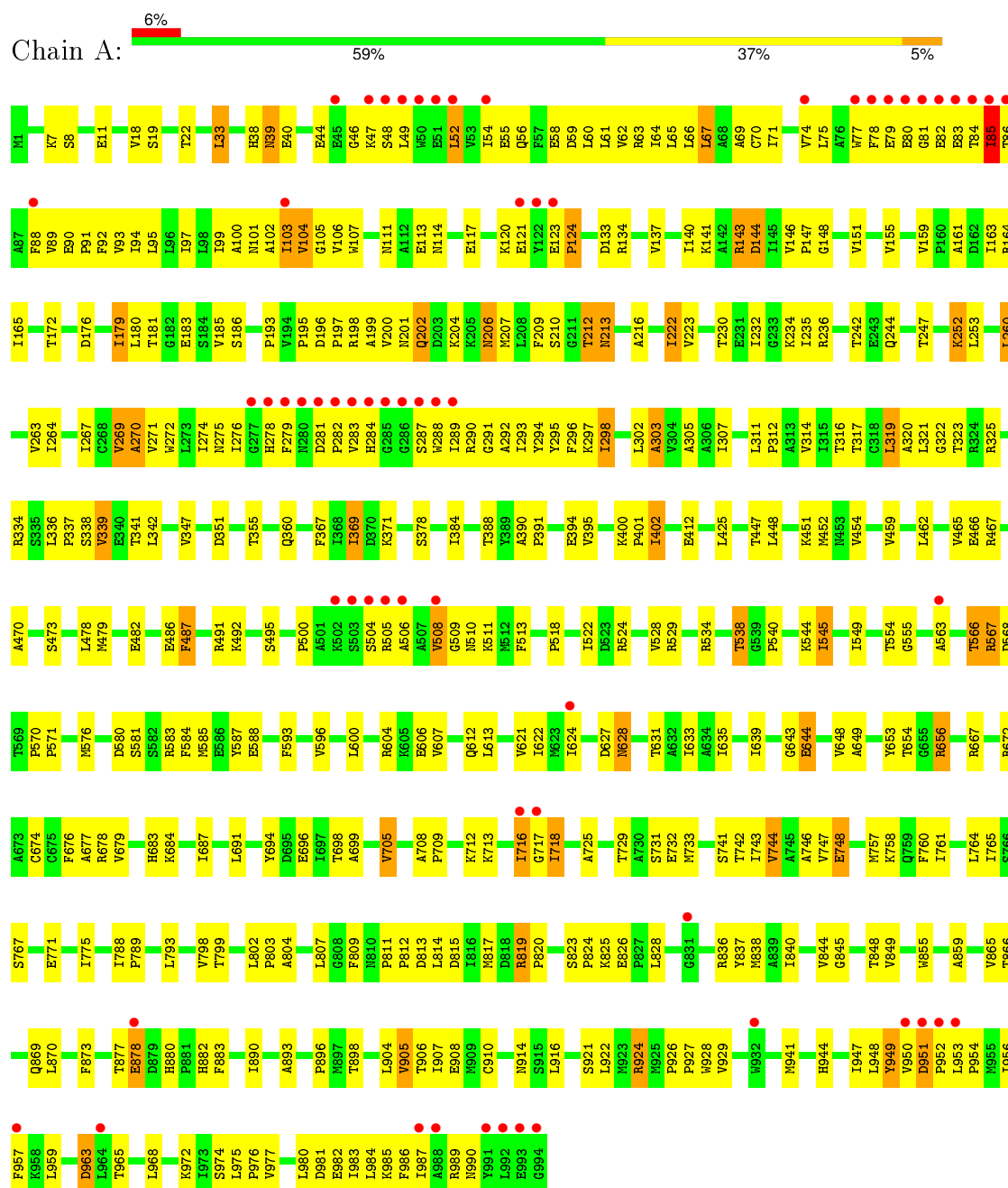
- Molecule 5 is water.

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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, $\alpha$ , $\beta$ , $\gamma$	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) 99.3 (29.35-2.65)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	0.27	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.64Å)	Xtriage
Refinement program	phenix.refine	Depositor
R, $R_{free}$	0.214 , 0.271 0.215 , 0.271	Depositor DCC
$R_{free}$ test set	1346 reflections (3.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 44779 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, MG, BEF

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	0.35	0/7812	0.56	1/10592 (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	121	GLU	N-CA-C	-5.70	95.60	111.00

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	7671	0	7764	338	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	338	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 22.

