



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:29 PM UTC

PDB ID : 2BBJ / pdb\_00002bbj  
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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

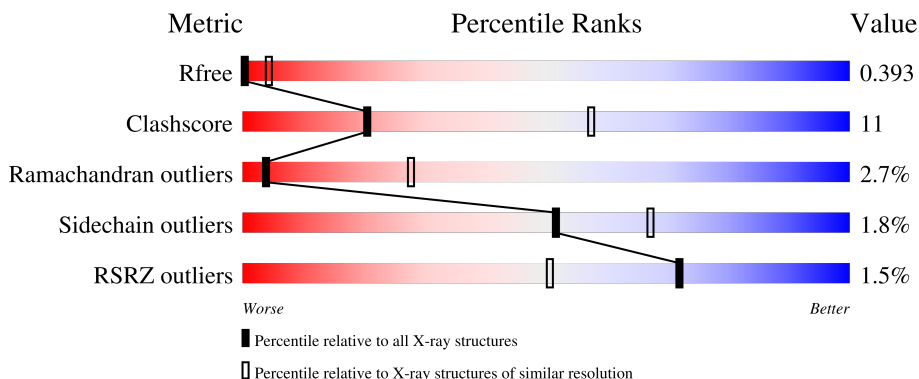
# 1 Overall quality at a glance i

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))
$R_{free}$	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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  $\geq 3$ , 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	354	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2%      71%      21%      • 6%</p>
1	B	354	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">%      66%      26%      • 6%</p>
1	D	354	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2%      70%      21%      • 6%</p>
1	E	354	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">%      68%      25%      • 6%</p>
1	F	354	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">%      72%      21%      • 6%</p>

## 2 Entry composition [i](#)

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.

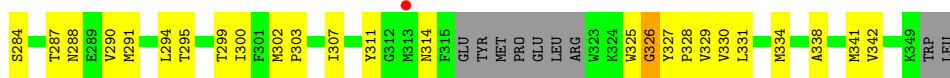
- Molecule 1 is a protein called divalent cation transport-related protein.

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

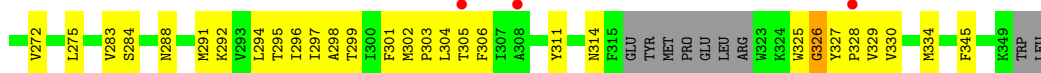
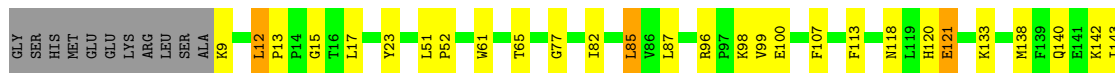
There are 15 discrepancies between the modelled and reference sequences:

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

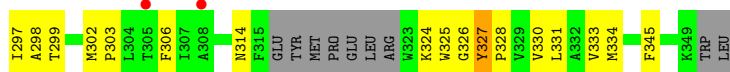
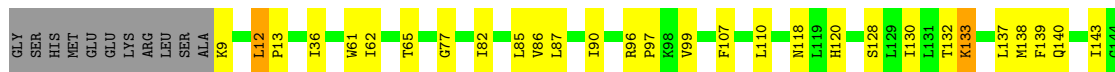




• Molecule 1: divalent cation transport-related protein



• 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 20.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-3.90) 94.8 (20.00-3.90)	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)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.361 , 0.406 0.347 , 0.393	Depositor DCC
$R_{free}$ test set	1394 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	141.8	Xtrriage
Anisotropy	0.233	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.017 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	163.0	wwPDB-VP

