



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:40 AM GMT

PDB ID : 2BBJ  
Title : Crystal structure of the CorA Mg<sup>2+</sup> transporter  
Authors : Lunin, V.V.; Dobrovetsky, E.; Khutoreskaya, G.; Zhang, R.; Joachimiak, A.;  
Bochkarev, A.; Maguire, M.E.; Edwards, A.M.; Koth, C.M.; Structural Ge-  
nomics Consortium (SGC)  
Deposited on : 2005-10-17  
Resolution : 3.90 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

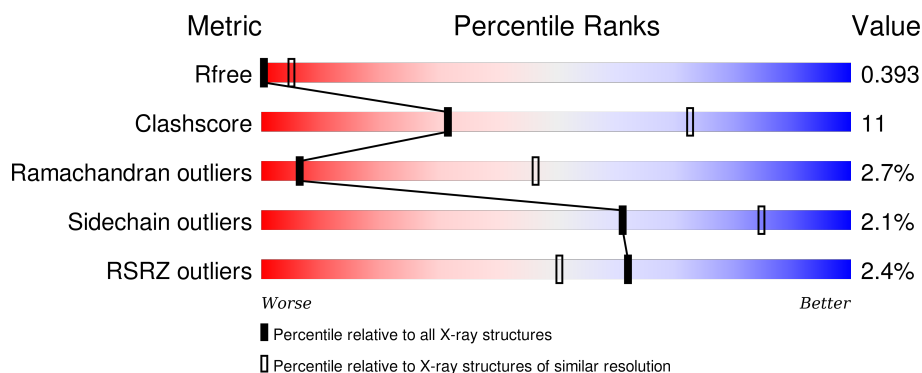
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	354	<div> <div>3%</div> <div>72%</div> <div>19%</div> <div>6%</div> </div>
1	B	354	<div> <div>2%</div> <div>66%</div> <div>25%</div> <div>6%</div> </div>
1	D	354	<div> <div>3%</div> <div>72%</div> <div>20%</div> <div>6%</div> </div>
1	E	354	<div> <div>2%</div> <div>69%</div> <div>23%</div> <div>6%</div> </div>
1	F	354	<div> <div>2%</div> <div>73%</div> <div>19%</div> <div>6%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13805 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 divalent cation transport-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2761	1799	449	504	9			
1	B	334	Total	C	N	O	S	0	0	0
			2761	1799	449	504	9			
1	D	334	Total	C	N	O	S	0	0	0
			2761	1799	449	504	9			
1	E	334	Total	C	N	O	S	0	0	0
			2761	1799	449	504	9			
1	F	334	Total	C	N	O	S	0	0	0
			2761	1799	449	504	9			

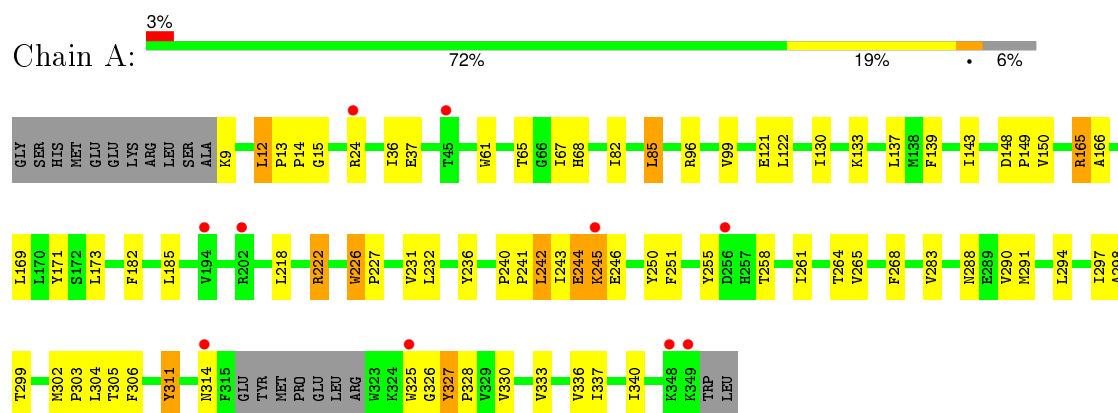
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP Q9WZ31
A	-1	SER	-	CLONING ARTIFACT	UNP Q9WZ31
A	0	HIS	-	CLONING ARTIFACT	UNP Q9WZ31
B	-2	GLY	-	CLONING ARTIFACT	UNP Q9WZ31
B	-1	SER	-	CLONING ARTIFACT	UNP Q9WZ31
B	0	HIS	-	CLONING ARTIFACT	UNP Q9WZ31
D	-2	GLY	-	CLONING ARTIFACT	UNP Q9WZ31
D	-1	SER	-	CLONING ARTIFACT	UNP Q9WZ31
D	0	HIS	-	CLONING ARTIFACT	UNP Q9WZ31
E	-2	GLY	-	CLONING ARTIFACT	UNP Q9WZ31
E	-1	SER	-	CLONING ARTIFACT	UNP Q9WZ31
E	0	HIS	-	CLONING ARTIFACT	UNP Q9WZ31
F	-2	GLY	-	CLONING ARTIFACT	UNP Q9WZ31
F	-1	SER	-	CLONING ARTIFACT	UNP Q9WZ31
F	0	HIS	-	CLONING ARTIFACT	UNP Q9WZ31