All (338) 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:718:ILE:HD12	1:A:733:MET:HE2	1.47	0.95
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: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
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:82:GLU:HG2	1:A:82:GLU:O	1.82	0.79
1:A:176:ASP:OD1	1:A:186:SER:HB3	1.82	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: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:279:PHE:CZ	1:A:291:GLY:HA3	2.22	0.75
1:A:196:ASP:HB3	1:A:199:ALA:HB2	1.68	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:206:ASN:HD22	1.41	0.67
1:A:983:ILE:O	1:A:987:ILE:HG12	1.95	0.67
1:A:914:ASN:HB3	1:A:981:ASP:OD2	1.94	0.67
1:A:338:SER:OG	1:A:732:GLU:HG2	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
1:A:906:THR:O	1:A:910:CYS:HB2	1.97	0.65
1:A:276:ILE:CG1	1:A:292:ALA:HB1	2.27	0.64
1:A:155:VAL:HG22	1:A:216:ALA:HA	1.77	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:529:ARG:HH22	1:A:568:ASP:CG	2.06	0.58
1:A:448:LEU:HG	1:A:452:MET:HE3	1.86	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: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: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:412:GLU:OE2	1:A:566:THR:HG21	2.04	0.56
1:A:336:LEU:O	1:A:339:VAL:HG13	2.05	0.56
1:A:209:PHE:O	1:A:212:THR:HB	2.06	0.56
1:A:201:ASN:HA	1:A:204:LYS:HD2	1.86	0.56
1:A:814:LEU:H	1:A:814:LEU:HD12	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:200:VAL:CG1	1:A:201:ASN:N	2.70	0.55
1:A:54:ILE:O	1:A:54:ILE:HG22	2.06	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:O	1:A:86:THR:HG22	2.07	0.55
1:A:914:ASN:H	1:A:914:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:725:ALA:O	1:A:729:THR:HG23	2.07	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:950:VAL:HB	1:A:953:LEU:HD12	1.91	0.53
1:A:836:ARG:HH22	1:A:985:LYS:HG3	1.73	0.53
1:A:491:ARG:NH1	1:A:588:GLU:CD	2.62	0.53
1:A:80:GLU:HB2	1:A:83:GLU:OE2	2.09	0.53
1:A:264:ILE:O	1:A:267:ILE:HG13	2.09	0.52
1:A:448:LEU:HG	1:A:452:MET:CE	2.39	0.52
1:A:141:LYS:NZ	1:A:141:LYS:HB2	2.24	0.52
1:A:80:GLU:O	1:A:82:GLU:N	2.42	0.52
1:A:951:ASP:CB	1:A:952:PRO:HD3	2.38	0.52
1:A:59:ASP:O	1:A:62:VAL:HG22	2.10	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:683:HIS:O	1:A:687:ILE:HG13	2.10	0.51
1:A:44:GLU:C	1:A:46:GLY:H	2.14	0.51
1:A:716:ILE:N	1:A:716:ILE:HD12	2.25	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:877:THR:HG22	1:A:878:GLU:N	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:953:LEU:HB2	1:A:954:PRO:HD3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:SER:C	1:A:288:TRP:CD1	2.86	0.49
1:A:321:LEU:CD2	1:A:809:PHE:HE1	2.25	0.49
1:A:508:VAL:HG12	1:A:508:VAL:O	2.12	0.49
1:A:77:TRP:HD1	1:A:78:PHE:HD2	1.51	0.49
1:A:717:GLY:O	1:A:731:SER:HB3	2.13	0.49
1:A:462:LEU:HD22	1:A:466:GLU:HB3	1.95	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:922:LEU:O	1:A:926:PRO:HA	2.13	0.49
1:A:633:ILE:HD13	1:A:648:VAL:HG21	1.94	0.49
