



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:00 PM GMT

PDB ID : 4UMV
Title : CRYSTAL STRUCTURE OF A ZINC-TRANSPORTING PIB-TYPE ATPASE IN THE E2P STATE
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Deposited on : 2014-05-21
Resolution : 3.20 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 (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

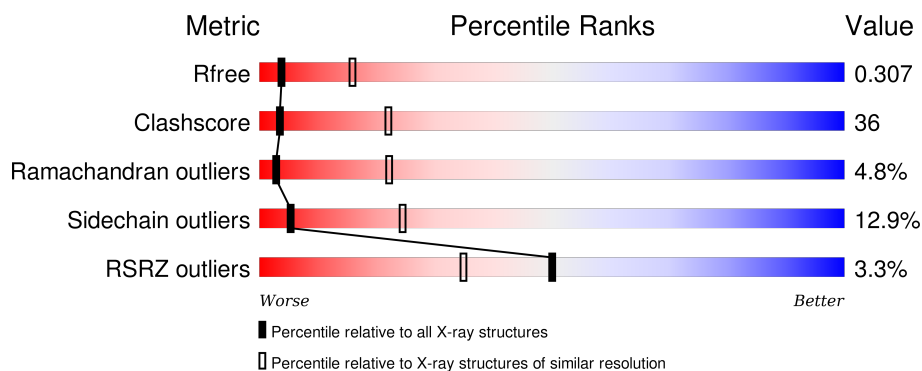
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	732	

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	BEF	A	1732	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4437 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.

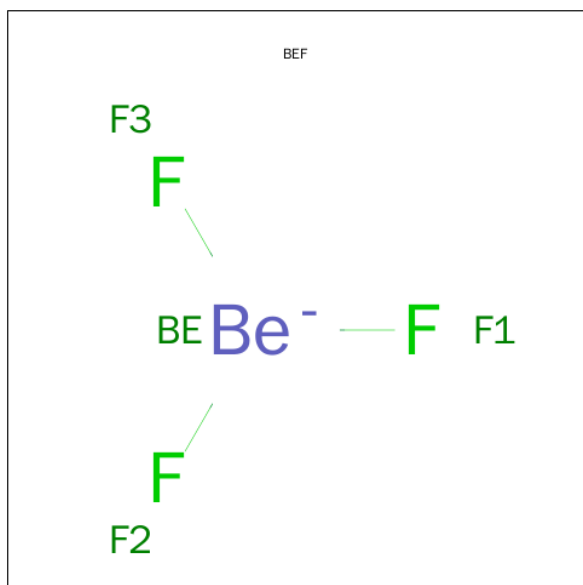
- Molecule 1 is a protein called ZINC-TRANSPORTING ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	7	0	0
			4432	2818	775	825	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).