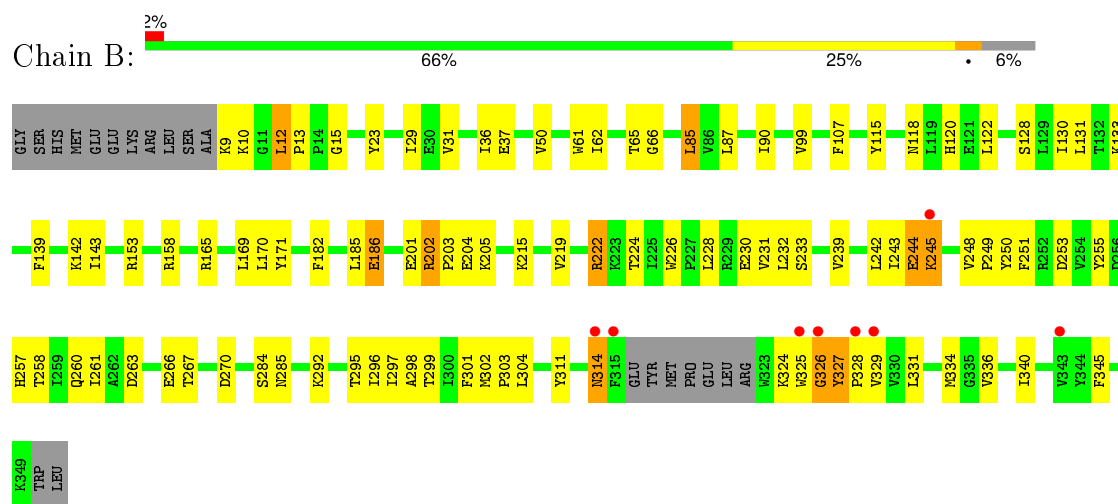
### 3 Residue-property plots [i](#)

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.

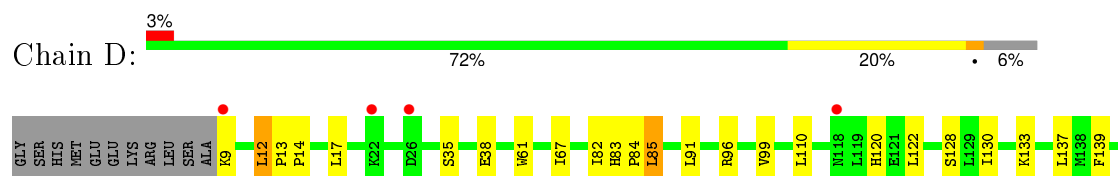
- Molecule 1: divalent cation transport-related protein

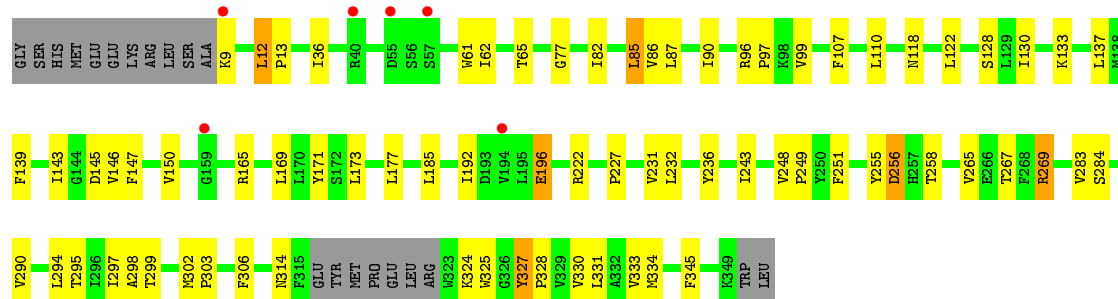


- Molecule 1: divalent cation transport-related protein



- Molecule 1: divalent cation transport-related protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.98Å 173.18Å 134.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.90 19.95 – 3.89	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-3.90) 95.5 (19.95-3.89)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 3.94Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.361 , 0.406 0.347 , 0.393	Depositor DCC
$R_{free}$ test set	1389 reflections (5.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	141.8	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 64.8	EDS
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 28309 reflections (0.011%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.37	0/2820	0.56	1/3822 (0.0%)
1	B	0.39	0/2820	0.60	2/3822 (0.1%)
1	D	0.37	0/2820	0.57	1/3822 (0.0%)
1	E	0.37	0/2820	0.56	1/3822 (0.0%)
1	F	0.37	0/2820	0.55	0/3822
All	All	0.37	0/14100	0.57	5/19110 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	ASN	CB-CA-C	-9.09	92.22	110.40
1	D	326	GLY	N-CA-C	7.08	130.81	113.10
1	B	326	GLY	N-CA-C	6.73	129.93	113.10
1	A	326	GLY	N-CA-C	6.68	129.80	113.10
1	E	326	GLY	N-CA-C	6.61	129.63	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2761	0	2804	72	0
1	B	2761	0	2804	73	0
1	D	2761	0	2804	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2761	0	2804	72	0
1	F	2761	0	2804	68	0
All	All	13805	0	14020	297	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 11.