1:A:837:TYR:C	1:A:837:TYR:CD1	2.86	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:269:VAL:O	1:A:270:ALA:C	2.51	0.48
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.94	0.48
1:A:165:ILE:HD12	1:A:206:ASN:C	2.33	0.48
1:A:288:TRP:CZ3	1:A:289:ILE:HD11	2.48	0.48
1:A:269:VAL:O	1:A:272:TRP:N	2.46	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: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:947:ILE:HA	1:A:953:LEU:CD1	2.43	0.47
1:A:319:LEU:O	1:A:322:GLY:N	2.47	0.47
1:A:486:GLU:CD	1:A:486:GLU:H	2.16	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:HG23	1:A:648:VAL:O	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:948:LEU:O	1:A:954:PRO:HG3	2.15	0.47
1:A:278:HIS:O	1:A:278:HIS:CG	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:PRO:HD3	1:A:509:GLY:O	2.15	0.47
1:A:269:VAL:O	1:A:271:VAL:N	2.47	0.46
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:491:ARG:HH11	1:A:588:GLU:CD	2.17	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:986:PHE:CD2	1:A:986:PHE:C	2.89	0.46
1:A:334:ARG:HH21	1:A:729:THR:HA	1.80	0.46
1:A:179:ILE:HG23	5:A:1010:HOH:O	2.14	0.46
1:A:974:SER:O	1:A:977:VAL:HG12	2.16	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: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:253:LEU:HD21	1:A:757:MET:HE1	1.97	0.45
1:A:49:LEU:O	1:A:52:LEU:HB2	2.16	0.45
1:A:206:ASN:N	1:A:206:ASN:HD22	2.04	0.45
1:A:18:VAL:HG12	1:A:19:SER:H	1.81	0.45
1:A:743:ILE:O	1:A:747:VAL:HG23	2.17	0.45
1:A:916:LEU:HA	1:A:916:LEU:HD23	1.73	0.45
1:A:989:ARG:NH1	1:A:990:ASN:HD21	2.15	0.45
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.99	0.45
1:A:141:LYS:HB2	1:A:141:LYS:HZ3	1.81	0.45
1:A:59:ASP:HB3	1:A:62:VAL:HG22	1.99	0.45
1:A:59:ASP:O	1:A:63:ARG:HG2	2.17	0.45
1:A:643:GLY:O	1:A:644:GLU:C	2.56	0.44
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:845:GLY:O	1:A:849:VAL:HG23	2.17	0.44
1:A:823:SER:HA	1:A:824:PRO:HD3	1.83	0.44
1:A:510:ASN:C	1:A:570:PRO:HG2	2.37	0.44
1:A:90:GLU:O	1:A:94:ILE:HG12	2.17	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:947:ILE:HD13	1:A:957:PHE:CE1	2.53	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:PRO:HG2	1:A:928:TRP:CE3	2.53	0.43
1:A:522:ILE:HD13	1:A:545:ILE:HG21	1.99	0.43
1:A:235:ILE:HG21	1:A:705:VAL:O	2.18	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:819:ARG:HG2	1:A:820:PRO:CD	2.46	0.43
1:A:804:ALA:O	1:A:807:LEU:HB2	2.18	0.43
1:A:495:SER:HA	1:A:513:PHE:O	2.17	0.43
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.84	0.43
1:A:282:PRO:CG	1:A:284:HIS:CD2	2.77	0.43
1:A:865:VAL:HB	1:A:869:GLN:NE2	2.33	0.43
1:A:518:PRO:HA	1:A:563:ALA:HB2	2.01	0.43
1:A:247:THR:OG1	1:A:337:PRO:HB2	2.18	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:290:ARG:NH1	1:A:291:GLY:O	2.52	0.43
1:A:274:ILE:HG23	1:A:275:ASN:OD1	2.19	0.43
1:A:478:LEU:C	1:A:479:MET:HG2	2.38	0.43
1:A:39:ASN:O	1:A:143:ARG:HA	2.18	0.43
1:A:287:SER:O	1:A:289:ILE:HG12	2.19	0.43