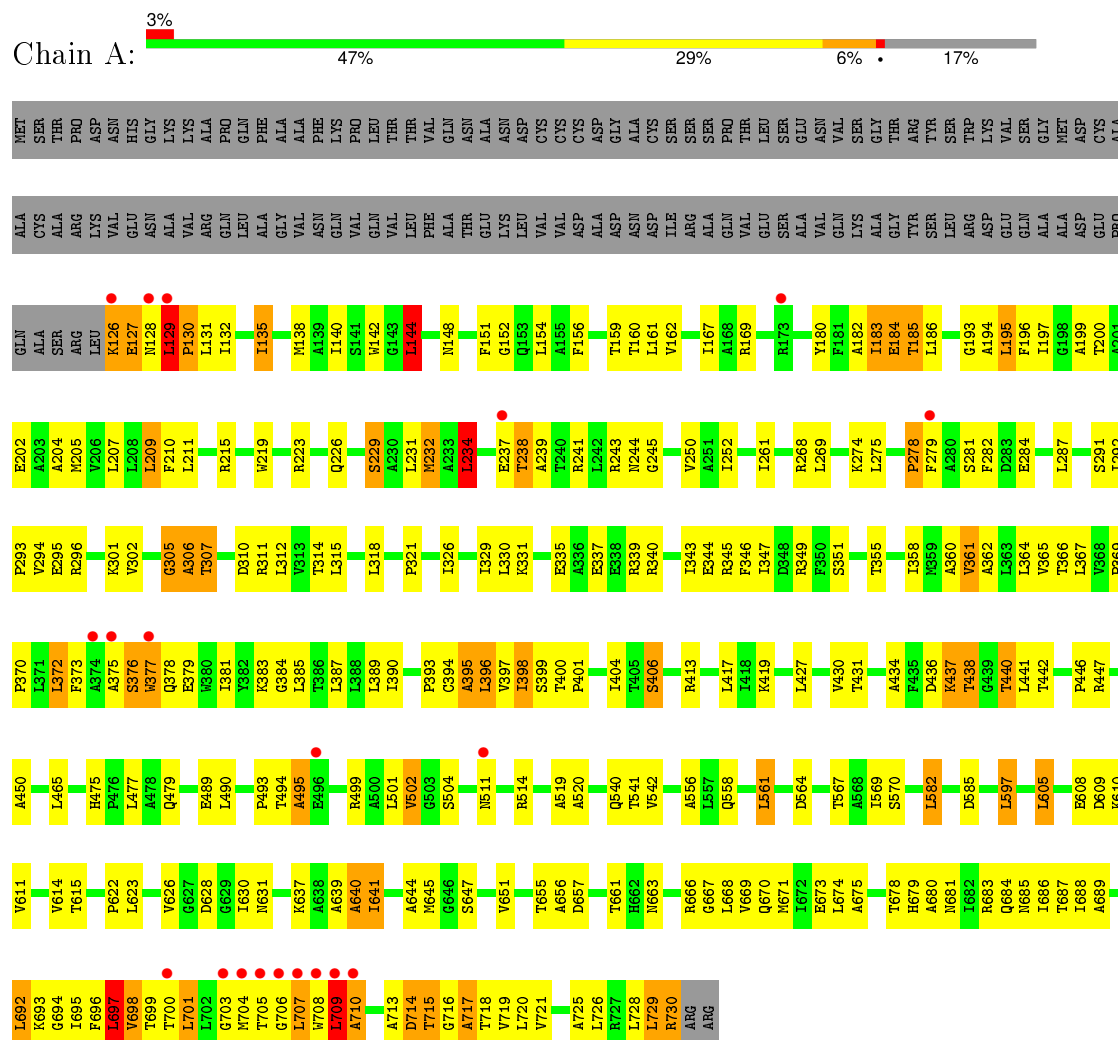


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Be	F	0	0
			4	1	3		

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: ZINC-TRANSPORTING ATPASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.46Å 60.97Å 141.52Å 90.00° 95.99° 90.00°	Depositor
Resolution (Å)	46.08 – 3.20 46.08 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.08-3.20) 99.2 (46.08-3.11)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.218 , 0.281 0.267 , 0.307	Depositor DCC
R_{free} test set	774 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 16804 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4437	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 5.59% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.40	2/4493 (0.0%)	0.71	11/6115 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	709	LEU	CA-C	6.67	1.70	1.52
1	A	130	PRO	N-CD	5.01	1.54	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	710	ALA	N-CA-CB	8.11	121.45	110.10
1	A	709	LEU	CA-C-O	6.91	134.61	120.10
1	A	709	LEU	CA-C-N	-6.69	102.47	117.20
1	A	692	LEU	CB-CA-C	-6.42	97.99	110.20
1	A	372	LEU	N-CA-C	-6.35	93.86	111.00
1	A	129	LEU	C-N-CD	5.75	140.47	128.40
1	A	701	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	697	LEU	N-CA-CB	5.52	121.44	110.40
1	A	714	ASP	N-CA-C	-5.50	96.16	111.00
1	A	144	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	697	LEU	N-CA-C	-5.12	97.17	111.00

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	4432	0	4628	329	1
2	A	1	0	0	0	0
3	A	4	0	0	0	0
All	All	4437	0	4628	329	1

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 36.