All (297) 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:E:314:ASN:ND2	1:F:314:ASN:HB2	1.60	1.15
1:F:77:GLY:HA2	1:F:82:ILE:HD12	1.33	1.09
1:D:314:ASN:CB	1:F:314:ASN:HD21	1.65	1.08
1:E:314:ASN:HD21	1:F:314:ASN:HB2	1.12	1.08
1:D:314:ASN:HB2	1:F:314:ASN:HD21	1.12	1.07
1:A:314:ASN:HD21	1:E:314:ASN:HB2	1.18	1.04
1:A:299:THR:HG23	1:B:297:ILE:HD13	1.38	1.01
1:A:314:ASN:CB	1:B:314:ASN:HD21	1.76	0.99
1:D:314:ASN:CB	1:F:314:ASN:ND2	2.27	0.97
1:E:314:ASN:HD21	1:F:314:ASN:CB	1.79	0.96
1:E:314:ASN:ND2	1:F:314:ASN:CB	2.37	0.87
1:E:77:GLY:HA2	1:E:82:ILE:HD12	1.56	0.86
1:B:185:LEU:HD11	1:B:261:ILE:HG23	1.55	0.86
1:D:12:LEU:H	1:D:13:PRO:CD	1.90	0.85
1:A:314:ASN:ND2	1:E:314:ASN:HB2	1.92	0.83
1:E:12:LEU:H	1:E:13:PRO:HD3	1.42	0.82
1:F:12:LEU:H	1:F:13:PRO:CD	1.93	0.82
1:B:284:SER:HB3	1:D:283:VAL:HG11	1.60	0.82
1:D:314:ASN:HB3	1:F:314:ASN:ND2	1.94	0.80
1:D:314:ASN:HB2	1:F:314:ASN:ND2	1.93	0.79
1:A:314:ASN:HB3	1:B:314:ASN:HD21	1.48	0.79
1:F:77:GLY:CA	1:F:82:ILE:HD12	2.13	0.79
1:F:77:GLY:HA2	1:F:82:ILE:CD1	2.12	0.76
1:A:314:ASN:CB	1:B:314:ASN:ND2	2.49	0.76
1:F:12:LEU:H	1:F:13:PRO:HD3	1.52	0.75
1:F:61:TRP:HB2	1:F:169:LEU:HD21	1.69	0.74
1:E:61:TRP:HB2	1:E:169:LEU:HD21	1.70	0.73
1:E:12:LEU:H	1:E:13:PRO:CD	2.01	0.73
1:B:12:LEU:H	1:B:13:PRO:CD	2.01	0.72
1:A:61:TRP:HB2	1:A:169:LEU:HD21	1.71	0.72
1:E:185:LEU:HD11	1:E:261:ILE:HG23	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:GLY:HA3	1:E:329:VAL:HB	1.74	0.70
1:B:327:TYR:HB3	1:B:328:PRO:HD3	1.73	0.69
1:B:12:LEU:H	1:B:13:PRO:HD3	1.58	0.69
1:A:314:ASN:HB2	1:B:314:ASN:HD21	1.56	0.68
1:B:165:ARG:HD3	1:B:243:ILE:HD13	1.73	0.68
1:F:171:TYR:HE1	1:F:251:PHE:HD1	1.41	0.68
1:D:284:SER:HB3	1:F:283:VAL:HG11	1.74	0.68
1:A:240:PRO:HB2	1:A:241:PRO:HD3	1.75	0.68
1:A:314:ASN:HB3	1:B:314:ASN:ND2	2.09	0.68
1:D:82:ILE:HD13	1:D:130:ILE:HD13	1.76	0.68
1:E:327:TYR:HB3	1:E:328:PRO:HD3	1.77	0.67
1:D:232:LEU:O	1:D:251:PHE:HZ	1.77	0.67
1:D:61:TRP:HB2	1:D:169:LEU:HD21	1.78	0.65
1:D:12:LEU:H	1:D:13:PRO:HD3	1.59	0.65
1:A:297:ILE:HD12	1:E:299:THR:HG23	1.78	0.65
1:D:326:GLY:HA3	1:D:329:VAL:HB	1.78	0.65
1:A:327:TYR:HB3	1:A:328:PRO:HD3	1.78	0.65
1:E:65:THR:HG21	1:E:143:ILE:HD13	1.78	0.65
1:B:61:TRP:HB2	1:B:169:LEU:HD21	1.77	0.65
1:F:12:LEU:N	1:F:13:PRO:CD	2.60	0.65
1:E:253:ASP:O	1:E:257:HIS:ND1	2.25	0.64
1:F:192:ILE:O	1:F:196:GLU:HB3	1.96	0.64
1:F:327:TYR:HB3	1:F:328:PRO:HD3	1.78	0.64
1:A:12:LEU:H	1:A:13:PRO:CD	2.10	0.64
1:A:314:ASN:HB2	1:B:314:ASN:ND2	2.12	0.63
1:F:99:VAL:CG2	1:F:231:VAL:HG13	2.28	0.63
1:A:306:PHE:CE1	1:B:304:LEU:HB3	2.34	0.63
1:E:297:ILE:CD1	1:F:299:THR:HG23	2.29	0.63
1:E:153:ARG:HA	1:E:158:ARG:HB2	1.80	0.63
1:E:288:ASN:HA	1:E:291:MET:HB2	1.82	0.62
1:A:294:LEU:HD13	1:E:295:THR:HA	1.82	0.62
1:A:244:GLU:HG3	1:A:245:LYS:H	1.64	0.61
1:B:297:ILE:O	1:B:301:PHE:HB2	2.01	0.61
1:F:298:ALA:O	1:F:302:MET:HB2	2.01	0.61
1:D:269:ARG:O	1:D:273:SER:HB2	2.01	0.60
1:E:240:PRO:HB2	1:E:241:PRO:HD3	1.84	0.60
1:B:292:LYS:O	1:B:296:ILE:HG13	2.02	0.59
1:A:304:LEU:HB3	1:E:306:PHE:CE1	2.38	0.59
1:A:302:MET:N	1:A:303:PRO:HD2	2.18	0.58
1:A:171:TYR:HB3	1:A:250:TYR:CE2	2.38	0.58
1:E:12:LEU:N	1:E:13:PRO:CD	2.64	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PHE:HB3	1:B:10:LYS:HG3	1.85	0.58
1:F:107:PHE:HD1	1:F:130:ILE:HG12	1.69	0.58
1:F:96:ARG:HD3	1:F:97:PRO:HD2	1.86	0.58