1:A:180:LEU:HD23	1:A:181:THR:HG23	2.01	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:621:VAL:C	1:A:622:ILE:HD12	2.40	0.42
1:A:667:ARG:NH1	1:A:694:TYR:CE2	2.88	0.42
1:A:183:GLU:HA	1:A:627:ASP:OD1	2.19	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:953:LEU:HD23	1:A:956:ILE:HD11	2.01	0.42
1:A:351:ASP:HA	1:A:624:ILE:O	2.19	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:716:ILE:H	1:A:716:ILE:HD12	1.85	0.42
1:A:232:ILE:HD13	1:A:232:ILE:HA	1.87	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:325:ARG:HG3	1:A:325:ARG:HH11	1.85	0.42
1:A:252:LYS:NZ	1:A:826:GLU:O	2.50	0.42
1:A:92:PHE:HA	1:A:95:LEU:HD12	2.02	0.42
1:A:877:THR:CG2	1:A:878:GLU:N	2.83	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:412:GLU:OE1	1:A:529:ARG:CD	2.68	0.41
1:A:336:LEU:N	1:A:337:PRO:HD2	2.35	0.41
1:A:500:PRO:HB2	1:A:506:ALA:HB2	2.02	0.41
1:A:390:ALA:HA	1:A:391:PRO:HD3	1.72	0.41
1:A:103:ILE:C	1:A:105:GLY:N	2.74	0.41
1:A:906:THR:HG22	1:A:974:SER:HB2	2.01	0.41
1:A:195:PRO:O	1:A:196:ASP:C	2.58	0.41
1:A:289:ILE:CG2	1:A:290:ARG:N	2.84	0.41
1:A:798:VAL:O	1:A:799:THR:C	2.59	0.41
1:A:159:VAL:HG12	1:A:161:ALA:O	2.21	0.41
1:A:8:SER:H	1:A:11:GLU:HB2	1.85	0.41
1:A:291:GLY:O	1:A:292:ALA:HB3	2.21	0.41
1:A:148:GLY:CA	1:A:222:ILE:HD11	2.50	0.41
1:A:146:VAL:C	1:A:147:PRO:O	2.57	0.41
1:A:654:THR:HA	1:A:677:ALA:O	2.21	0.41
1:A:963:ASP:C	1:A:963:ASP:OD2	2.57	0.41
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.92	0.41
1:A:975:LEU:HB2	1:A:976:PRO:HD3	2.03	0.41
1:A:48:SER:CB	1:A:52:LEU:HD12	2.42	0.41
1:A:922:LEU:HD13	1:A:982:GLU:OE1	2.20	0.41
1:A:75:LEU:HD23	1:A:75:LEU:O	2.20	0.41
1:A:400:LYS:HA	1:A:401:PRO:HD3	1.83	0.41
1:A:360:GLN:OE1	1:A:388:THR:HB	2.21	0.41
1:A:947:ILE:HA	1:A:953:LEU:HD13	2.01	0.41
1:A:529:ARG:NH2	1:A:568:ASP:OD1	2.50	0.41
1:A:518:PRO:HA	1:A:563:ALA:CB	2.51	0.41
1:A:78:PHE:CD1	1:A:78:PHE:C	2.94	0.41
1:A:140:ILE:HG22	1:A:141:LYS:O	2.20	0.41
1:A:926:PRO:HD2	1:A:929:VAL:HG23	2.03	0.41
1:A:367:PHE:C	1:A:367:PHE:CD2	2.94	0.41
1:A:511:LYS:HE2	5:A:1039:HOH:O	2.21	0.41
1:A:242:THR:HG23	1:A:713:LYS:HD2	2.02	0.41
1:A:302:LEU:O	1:A:305:ALA:HB3	2.21	0.40
1:A:69:ALA:HB2	1:A:94:ILE:HG21	2.03	0.40
1:A:534:ARG:HH21	1:A:568:ASP:HB2	1.86	0.40
1:A:44:GLU:C	1:A:46:GLY:N	2.74	0.40
1:A:275:ASN:HB3	1:A:295:TYR:CE2	2.56	0.40
1:A:948:LEU:HB2	1:A:949:TYR:HD1	1.87	0.40
1:A:92:PHE:O	1:A:95:LEU:HB2	2.21	0.40
1:A:500:PRO:HB2	1:A:506:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:ILE:O	1:A:765:ILE:HG22	2.21	0.40
1:A:844:VAL:O	1:A:848:THR:HG23	2.21	0.40
1:A:200:VAL:CG1	1:A:201:ASN:H	2.33	0.40
1:A:84:THR:O	1:A:86:THR:N	2.48	0.40
1:A:941:MET:O	1:A:944:HIS:HB3	2.21	0.40
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.90	0.40
1:A:319:LEU:O	1:A:321:LEU:N	2.55	0.40
1:A:47:LYS:O	1:A:47:LYS:HG3	2.21	0.40
1:A:319:LEU:O	1:A:320:ALA:C	2.58	0.40
1:A:351:ASP:O	1:A:355:THR:HB	2.21	0.40
1:A:252:LYS:HD2	1:A:252:LYS:HA	1.70	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	992/994 (100%)	895 (90%)	76 (8%)	21 (2%)	<b>9</b> <b>20</b>