All (329) 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:693:LYS:HA	1:A:696:PHE:CE2	1.16	1.66
1:A:709:LEU:CA	1:A:713:ALA:HB2	1.26	1.58
1:A:129:LEU:CD2	1:A:132:ILE:CB	1.84	1.52
1:A:709:LEU:CB	1:A:713:ALA:HB2	1.39	1.49
1:A:693:LYS:CA	1:A:696:PHE:CE2	2.05	1.37
1:A:183:ILE:O	1:A:185:THR:N	1.56	1.37
1:A:709:LEU:HA	1:A:713:ALA:CB	1.59	1.32
1:A:709:LEU:CB	1:A:713:ALA:CB	2.07	1.31
1:A:709:LEU:HB2	1:A:713:ALA:CB	1.62	1.29
1:A:142:TRP:CZ2	1:A:205:MET:CE	2.20	1.25
1:A:693:LYS:HD2	1:A:696:PHE:CZ	1.70	1.24
1:A:129:LEU:HD22	1:A:132:ILE:CB	1.56	1.24
1:A:142:TRP:HZ2	1:A:205:MET:CE	1.49	1.24
1:A:693:LYS:CA	1:A:696:PHE:HE2	1.41	1.23
1:A:142:TRP:CZ2	1:A:205:MET:HE1	1.74	1.21
1:A:709:LEU:CA	1:A:713:ALA:CB	2.11	1.21
1:A:708:TRP:O	1:A:709:LEU:CG	1.90	1.18
1:A:393:PRO:CG	1:A:693:LYS:HG3	1.76	1.15
1:A:129:LEU:HD21	1:A:132:ILE:CB	1.75	1.15
1:A:708:TRP:O	1:A:709:LEU:HG	0.98	1.13
1:A:693:LYS:HD2	1:A:696:PHE:CE2	1.85	1.12
1:A:237:GLU:HG2	1:A:252:ILE:HD12	1.31	1.12
1:A:183:ILE:O	1:A:184:GLU:C	1.92	1.07
1:A:396:LEU:HD12	1:A:397:VAL:N	1.70	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ASP:O	1:A:717:ALA:N	1.89	1.04
1:A:279:PHE:CZ	1:A:501:LEU:HA	1.93	1.02
1:A:692:LEU:O	1:A:696:PHE:CD2	2.13	1.01
1:A:393:PRO:HG3	1:A:693:LYS:HG3	1.40	1.01
1:A:693:LYS:HA	1:A:696:PHE:CZ	1.97	0.99
1:A:707:LEU:HG	1:A:708:TRP:H	1.28	0.98
1:A:705:THR:N	1:A:706:GLY:HA2	1.78	0.98
1:A:183:ILE:O	1:A:186:LEU:N	1.99	0.96
1:A:714:ASP:O	1:A:716:GLY:N	1.99	0.95
1:A:148:ASN:HD21	1:A:151:PHE:HD2	1.05	0.95
1:A:692:LEU:O	1:A:696:PHE:HD2	1.47	0.94
1:A:393:PRO:HD2	1:A:396:LEU:HD21	1.50	0.93
1:A:709:LEU:HA	1:A:713:ALA:HB2	0.94	0.92
1:A:376:SER:O	1:A:378:GLN:N	2.04	0.91
1:A:138:MET:HE1	1:A:204:ALA:HB1	1.53	0.90
1:A:704:MET:N	1:A:705:THR:HB	1.87	0.90
1:A:685:ASN:HB3	1:A:721:VAL:HG13	1.54	0.88
1:A:369:PRO:O	1:A:372:LEU:O	1.92	0.88
1:A:395:ALA:O	1:A:397:VAL:N	2.06	0.88
1:A:709:LEU:HB2	1:A:713:ALA:HB1	1.55	0.87
1:A:138:MET:CE	1:A:204:ALA:HB1	2.03	0.87
1:A:183:ILE:HG23	1:A:184:GLU:N	1.89	0.86
1:A:142:TRP:CH2	1:A:205:MET:CE	2.59	0.86
1:A:183:ILE:HG23	1:A:184:GLU:H	1.41	0.86
1:A:693:LYS:CD	1:A:696:PHE:CZ	2.57	0.85
1:A:142:TRP:CH2	1:A:205:MET:HE3	2.11	0.85
1:A:129:LEU:HD23	1:A:132:ILE:CB	2.02	0.85
1:A:183:ILE:CG2	1:A:184:GLU:H	1.88	0.85
1:A:241:ARG:HH21	1:A:243:ARG:NH1	1.74	0.85
1:A:237:GLU:CD	1:A:238:THR:N	2.30	0.85
1:A:268:ARG:HB3	1:A:306:ALA:H	1.43	0.84
1:A:369:PRO:O	1:A:373:PHE:HB2	1.76	0.84
1:A:183:ILE:C	1:A:185:THR:N	2.25	0.83
1:A:372:LEU:HB2	1:A:373:PHE:CD1	2.13	0.83
1:A:142:TRP:CZ2	1:A:205:MET:HE3	2.14	0.83
1:A:709:LEU:HA	1:A:713:ALA:CA	2.09	0.82
1:A:142:TRP:HD1	1:A:156:PHE:CZ	1.97	0.82
1:A:696:PHE:HA	1:A:699:THR:OG1	1.77	0.82
1:A:709:LEU:HB3	1:A:713:ALA:HB2	1.61	0.81
1:A:370:PRO:HA	1:A:375:ALA:H	1.45	0.80
1:A:183:ILE:CG2	1:A:184:GLU:N	2.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:GLU:HG2	1:A:383:LYS:HZ3	1.46	0.80
1:A:393:PRO:HG2	1:A:693:LYS:HG3	1.61	0.79
1:A:390:ILE:HD11	1:A:693:LYS:NZ	1.97	0.79
1:A:693:LYS:HD2	1:A:696:PHE:HZ	1.40	0.79
1:A:344:GLU:HG3	1:A:349:ARG:HH21	1.48	0.79
1:A:376:SER:O	1:A:377:TRP:C	2.21	0.78
1:A:396:LEU:HD12	1:A:397:VAL:H	1.48	0.76
1:A:437:LYS:HA	1:A:441:LEU:HB2	1.68	0.76
1:A:499:ARG:HG3	1:A:501:LEU:HG	1.67	0.76
1:A:714:ASP:C	1:A:716:GLY:N	2.39	0.75
1:A:396:LEU:HA	1:A:399:SER:OG	1.87	0.74
1:A:195:LEU:O	1:A:195:LEU:HD13	1.86	0.74
1:A:708:TRP:C	1:A:709:LEU:HG	2.05	0.74
1:A:729:LEU:HD12	1:A:729:LEU:N	2.03	0.74
1:A:714:ASP:O	1:A:715:THR:C	2.25	0.74
1:A:707:LEU:HG	1:A:708:TRP:N	2.02	0.74
1:A:695:ILE:O	1:A:698:VAL:HG23	1.87	0.73
1:A:237:GLU:CD	1:A:238:THR:H	1.90	0.73