1:B:253:ASP:O	1:B:257:HIS:ND1	2.36	0.58
1:E:171:TYR:HB3	1:E:250:TYR:HE2	1.68	0.57
1:E:222:ARG:NE	1:E:266:GLU:OE1	2.36	0.57
1:D:128:SER:HB2	1:D:139:PHE:HB2	1.87	0.57
1:F:302:MET:H	1:F:303:PRO:HD2	1.70	0.57
1:B:23:TYR:CZ	1:B:142:LYS:HD3	2.40	0.57
1:F:171:TYR:CE1	1:F:251:PHE:HD1	2.22	0.57
1:E:85:LEU:HD23	1:E:85:LEU:H	1.70	0.57
1:D:187:LYS:O	1:D:191:GLU:HG2	2.04	0.57
1:A:96:ARG:HD2	1:A:227:PRO:HG3	1.86	0.57
1:B:231:VAL:HG12	1:B:232:LEU:HD12	1.87	0.56
1:B:255:TYR:HA	1:B:258:THR:HG22	1.88	0.56
1:E:171:TYR:HB3	1:E:250:TYR:CE2	2.41	0.56
1:E:244:GLU:HG3	1:E:245:LYS:H	1.71	0.56
1:B:299:THR:HG21	1:B:345:PHE:CE1	2.41	0.55
1:B:12:LEU:N	1:B:13:PRO:CD	2.68	0.55
1:B:331:LEU:HA	1:B:334:MET:HB2	1.88	0.55
1:E:288:ASN:O	1:E:292:LYS:HG3	2.06	0.55
1:B:171:TYR:HB3	1:B:250:TYR:HE2	1.70	0.55
1:A:185:LEU:HD11	1:A:261:ILE:HG23	1.87	0.55
1:E:304:LEU:HB3	1:F:306:PHE:CE1	2.41	0.55
1:F:65:THR:HG21	1:F:143:ILE:HD13	1.89	0.55
1:F:171:TYR:HE1	1:F:251:PHE:CD1	2.24	0.55
1:F:99:VAL:HG23	1:F:231:VAL:HG13	1.88	0.55
1:E:297:ILE:O	1:E:301:PHE:HB2	2.06	0.55
1:B:260:GLN:HA	1:D:96:ARG:HH21	1.72	0.55
1:A:283:VAL:HG11	1:E:284:SER:HB3	1.89	0.55
1:D:171:TYR:HB3	1:D:250:TYR:CE2	2.42	0.55
1:B:326:GLY:HA2	1:B:329:VAL:HB	1.87	0.55
1:B:224:THR:O	1:B:228:LEU:HD13	2.06	0.55
1:B:244:GLU:HG3	1:B:245:LYS:H	1.72	0.55
1:D:253:ASP:O	1:D:257:HIS:ND1	2.40	0.55
1:B:107:PHE:HD1	1:B:130:ILE:HG12	1.73	0.54
1:A:297:ILE:O	1:A:297:ILE:HG22	2.08	0.54
1:E:298:ALA:O	1:E:302:MET:HB2	2.08	0.54
1:A:236:TYR:HB2	1:A:251:PHE:CE2	2.43	0.53
1:E:242:LEU:CD1	1:E:243:ILE:H	2.22	0.53
1:E:113:PHE:HE2	1:E:224:THR:HG21	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:HG23	1:B:297:ILE:CD1	2.26	0.53
1:D:12:LEU:H	1:D:13:PRO:HD2	1.71	0.53
1:D:99:VAL:CG2	1:D:231:VAL:HG13	2.38	0.53
1:D:85:LEU:H	1:D:85:LEU:HD23	1.73	0.53
1:F:128:SER:HB2	1:F:139:PHE:HB2	1.91	0.52
1:B:267:THR:HG23	1:D:219:VAL:HG11	1.91	0.52
1:B:222:ARG:O	1:B:226:TRP:HB2	2.09	0.52
1:B:263:ASP:HB2	1:D:96:ARG:NH2	2.25	0.52
1:B:266:GLU:O	1:B:270:ASP:HB2	2.10	0.52
1:E:229:ARG:HD2	1:E:259:ILE:HG13	1.91	0.52
1:B:153:ARG:HA	1:B:158:ARG:HB2	1.92	0.52
1:D:120:HIS:CD2	1:D:210:ARG:HD3	2.44	0.52
1:D:327:TYR:H	1:D:328:PRO:CD	2.22	0.52
1:E:330:VAL:O	1:E:334:MET:HG2	2.09	0.52
1:F:231:VAL:HG12	1:F:232:LEU:HD12	1.93	0.51
1:D:240:PRO:O	1:D:242:LEU:HD23	2.11	0.51
1:B:85:LEU:HD23	1:B:85:LEU:H	1.76	0.51
1:B:128:SER:HB2	1:B:139:PHE:HB2	1.91	0.51
1:D:288:ASN:HA	1:D:291:MET:HB2	1.92	0.51
1:E:219:VAL:HG12	1:F:267:THR:HG23	1.92	0.51
1:E:120:HIS:O	1:E:121:GLU:CB	2.59	0.51
1:B:202:ARG:N	1:B:203:PRO:HD3	2.26	0.51
1:A:130:ILE:HB	1:A:137:LEU:HB2	1.93	0.51
1:E:327:TYR:H	1:E:328:PRO:CD	2.24	0.50
1:F:302:MET:N	1:F:303:PRO:HD2	2.25	0.50
1:A:298:ALA:O	1:A:302:MET:HB2	2.12	0.50
1:D:12:LEU:N	1:D:13:PRO:CD	2.61	0.50
1:D:327:TYR:HB3	1:D:328:PRO:HD3	1.93	0.49
1:B:295:THR:HG21	1:D:290:VAL:HG13	1.94	0.49
1:A:171:TYR:HB3	1:A:250:TYR:HE2	1.77	0.49
1:E:294:LEU:HD13	1:F:295:THR:HA	1.94	0.49
1:E:314:ASN:HD21	1:F:314:ASN:CG	2.13	0.49
1:D:222:ARG:O	1:D:226:TRP:HB2	2.12	0.49
1:B:314:ASN:CB	1:D:314:ASN:HD21	2.26	0.49
1:F:232:LEU:O	1:F:251:PHE:HZ	1.95	0.49
1:F:236:TYR:HB2	1:F:251:PHE:CE2	2.48	0.49
1:A:171:TYR:HE1	1:A:251:PHE:HD1	1.60	0.49
1:B:263:ASP:HB2	1:D:96:ARG:HH22	1.77	0.49
1:B:298:ALA:O	1:B:302:MET:HB3	2.12	0.49
1:A:85:LEU:HD23	1:A:85:LEU:H	1.78	0.49