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	124	PRO
1	A	270	ALA
1	A	508	VAL
1	A	649	ALA
1	A	924	ARG
1	A	951	ASP
1	A	81	GLY
1	A	85	ILE
1	A	269	VAL

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Mol	Chain	Res	Type
1	A	487	PHE
1	A	644	GLU
1	A	905	VAL
1	A	293	ILE
1	A	921	SER
1	A	133	ASP
1	A	303	ALA
1	A	758	LYS
1	A	878	GLU
1	A	904	LEU
1	A	319	LEU

### 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	840/840 (100%)	771 (92%)	69 (8%)	14	29

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
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
1	A	101	ASN
1	A	103	ILE
1	A	104	VAL
1	A	137	VAL
1	A	143	ARG
1	A	144	ASP
1	A	164	ARG

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Mol	Chain	Res	Type
1	A	172	THR
1	A	179	ILE
1	A	185	VAL
1	A	202	GLN
1	A	206	ASN
1	A	212	THR
1	A	213	ASN
1	A	222	ILE
1	A	236	ARG
1	A	252	LYS
1	A	260	LEU
1	A	263	VAL
1	A	298	ILE
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	538	THR
1	A	544	LYS
1	A	545	ILE
1	A	566	THR
1	A	567	ARG
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

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Mol	Chain	Res	Type
1	A	744	VAL
1	A	748	GLU
1	A	813	ASP
1	A	815	ASP
1	A	819	ARG
1	A	825	LYS
1	A	828	LEU
1	A	838	MET
1	A	890	ILE
1	A	949	TYR
1	A	963	ASP
1	A	965	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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	628	ASN
1	A	869	GLN
1	A	872	HIS
1	A	882	HIS
1	A	990	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 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	0.00	-	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BEF	A	998	1	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	994/994 (100%)	-0.02	62 (6%)	24 22	8, 49, 133, 318	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	VAL	15.9
1	A	287	SER	12.2
1	A	505	ARG	10.9
1	A	78	PHE	10.7
1	A	81	GLY	10.5
1	A	122	TYR	9.8
1	A	285	GLY	9.1
1	A	85	ILE	8.5
1	A	288	TRP	8.4
1	A	506	ALA	8.3
1	A	48	SER	8.2
1	A	84	THR	7.8
1	A	286	GLY	7.8
1	A	80	GLU	7.7
1	A	994	GLY	7.7
1	A	86	THR	7.1
1	A	991	TYR	6.9
1	A	121	GLU	6.8
1	A	280	ASN	6.8
1	A	504	SER	6.7
1	A	50	TRP	6.4
1	A	83	GLU	6.1
1	A	951	ASP	6.0
1	A	281	ASP	6.0
1	A	279	PHE	5.3
1	A	284	HIS	5.1
1	A	49	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	503	SER	4.8
1	A	993	GLU	4.8
1	A	289	ILE	4.6
1	A	79	GLU	4.6
1	A	82	GLU	4.3
1	A	123	GLU	4.1
1	A	88	PHE	4.1
1	A	74	VAL	3.9
1	A	508	VAL	3.9
1	A	278	HIS	3.5
1	A	282	PRO	3.4
1	A	953	LEU	3.4
1	A	987	ILE	3.2
1	A	952	PRO	3.2
1	A	957	PHE	3.0
1	A	502	LYS	2.9
1	A	45	GLU	2.9
1	A	988	ALA	2.8
1	A	52	LEU	2.8
1	A	47	LYS	2.7
1	A	964	LEU	2.7
1	A	992	LEU	2.7
1	A	77	TRP	2.7
1	A	831	GLY	2.6
1	A	277	GLY	2.5
1	A	54	ILE	2.5
1	A	563	ALA	2.4
1	A	103	ILE	2.4
1	A	51	GLU	2.3
1	A	878	GLU	2.3
1	A	950	VAL	2.2
1	A	624	ILE	2.2
1	A	716	ILE	2.1
1	A	717	GLY	2.1
1	A	932	TRP	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NA	A	995	1/1	0.96	0.84	9.52	69,69,69,69	0
3	MG	A	996	1/1	0.98	0.17	0.97	13,13,13,13	0
4	BEF	A	998	4/4	0.98	0.20	0.85	30,35,37,45	0
3	MG	A	997	1/1	0.81	0.33	-	98,98,98,98	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.