1:A:390:ILE:CD1	1:A:693:LYS:HZ1	2.02	0.73
1:A:703:GLY:C	1:A:705:THR:HB	2.08	0.73
1:A:639:ALA:O	1:A:641:ILE:N	2.22	0.73
1:A:390:ILE:HD11	1:A:693:LYS:HZ2	1.54	0.72
1:A:372:LEU:O	1:A:373:PHE:HB2	1.90	0.72
1:A:372:LEU:HB2	1:A:373:PHE:HD1	1.54	0.72
1:A:183:ILE:O	1:A:185:THR:CA	2.38	0.72
1:A:704:MET:HA	1:A:705:THR:C	2.10	0.72
1:A:704:MET:C	1:A:706:GLY:HA2	2.10	0.72
1:A:194:ALA:HA	1:A:197:ILE:HG12	1.70	0.72
1:A:705:THR:N	1:A:706:GLY:CA	2.50	0.71
1:A:142:TRP:HZ2	1:A:205:MET:HE1	1.12	0.71
1:A:729:LEU:HD12	1:A:729:LEU:H	1.53	0.70
1:A:226:GLN:HA	1:A:229:SER:HB2	1.72	0.70
1:A:142:TRP:CD1	1:A:156:PHE:CZ	2.79	0.69
1:A:279:PHE:HZ	1:A:501:LEU:HA	1.53	0.69
1:A:670:GLN:NE2	1:A:673:GLU:OE1	2.25	0.69
1:A:142:TRP:CH2	1:A:205:MET:HE1	2.26	0.68
1:A:183:ILE:C	1:A:185:THR:H	1.97	0.68
1:A:210:PHE:HB2	1:A:397:VAL:HG11	1.74	0.68
1:A:305:GLY:HA3	1:A:326:ILE:HD11	1.75	0.67
1:A:390:ILE:CD1	1:A:693:LYS:NZ	2.56	0.67
1:A:241:ARG:HH21	1:A:243:ARG:HH11	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASN:ND2	1:A:151:PHE:CD2	2.60	0.67
1:A:709:LEU:HA	1:A:713:ALA:N	2.09	0.67
1:A:694:GLY:O	1:A:697:LEU:HB3	1.95	0.67
1:A:278:PRO:HG2	1:A:311:ARG:NH2	2.10	0.67
1:A:142:TRP:CD1	1:A:156:PHE:CE1	2.83	0.66
1:A:269:LEU:N	1:A:269:LEU:HD12	2.10	0.66
1:A:693:LYS:CD	1:A:696:PHE:HZ	2.01	0.66
1:A:430:VAL:HA	1:A:622:PRO:HB2	1.77	0.66
1:A:390:ILE:HD12	1:A:693:LYS:HZ1	1.60	0.66
1:A:129:LEU:O	1:A:129:LEU:HD22	1.95	0.66
1:A:129:LEU:O	1:A:129:LEU:HD13	1.95	0.66
1:A:395:ALA:O	1:A:396:LEU:HG	1.95	0.66
1:A:693:LYS:C	1:A:696:PHE:CE2	2.69	0.66
1:A:148:ASN:ND2	1:A:151:PHE:HD2	1.87	0.65
1:A:156:PHE:HA	1:A:159:THR:HG22	1.77	0.65
1:A:696:PHE:O	1:A:697:LEU:O	2.15	0.65
1:A:696:PHE:O	1:A:697:LEU:C	2.35	0.65
1:A:692:LEU:HA	1:A:695:ILE:HD12	1.78	0.65
1:A:215:ARG:NH1	1:A:219:TRP:HB2	2.10	0.65
1:A:376:SER:C	1:A:378:GLN:N	2.50	0.64
1:A:707:LEU:CD1	1:A:708:TRP:HD1	2.10	0.64
1:A:142:TRP:HD1	1:A:156:PHE:HZ	1.45	0.64
1:A:400:THR:HG23	1:A:401:PRO:HD3	1.79	0.64
1:A:707:LEU:HG	1:A:708:TRP:HD1	1.63	0.63
1:A:450:ALA:HB3	1:A:556:ALA:HB3	1.79	0.63
1:A:430:VAL:HG11	1:A:641:ILE:HD11	1.80	0.63
1:A:442:THR:HA	1:A:561:LEU:HA	1.81	0.62
1:A:707:LEU:CG	1:A:708:TRP:H	2.07	0.62
1:A:182:ALA:O	1:A:183:ILE:HG22	1.99	0.62
1:A:142:TRP:HZ2	1:A:205:MET:HE2	1.57	0.62
1:A:138:MET:HE3	1:A:204:ALA:HB1	1.82	0.62
1:A:331:LYS:O	1:A:335:GLU:HB2	1.99	0.61
1:A:210:PHE:HB2	1:A:397:VAL:CG1	2.30	0.61
1:A:417:LEU:CD1	1:A:661:THR:HG23	2.31	0.61
1:A:693:LYS:CE	1:A:696:PHE:HZ	2.13	0.61
1:A:605:LEU:HB2	1:A:609:ASP:HB2	1.81	0.61
1:A:183:ILE:HG22	1:A:184:GLU:OE1	2.01	0.61
1:A:705:THR:HG22	1:A:705:THR:O	2.01	0.60
1:A:379:GLU:HG2	1:A:383:LYS:NZ	2.15	0.60
1:A:396:LEU:CD1	1:A:397:VAL:N	2.57	0.60
1:A:215:ARG:HH12	1:A:219:TRP:HB2	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:THR:O	1:A:663:ASN:N	2.34	0.60
1:A:626:VAL:HG21	1:A:668:LEU:HD21	1.83	0.60
1:A:700:THR:HA	1:A:704:MET:O	2.01	0.60
1:A:706:GLY:O	1:A:707:LEU:HB2	2.02	0.59
1:A:360:ALA:O	1:A:364:LEU:HD23	2.02	0.59
1:A:239:ALA:HB1	1:A:261:ILE:HD11	1.85	0.59
1:A:717:ALA:O	1:A:719:VAL:N	2.35	0.58
1:A:707:LEU:CD1	1:A:708:TRP:CD1	2.86	0.58
1:A:194:ALA:HB1	1:A:199:ALA:HB3	1.85	0.58
1:A:708:TRP:H	1:A:708:TRP:HD1	1.51	0.58
1:A:241:ARG:NH2	1:A:243:ARG:NH1	2.49	0.58
1:A:569:ILE:HG13	1:A:597:LEU:HD22	1.86	0.58
1:A:697:LEU:HD11	1:A:701:LEU:HD21	1.85	0.58
1:A:219:TRP:CH2	1:A:223:ARG:HD2	2.39	0.58
1:A:379:GLU:CG	1:A:383:LYS:NZ	2.67	0.57
1:A:142:TRP:HH2	1:A:205:MET:HE3	1.68	0.57
1:A:396:LEU:CD1	1:A:397:VAL:HG23	2.35	0.57
1:A:183:ILE:O	1:A:185:THR:C	2.42	0.56
1:A:540:GLN:NE2	1:A:558:GLN:OE1	2.35	0.56
1:A:730:ARG:O	1:A:730:ARG:HG3	2.04	0.56