1:B:314:ASN:CG	1:D:314:ASN:HD21	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:O	1:A:226:TRP:HB2	2.12	0.49
1:D:331:LEU:HA	1:D:334:MET:HB2	1.94	0.48
1:A:333:VAL:O	1:A:337:ILE:HG13	2.12	0.48
1:F:255:TYR:O	1:F:258:THR:HG22	2.14	0.48
1:F:327:TYR:H	1:F:328:PRO:CD	2.27	0.48
1:B:171:TYR:HB3	1:B:250:TYR:CE2	2.49	0.48
1:A:240:PRO:HB2	1:A:241:PRO:CD	2.42	0.48
1:A:236:TYR:HB2	1:A:251:PHE:CZ	2.49	0.48
1:B:295:THR:HA	1:D:294:LEU:HD13	1.94	0.48
1:E:302:MET:N	1:E:303:PRO:HD2	2.28	0.48
1:A:299:THR:CG2	1:B:297:ILE:HD13	2.27	0.48
1:F:331:LEU:HA	1:F:334:MET:HB2	1.95	0.48
1:B:99:VAL:CG2	1:B:231:VAL:HG13	2.44	0.48
1:D:269:ARG:O	1:D:269:ARG:HD3	2.13	0.47
1:E:314:ASN:HD22	1:F:314:ASN:HB2	1.65	0.47
1:F:165:ARG:HD3	1:F:243:ILE:HD13	1.95	0.47
1:E:77:GLY:HA2	1:E:82:ILE:CD1	2.38	0.47
1:A:302:MET:N	1:A:303:PRO:CD	2.78	0.47
1:E:242:LEU:HD12	1:E:243:ILE:H	1.79	0.47
1:F:85:LEU:H	1:F:85:LEU:HD23	1.78	0.47
1:A:264:THR:O	1:A:268:PHE:HD1	1.97	0.47
1:A:297:ILE:CD1	1:E:299:THR:HG23	2.44	0.47
1:E:99:VAL:CG2	1:E:231:VAL:HG13	2.44	0.47
1:B:336:VAL:O	1:B:340:ILE:HG13	2.14	0.47
1:F:130:ILE:HB	1:F:137:LEU:HB2	1.95	0.47
1:D:295:THR:HA	1:F:294:LEU:HD13	1.96	0.47
1:B:31:VAL:HG22	1:B:62:ILE:HG23	1.97	0.46
1:A:65:THR:HG21	1:A:143:ILE:HD13	1.97	0.46
1:F:185:LEU:HD21	1:F:265:VAL:HG22	1.96	0.46
1:B:249:PRO:HB2	1:D:85:LEU:HD11	1.97	0.46
1:D:270:ASP:OD1	1:F:269:ARG:NH1	2.49	0.46
1:A:255:TYR:HA	1:A:258:THR:HG22	1.98	0.46
1:A:182:PHE:HD2	1:B:10:LYS:HE2	1.81	0.46
1:D:300:ILE:HG12	1:D:341:MET:HB2	1.96	0.46
1:F:86:VAL:O	1:F:90:ILE:HG13	2.16	0.45
1:E:283:VAL:HG11	1:F:284:SER:HB3	1.98	0.45
1:E:298:ALA:O	1:E:302:MET:CB	2.64	0.45
1:E:255:TYR:HA	1:E:258:THR:HG22	1.97	0.45
1:E:120:HIS:HD2	1:E:210:ARG:HE	1.63	0.45
1:A:218:LEU:HD21	1:A:268:PHE:HB3	1.99	0.45
1:D:244:GLU:HG3	1:D:245:LYS:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:TYR:N	1:D:328:PRO:CD	2.79	0.45
1:B:201:GLU:O	1:B:202:ARG:HB2	2.16	0.45
1:B:302:MET:N	1:B:303:PRO:HD2	2.32	0.45
1:A:99:VAL:CG2	1:A:231:VAL:HG13	2.46	0.45
1:D:35:SER:OG	1:D:38:GLU:HG2	2.16	0.45
1:A:67:ILE:HG21	1:A:139:PHE:HB3	1.99	0.45
1:E:100:GLU:HB2	1:E:107:PHE:HB3	1.99	0.45
1:F:299:THR:HG21	1:F:345:PHE:HE1	1.80	0.45
1:A:14:PRO:HD3	1:E:153:ARG:HD3	1.98	0.45
1:A:82:ILE:HD13	1:A:130:ILE:HD13	1.99	0.45
1:A:261:ILE:O	1:A:265:VAL:HG23	2.17	0.45
1:A:302:MET:H	1:A:303:PRO:HD2	1.82	0.45
1:A:36:ILE:HG23	1:A:37:GLU:HG3	1.99	0.45
1:F:330:VAL:O	1:F:333:VAL:HG12	2.17	0.45
1:F:299:THR:HG21	1:F:345:PHE:CE1	2.52	0.45
1:A:314:ASN:OD1	1:E:314:ASN:OD1	2.35	0.45
1:D:202:ARG:HE	1:D:202:ARG:HA	1.81	0.45
1:D:302:MET:N	1:D:303:PRO:HD2	2.32	0.45
1:A:327:TYR:H	1:A:328:PRO:CD	2.31	0.44
1:D:67:ILE:HG21	1:D:139:PHE:HB3	1.98	0.44
1:D:311:TYR:CZ	1:D:330:VAL:HG21	2.52	0.44
1:E:98:LYS:HD3	1:F:256:ASP:OD1	2.17	0.44
1:D:307:ILE:O	1:D:311:TYR:HB2	2.17	0.44
1:F:145:ASP:HB2	1:F:147:PHE:CD2	2.52	0.44
1:F:248:VAL:N	1:F:249:PRO:HD2	2.33	0.44
1:D:232:LEU:O	1:D:251:PHE:CZ	2.65	0.44
1:F:302:MET:N	1:F:303:PRO:CD	2.81	0.44
1:D:338:ALA:O	1:D:342:VAL:HG23	2.17	0.44
1:B:115:TYR:OH	1:B:120:HIS:ND1	2.50	0.44
1:B:327:TYR:O	1:B:331:LEU:HB2	2.18	0.44
1:E:96:ARG:NH1	1:E:223:LYS:O	2.51	0.44
1:E:195:LEU:O	1:E:199:VAL:HG23	2.18	0.44
1:B:239:VAL:HG11	1:B:248:VAL:HG22	2.00	0.44
1:E:17:LEU:HD11	1:E:87:LEU:HB3	2.00	0.43