1:A:373:PHE:N	1:A:373:PHE:CD1	2.72	0.56
1:A:647:SER:HB3	1:A:663:ASN:HD21	1.70	0.56
1:A:708:TRP:CD1	1:A:708:TRP:N	2.73	0.56
1:A:142:TRP:CD1	1:A:156:PHE:HZ	2.22	0.56
1:A:514:ARG:HG3	1:A:514:ARG:O	2.05	0.56
1:A:128:ASN:ND2	1:A:215:ARG:HH21	2.04	0.55
1:A:697:LEU:CD1	1:A:701:LEU:CD2	2.84	0.55
1:A:329:ILE:HG21	1:A:630:ILE:HG22	1.88	0.55
1:A:361:VAL:O	1:A:365:VAL:HG13	2.07	0.55
1:A:237:GLU:CG	1:A:238:THR:H	2.19	0.55
1:A:144:LEU:HD13	1:A:152:GLY:HA2	1.89	0.55
1:A:379:GLU:CG	1:A:383:LYS:HZ3	2.16	0.54
1:A:396:LEU:CD1	1:A:397:VAL:H	2.19	0.54
1:A:434:ALA:HB1	1:A:582:LEU:HD22	1.89	0.54
1:A:693:LYS:HD3	1:A:714:ASP:CG	2.28	0.54
1:A:142:TRP:HD1	1:A:156:PHE:CE1	2.22	0.54
1:A:501:LEU:HD12	1:A:502:VAL:CG1	2.37	0.54
1:A:129:LEU:N	1:A:130:PRO:HD3	2.24	0.53
1:A:436:ASP:OD1	1:A:437:LYS:N	2.40	0.53
1:A:292:ILE:HG23	1:A:293:PRO:HD2	1.91	0.53
1:A:494:THR:HG22	1:A:495:ALA:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:LEU:CA	1:A:713:ALA:HB3	2.30	0.53
1:A:714:ASP:C	1:A:716:GLY:H	2.09	0.53
1:A:376:SER:C	1:A:378:GLN:H	2.10	0.53
1:A:697:LEU:HD13	1:A:701:LEU:HD23	1.91	0.52
1:A:707:LEU:CG	1:A:708:TRP:HD1	2.21	0.52
1:A:680:ALA:O	1:A:684:GLN:HG3	2.09	0.52
1:A:709:LEU:HB2	1:A:713:ALA:HB3	1.78	0.52
1:A:709:LEU:C	1:A:713:ALA:CB	2.77	0.52
1:A:693:LYS:CA	1:A:696:PHE:CZ	2.76	0.52
1:A:697:LEU:HD11	1:A:701:LEU:CD2	2.40	0.52
1:A:372:LEU:C	1:A:373:PHE:HD1	2.13	0.52
1:A:614:VAL:CG1	1:A:639:ALA:HB2	2.39	0.52
1:A:370:PRO:HB3	1:A:375:ALA:O	2.10	0.52
1:A:717:ALA:O	1:A:720:LEU:N	2.41	0.52
1:A:183:ILE:HG22	1:A:184:GLU:H	1.74	0.52
1:A:372:LEU:CB	1:A:373:PHE:HD1	2.20	0.51
1:A:396:LEU:HA	1:A:399:SER:CB	2.40	0.51
1:A:373:PHE:N	1:A:373:PHE:HD1	2.08	0.51
1:A:395:ALA:HB1	1:A:721:VAL:HG21	1.93	0.51
1:A:292:ILE:CG2	1:A:293:PRO:HD2	2.39	0.51
1:A:337:GLU:HA	1:A:340:ARG:HG3	1.92	0.51
1:A:709:LEU:CB	1:A:713:ALA:HB1	2.19	0.51
1:A:379:GLU:HG2	1:A:379:GLU:O	2.10	0.51
1:A:269:LEU:CD1	1:A:269:LEU:N	2.73	0.51
1:A:511:ASN:O	1:A:511:ASN:OD1	2.29	0.51
1:A:237:GLU:CG	1:A:238:THR:N	2.74	0.51
1:A:637:LYS:HG2	1:A:655:THR:CG2	2.40	0.51
1:A:358:ILE:HA	1:A:361:VAL:HG13	1.93	0.51
1:A:195:LEU:HD13	1:A:195:LEU:C	2.30	0.50
1:A:269:LEU:HD22	1:A:302:VAL:HG12	1.94	0.50
1:A:692:LEU:O	1:A:696:PHE:CE2	2.62	0.50
1:A:138:MET:HE3	1:A:204:ALA:CB	2.41	0.50
1:A:241:ARG:HA	1:A:261:ILE:HD12	1.92	0.50
1:A:614:VAL:HG13	1:A:639:ALA:HB2	1.94	0.50
1:A:209:LEU:HD13	1:A:394:CYS:HB3	1.93	0.50
1:A:667:GLY:O	1:A:671:MET:N	2.42	0.50
1:A:126:LYS:HD2	1:A:126:LYS:C	2.32	0.50
1:A:400:THR:O	1:A:404:ILE:HG12	2.12	0.49
1:A:564:ASP:HB2	1:A:666:ARG:HG3	1.93	0.49
1:A:396:LEU:HD11	1:A:397:VAL:HG23	1.93	0.49
1:A:269:LEU:CD2	1:A:302:VAL:HG12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:LEU:C	1:A:713:ALA:HB3	2.33	0.49
1:A:698:VAL:HA	1:A:701:LEU:HG	1.94	0.49
1:A:726:LEU:C	1:A:728:LEU:H	2.16	0.49
1:A:693:LYS:CE	1:A:696:PHE:CZ	2.95	0.49
1:A:367:LEU:HD23	1:A:377:TRP:HZ3	1.77	0.48
1:A:661:THR:C	1:A:663:ASN:H	2.17	0.48
1:A:697:LEU:CD1	1:A:701:LEU:HD23	2.43	0.48
1:A:138:MET:CE	1:A:204:ALA:CB	2.84	0.48
1:A:501:LEU:HD12	1:A:502:VAL:HG13	1.95	0.48
1:A:184:GLU:N	1:A:184:GLU:OE1	2.45	0.48
1:A:406:SER:HB3	1:A:728:LEU:HD12	1.96	0.48
1:A:696:PHE:CD1	1:A:697:LEU:N	2.82	0.47
1:A:159:THR:HA	1:A:162:VAL:HG22	1.96	0.47
1:A:131:LEU:CD1	1:A:135:ILE:HD11	2.43	0.47
1:A:372:LEU:O	1:A:373:PHE:CB	2.60	0.47
1:A:268:ARG:HG2	1:A:306:ALA:HA	1.97	0.46
1:A:275:LEU:HA	1:A:315:LEU:HD13	1.97	0.46
1:A:142:TRP:CD1	1:A:156:PHE:HE1	2.30	0.46
1:A:243:ARG:O	1:A:245:GLY:N	2.41	0.46
1:A:644:ALA:HB2	1:A:656:ALA:HB2	1.98	0.46
1:A:268:ARG:HG2	1:A:307:THR:OG1	2.16	0.46
1:A:372:LEU:C	1:A:373:PHE:CD1	2.88	0.46
1:A:697:LEU:HD13	1:A:697:LEU:C	2.37	0.45
1:A:241:ARG:NH2	1:A:243:ARG:HH11	2.13	0.45
1:A:396:LEU:O	1:A:399:SER:HB2	2.17	0.45
1:A:398:ILE:HA	1:A:398:ILE:HD12	1.70	0.45
1:A:129:LEU:N	1:A:130:PRO:CD	2.80	0.45
1:A:160:THR:OG1	1:A:204:ALA:HB2	2.16	0.45
1:A:241:ARG:CZ	1:A:250:VAL:HG11	2.47	0.44
1:A:709:LEU:O	1:A:713:ALA:HB3	2.17	0.44
1:A:366:THR:OG1	1:A:384:GLY:HA3	2.17	0.44
1:A:387:LEU:HA	1:A:390:ILE:HG22	1.98	0.44
1:A:675:ALA:O	1:A:678:THR:HB	2.17	0.44
1:A:193:GLY:HA2	1:A:385:LEU:HD13	1.99	0.44
1:A:396:LEU:HD12	1:A:397:VAL:HG23	2.00	0.44
1:A:140:ILE:O	1:A:144:LEU:HD12	2.18	0.44
1:A:126:LYS:HA	1:A:127:GLU:HB2	2.00	0.44
1:A:693:LYS:O	1:A:696:PHE:CE2	2.70	0.44
1:A:693:LYS:NZ	1:A:696:PHE:CZ	2.84	0.44
1:A:398:ILE:O	1:A:401:PRO:HD2	2.18	0.44
1:A:232:MET:H	1:A:232:MET:HG2	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:HG22	1:A:355:THR:HG21	1.99	0.43
1:A:630:ILE:HG23	1:A:651:VAL:HG21	2.00	0.43
1:A:637:LYS:HD3	1:A:655:THR:HG23	2.00	0.43
1:A:274:LYS:HB2	1:A:318:LEU:HD21	1.99	0.43
1:A:697:LEU:HD13	1:A:701:LEU:CD2	2.46	0.43
1:A:268:ARG:HE	1:A:306:ALA:N	2.17	0.43
1:A:696:PHE:CG	1:A:697:LEU:N	2.87	0.43
1:A:362:ALA:O	1:A:365:VAL:HG22	2.18	0.43
1:A:269:LEU:HD21	1:A:302:VAL:CG1	2.49	0.43
1:A:694:GLY:O	1:A:697:LEU:CB	2.66	0.43
1:A:377:TRP:O	1:A:381:ILE:HD12	2.19	0.43
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.74	0.43
1:A:440:THR:HB	1:A:645:MET:HG3	2.01	0.42
1:A:393:PRO:HD2	1:A:396:LEU:CD2	2.35	0.42
1:A:685:ASN:O	1:A:688:ILE:HG12	2.20	0.42
1:A:605:LEU:HD13	1:A:610:LYS:HG2	2.00	0.42
1:A:126:LYS:HA	1:A:127:GLU:CB	2.50	0.42
1:A:697:LEU:CD1	1:A:701:LEU:HD21	2.45	0.42
1:A:437:LYS:HG3	1:A:438:THR:H	1.85	0.42
1:A:287:LEU:O	1:A:631:ASN:ND2	2.51	0.42
1:A:135:ILE:H	1:A:135:ILE:HG12	1.52	0.42
1:A:611:VAL:O	1:A:615:THR:HG23	2.20	0.42
1:A:345:ARG:HB3	1:A:345:ARG:HE	1.67	0.42
1:A:393:PRO:HG2	1:A:693:LYS:CG	2.40	0.42
1:A:693:LYS:O	1:A:696:PHE:CZ	2.73	0.42
1:A:281:SER:HB3	1:A:295:GLU:OE1	2.20	0.42
1:A:684:GLN:O	1:A:688:ILE:HG23	2.20	0.41
1:A:279:PHE:CE2	1:A:501:LEU:HA	2.47	0.41
1:A:436:ASP:O	1:A:440:THR:HG23	2.21	0.41
1:A:310:ASP:O	1:A:311:ARG:HB3	2.20	0.41
1:A:372:LEU:HB2	1:A:373:PHE:CE1	2.54	0.41
1:A:641:ILE:HG22	1:A:657:ASP:HB2	2.01	0.41
1:A:194:ALA:CB	1:A:389:LEU:HD22	2.50	0.41
1:A:269:LEU:HD21	1:A:302:VAL:HG11	2.02	0.41
1:A:623:LEU:O	1:A:640:ALA:HB3	2.20	0.41
1:A:709:LEU:HB3	1:A:713:ALA:CB	2.28	0.41
1:A:499:ARG:CZ	1:A:501:LEU:HD23	2.51	0.41
1:A:268:ARG:HB3	1:A:306:ALA:N	2.23	0.41
1:A:440:THR:HG22	1:A:628:ASP:OD1	2.21	0.41
1:A:284:GLU:OE2	1:A:294:VAL:HG21	2.20	0.41
1:A:645:MET:HB3	1:A:663:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASN:HD21	1:A:215:ARG:HH21	1.67	0.41
1:A:681:ASN:OD1	1:A:725:ALA:HA	2.20	0.41
1:A:475:HIS:O	1:A:479:GLN:HG3	2.21	0.41
1:A:707:LEU:O	1:A:710:ALA:HB2	2.21	0.41
1:A:501:LEU:O	1:A:502:VAL:HG22	2.20	0.41
1:A:202:GLU:N	1:A:202:GLU:OE1	2.42	0.41
1:A:707:LEU:HD11	1:A:708:TRP:CD1	2.56	0.41
1:A:291:SER:OG	1:A:585:ASP:OD2	2.21	0.41
1:A:686:ILE:HG22	1:A:687:THR:N	2.35	0.41
1:A:700:THR:HA	1:A:704:MET:C	2.40	0.40
1:A:243:ARG:HB3	1:A:244:ASN:H	1.64	0.40
1:A:695:ILE:O	1:A:698:VAL:CG2	2.64	0.40
1:A:707:LEU:H	1:A:710:ALA:HB2	1.86	0.40
1:A:282:PHE:O	1:A:293:PRO:HA	2.21	0.40
1:A:395:ALA:C	1:A:396:LEU:HG	2.42	0.40
1:A:351:SER:HB2	1:A:355:THR:OG1	2.22	0.40
1:A:234:LEU:HD12	1:A:234:LEU:HA	1.88	0.40
1:A:446:PRO:HG3	1:A:477:LEU:HD23	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:NH2	1:A:489:GLU:O[1_455]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	603/732 (82%)	502 (83%)	72 (12%)	29 (5%)	3 22