1:D:185:LEU:HD11	1:D:261:ILE:HG23	2.00	0.43
1:E:248:VAL:N	1:E:249:PRO:HD2	2.33	0.43
1:A:311:TYR:CE2	1:A:330:VAL:HG21	2.53	0.43
1:D:314:ASN:HB3	1:F:314:ASN:HD22	1.80	0.43
1:D:171:TYR:HB3	1:D:250:TYR:HE2	1.83	0.43
1:A:12:LEU:H	1:A:13:PRO:HD2	1.81	0.43
1:E:222:ARG:HG3	1:E:223:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:HE	1:B:202:ARG:HA	1.83	0.43
1:B:65:THR:HG21	1:B:143:ILE:HD13	2.01	0.43
1:B:215:LYS:O	1:B:219:VAL:HG23	2.18	0.43
1:E:23:TYR:CE1	1:E:142:LYS:HD3	2.54	0.43
1:D:244:GLU:O	1:D:246:GLU:N	2.51	0.42
1:B:36:ILE:HG23	1:B:37:GLU:HG3	2.00	0.42
1:A:243:ILE:HG13	1:A:243:ILE:O	2.20	0.42
1:E:272:VAL:HA	1:E:275:LEU:HB2	2.01	0.42
1:B:230:GLU:HA	1:B:233:SER:HB2	2.02	0.42
1:D:171:TYR:HE1	1:D:251:PHE:HD1	1.68	0.42
1:D:244:GLU:C	1:D:246:GLU:H	2.23	0.42
1:B:87:LEU:HA	1:B:90:ILE:HD12	2.00	0.42
1:A:336:VAL:O	1:A:340:ILE:HG13	2.19	0.42
1:A:165:ARG:HB3	1:A:166:ALA:H	1.62	0.42
1:D:83:HIS:HA	1:D:84:PRO:HD3	1.91	0.42
1:B:302:MET:H	1:B:303:PRO:HD2	1.85	0.41
1:A:24:ARG:HA	1:A:68:HIS:CG	2.55	0.41
1:D:156:TYR:N	1:D:156:TYR:CD1	2.87	0.41
1:F:150:VAL:HG21	1:F:173:LEU:HD23	2.01	0.41
1:B:182:PHE:O	1:B:186:GLU:HB2	2.20	0.41
1:F:227:PRO:O	1:F:231:VAL:N	2.53	0.41
1:A:311:TYR:HE2	1:A:330:VAL:HG21	1.86	0.41
1:A:148:ASP:N	1:A:149:PRO:CD	2.84	0.41
1:F:62:ILE:HB	1:F:137:LEU:HD23	2.02	0.41
1:F:110:LEU:HD13	1:F:177:LEU:HD23	2.02	0.41
1:A:288:ASN:HA	1:A:291:MET:HB2	2.02	0.41
1:B:29:ILE:HG21	1:B:50:VAL:HG21	2.02	0.41
1:E:302:MET:HA	1:E:305:THR:HG22	2.02	0.41
1:E:51:LEU:N	1:E:52:PRO:CD	2.83	0.41
1:A:290:VAL:HG13	1:E:295:THR:HG21	2.02	0.41
1:B:171:TYR:CE1	1:B:251:PHE:CD1	3.08	0.41
1:E:165:ARG:HB3	1:E:166:ALA:H	1.72	0.41
1:B:204:GLU:HB3	1:B:205:LYS:H	1.62	0.41
1:A:244:GLU:O	1:A:246:GLU:N	2.52	0.41
1:E:244:GLU:HG3	1:E:245:LYS:N	2.34	0.41
1:A:298:ALA:O	1:A:302:MET:CB	2.68	0.41
1:E:292:LYS:O	1:E:296:ILE:HG13	2.20	0.41
1:D:299:THR:HG23	1:F:297:ILE:CD1	2.50	0.41
1:D:122:LEU:H	1:D:122:LEU:HD23	1.86	0.41
1:E:171:TYR:HE1	1:E:251:PHE:HD1	1.69	0.41
1:F:171:TYR:CE1	1:F:251:PHE:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:MET:HA	1:A:305:THR:HG22	2.04	0.40
1:A:231:VAL:HG12	1:A:232:LEU:HD12	2.03	0.40
1:A:150:VAL:HG21	1:A:173:LEU:HD23	2.03	0.40
1:B:324:LYS:O	1:B:325:TRP:HB2	2.20	0.40
1:A:232:LEU:HB3	1:A:255:TYR:HD1	1.86	0.40
1:B:115:TYR:HD1	1:B:122:LEU:HB3	1.85	0.40
1:D:224:THR:O	1:D:228:LEU:HB2	2.21	0.40
1:A:122:LEU:H	1:A:122:LEU:HD23	1.86	0.40
1:F:77:GLY:HA3	1:F:87:LEU:HD21	2.03	0.40
1:D:17:LEU:HB3	1:D:91:LEU:HD12	2.04	0.40
1:E:148:ASP:N	1:E:149:PRO:CD	2.84	0.40
1:D:130:ILE:HB	1:D:137:LEU:HB2	2.03	0.40
1:E:299:THR:HG21	1:E:345:PHE:HE1	1.87	0.40
1:A:226:TRP:N	1:A:227:PRO:HD2	2.37	0.40
1:B:244:GLU:CG	1:B:245:LYS:H	2.33	0.40
1:D:110:LEU:HD21	1:D:231:VAL:HG11	2.04	0.40
1:D:291:MET:HB3	1:F:290:VAL:HG11	2.03	0.40
1:D:270:ASP:CG	1:F:269:ARG:HH12	2.25	0.40
1:A:99:VAL:HG23	1:A:231:VAL:HG13	2.04	0.40
1:B:131:LEU:HD22	1:B:170:LEU:HD22	2.03	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	330/354 (93%)	293 (89%)	27 (8%)	10 (3%)	5	44
1	B	330/354 (93%)	289 (88%)	32 (10%)	9 (3%)	6	46
1	D	330/354 (93%)	292 (88%)	30 (9%)	8 (2%)	7	49
1	E	330/354 (93%)	291 (88%)	30 (9%)	9 (3%)	6	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	330/354 (93%)	290 (88%)	32 (10%)	8 (2%)	7	49
All	All	1650/1770 (93%)	1455 (88%)	151 (9%)	44 (3%)	6	46