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	195	LEU
1	A	234	LEU
1	A	377	TRP
1	A	396	LEU
1	A	419	LYS
1	A	495	ALA
1	A	640	ALA
1	A	689	ALA
1	A	717	ALA
1	A	718	THR
1	A	183	ILE
1	A	376	SER
1	A	520	ALA
1	A	715	THR
1	A	339	ARG
1	A	395	ALA
1	A	493	PRO
1	A	502	VAL
1	A	697	LEU
1	A	707	LEU
1	A	278	PRO
1	A	438	THR
1	A	709	LEU
1	A	321	PRO
1	A	519	ALA
1	A	306	ALA
1	A	305	GLY
1	A	129	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	448/553 (81%)	390 (87%)	58 (13%)	5	24

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LYS
1	A	127	GLU
1	A	135	ILE
1	A	144	LEU
1	A	154	LEU
1	A	161	LEU
1	A	167	ILE
1	A	169	ARG
1	A	180	TYR
1	A	185	THR
1	A	196	PHE
1	A	200	THR
1	A	207	LEU
1	A	209	LEU
1	A	211	LEU
1	A	229	SER
1	A	231	LEU
1	A	232	MET
1	A	234	LEU
1	A	238	THR
1	A	296	ARG
1	A	301	LYS
1	A	307	THR
1	A	312	LEU
1	A	314	THR
1	A	330	LEU
1	A	343	ILE
1	A	346	PHE
1	A	347	ILE
1	A	361	VAL
1	A	398	ILE
1	A	406	SER
1	A	413	ARG
1	A	427	LEU
1	A	431	THR
1	A	437	LYS
1	A	440	THR
1	A	447	ARG
1	A	465	LEU
1	A	490	LEU
1	A	504	SER
1	A	541	THR
1	A	542	VAL

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Mol	Chain	Res	Type
1	A	561	LEU
1	A	567	THR
1	A	570	SER
1	A	582	LEU
1	A	597	LEU
1	A	605	LEU
1	A	608	GLU
1	A	641	ILE
1	A	669	VAL
1	A	674	LEU
1	A	679	HIS
1	A	683	ARG
1	A	698	VAL
1	A	729	LEU
1	A	730	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	426	GLN

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 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
3	BEF	A	1732	1,2	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
3	BEF	A	1732	1,2	-	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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	605/732 (82%)	-0.09	20 (3%)	50	35	24, 59, 102, 131	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	703	GLY	7.1
1	A	708	TRP	6.7
1	A	707	LEU	6.2
1	A	709	LEU	5.7
1	A	705	THR	5.3
1	A	706	GLY	5.0
1	A	237	GLU	3.0
1	A	511	ASN	2.9
1	A	375	ALA	2.8
1	A	496	GLU	2.8
1	A	128	ASN	2.7
1	A	374	ALA	2.7
1	A	129	LEU	2.7
1	A	704	MET	2.6
1	A	700	THR	2.5
1	A	279	PHE	2.3
1	A	126	LYS	2.2
1	A	710	ALA	2.2
1	A	173	ARG	2.1
1	A	377	TRP	2.1

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(\AA^2)	Q<0.9
3	BEF	A	1732	4/4	0.90	0.36	6.55	64,74,75,96	0
2	MG	A	1731	1/1	0.75	0.14	-1.42	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.