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	GLU
1	B	244	GLU
1	D	245	LYS
1	E	121	GLU
1	A	15	GLY
1	A	245	LYS
1	D	242	LEU
1	D	244	GLU
1	E	15	GLY
1	F	36	ILE
1	A	12	LEU
1	A	133	LYS
1	A	325	TRP
1	A	327	TYR
1	B	12	LEU
1	B	327	TYR
1	D	12	LEU
1	D	133	LYS
1	D	325	TRP
1	E	245	LYS
1	F	118	ASN
1	F	133	LYS
1	F	325	TRP
1	A	165	ARG
1	A	242	LEU
1	B	133	LYS
1	B	202	ARG
1	E	12	LEU
1	E	133	LYS
1	E	325	TRP
1	A	121	GLU
1	B	118	ASN
1	B	245	LYS
1	E	118	ASN
1	F	12	LEU
1	F	327	TYR

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Mol	Chain	Res	Type
1	B	15	GLY
1	E	244	GLU
1	F	324	LYS
1	D	14	PRO
1	B	66	GLY
1	D	243	ILE
1	E	239	VAL
1	F	146	VAL

### 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	312/332 (94%)	306 (98%)	6 (2%)	65	86
1	B	312/332 (94%)	305 (98%)	7 (2%)	60	84
1	D	312/332 (94%)	306 (98%)	6 (2%)	65	86
1	E	312/332 (94%)	306 (98%)	6 (2%)	65	86
1	F	312/332 (94%)	305 (98%)	7 (2%)	60	84
All	All	1560/1660 (94%)	1528 (98%)	32 (2%)	61	85

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	85	LEU
1	A	222	ARG
1	A	226	TRP
1	A	242	LEU
1	A	311	TYR
1	B	9	LYS
1	B	85	LEU
1	B	186	GLU
1	B	222	ARG
1	B	242	LEU

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Mol	Chain	Res	Type
1	B	285	ASN
1	B	311	TYR
1	D	9	LYS
1	D	85	LEU
1	D	196	GLU
1	D	222	ARG
1	D	242	LEU
1	D	269	ARG
1	E	9	LYS
1	E	85	LEU
1	E	210	ARG
1	E	222	ARG
1	E	251	PHE
1	E	311	TYR
1	F	9	LYS
1	F	85	LEU
1	F	122	LEU
1	F	196	GLU
1	F	222	ARG
1	F	256	ASP
1	F	269	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	94	HIS
1	A	95	GLN
1	A	140	GLN
1	A	217	ASN
1	B	33	ASN
1	B	104	ASN
1	B	134	ASN
1	B	217	ASN
1	B	285	ASN
1	B	288	ASN
1	D	33	ASN
1	D	95	GLN
1	D	104	ASN
1	D	120	HIS
1	D	140	GLN
1	D	217	ASN

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Mol	Chain	Res	Type
1	D	285	ASN
1	D	314	ASN
1	E	33	ASN
1	E	95	GLN
1	E	217	ASN
1	E	314	ASN
1	F	95	GLN
1	F	104	ASN
1	F	140	GLN
1	F	217	ASN
1	F	314	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 ⓘ

There are no ligands in this entry.

## 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	334/354 (94%)	-0.06	10 (2%) 54 40	157, 163, 169, 171	0
1	B	334/354 (94%)	0.01	8 (2%) 62 50	157, 163, 169, 563	0
1	D	334/354 (94%)	-0.04	9 (2%) 58 46	157, 163, 169, 172	0
1	E	334/354 (94%)	-0.09	7 (2%) 67 56	157, 163, 169, 172	0
1	F	334/354 (94%)	-0.09	6 (1%) 71 61	157, 163, 169, 172	0
All	All	1670/1770 (94%)	-0.05	40 (2%) 62 50	157, 163, 169, 563	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	328	PRO	3.7
1	D	194	VAL	3.5
1	A	349	LYS	3.5
1	B	314	ASN	3.4
1	D	22	LYS	3.3
1	D	26	ASP	3.2
1	D	314	ASN	3.2
1	A	314	ASN	3.1
1	F	55	ASP	2.9
1	A	256	ASP	2.8
1	D	328	PRO	2.7
1	A	194	VAL	2.7
1	B	326	GLY	2.7
1	A	325	TRP	2.7
1	A	45	THR	2.6
1	B	245	LYS	2.6
1	B	325	TRP	2.6
1	E	314	ASN	2.6
1	F	40	ARG	2.5
1	D	118	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	348	LYS	2.4
1	E	9	LYS	2.4
1	A	245	LYS	2.4
1	B	329	VAL	2.3
1	F	9	LYS	2.3
1	B	315	PHE	2.2
1	D	324	LYS	2.2
1	E	328	PRO	2.2
1	F	194	VAL	2.2
1	B	343	VAL	2.2
1	E	327	TYR	2.2
1	A	202	ARG	2.1
1	D	143	ILE	2.1
1	F	57	SER	2.1
1	F	159	GLY	2.1
1	E	315	PHE	2.1
1	E	313	MET	2.0
1	A	24	ARG	2.0
1	E	25	GLU	2.0
1	D	9	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.