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.50	0/2820	0.89	1/3822 (0.0%)
1	B	0.53	0/2820	0.93	5/3822 (0.1%)
1	D	0.52	1/2820 (0.0%)	0.92	5/3822 (0.1%)
1	E	0.50	1/2820 (0.0%)	0.88	2/3822 (0.1%)
1	F	0.51	0/2820	0.89	3/3822 (0.1%)
All	All	0.51	2/14100 (0.0%)	0.90	16/19110 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	248	VAL	CA-CB	5.51	1.56	1.54
1	E	248	VAL	CA-CB	5.12	1.56	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	GLY	N-CA-C	12.07	129.80	110.97
1	B	314	ASN	CB-CA-C	-11.79	92.22	110.37
1	D	326	GLY	N-CA-C	10.93	130.81	111.25
1	E	326	GLY	N-CA-C	10.63	129.63	110.71
1	F	326	GLY	N-CA-C	9.63	125.31	110.96
1	B	326	GLY	N-CA-C	7.07	129.93	113.18
1	B	83	HIS	CA-C-N	6.53	128.00	119.84
1	B	83	HIS	C-N-CA	6.53	128.00	119.84
1	B	314	ASN	N-CA-C	6.53	123.83	114.16
1	F	242	LEU	N-CA-C	6.49	119.05	108.08
1	F	120	HIS	N-CA-C	5.62	117.17	110.19
1	D	224	THR	N-CA-C	-5.42	108.44	114.62
1	D	120	HIS	N-CA-C	5.36	116.84	110.19
1	E	205	LYS	N-CA-C	5.35	116.80	110.97
1	D	287	THR	N-CA-C	-5.27	104.97	111.40
1	D	113	PHE	N-CA-C	5.18	117.68	109.24

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	2761	0	2804	77	0
1	B	2761	0	2804	76	0
1	D	2761	0	2804	73	0
1	E	2761	0	2804	74	0
1	F	2761	0	2804	73	0
All	All	13805	0	14020	312	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 (312) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:297:ILE:HD12	1:E:299:THR:HG23	1.78	0.65
1:D:12:LEU:H	1:D:13:PRO:HD3	1.59	0.65
1:A:327:TYR:HB3	1:A:328:PRO:HD3	1.78	0.65
1:D:326:GLY:HA3	1:D:329:VAL:HB	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:153:ARG:HA	1:E:158:ARG:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:ILE:CD1	1:F:299:THR:HG23	2.29	0.63
1:F:138:MET:HE3	1:F:140:GLN:HE21	1.62	0.62
1:E:288:ASN:HA	1:E:291:MET:HB2	1.82	0.62
1:A:291:MET:HE3	1:B:290:VAL:HG12	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:299:THR:HG22	1:A:341:MET:HE2	1.85	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:A:182:PHE:HB3	1:B:10:LYS:HG3	1.85	0.58
1:E:12:LEU:N	1:E:13:PRO:CD	2.64	0.58
1:F:107:PHE:HD1	1:F:130:ILE:HG12	1.69	0.58
1:B:253:ASP:O	1:B:257:HIS:ND1	2.36	0.58
1:F:96:ARG:HD3	1:F:97:PRO:HD2	1.86	0.58
1:E:171:TYR:HB3	1:E:250:TYR:HE2	1.68	0.57
1:D:128:SER:HB2	1:D:139:PHE:HB2	1.87	0.57
1:E:222:ARG:NE	1:E:266:GLU:OE1	2.36	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:D:187:LYS:O	1:D:191:GLU:HG2	2.04	0.57
1:E:85:LEU:HD23	1:E:85:LEU:H	1.70	0.57
1:F:171:TYR:CE1	1:F:251:PHE:HD1	2.22	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:A:185:LEU:HD11	1:A:261:ILE:HG23	1.87	0.55
1:B:12:LEU:N	1:B:13:PRO:CD	2.68	0.55
1:B:171:TYR:HB3	1:B:250:TYR:HE2	1.70	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:E:304:LEU:HB3	1:F:306:PHE:CE1	2.41	0.55
1:E:314:ASN:HD21	1:F:314:ASN:CG	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:THR:HG21	1:F:143:ILE:HD13	1.89	0.55
1:E:297:ILE:O	1:E:301:PHE:HB2	2.06	0.55
1:F:99:VAL:HG23	1:F:231:VAL:HG13	1.88	0.55
1:F:171:TYR:HE1	1:F:251:PHE:CD1	2.24	0.55
1:A:283:VAL:HG11	1:E:284:SER:HB3	1.89	0.55
1:B:260:GLN:HA	1:D:96:ARG:HH21	1.72	0.55
1:B:326:GLY:HA2	1:B:329:VAL:HB	1.87	0.55
1:D:171:TYR:HB3	1:D:250:TYR:CE2	2.42	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:113:PHE:HE2	1:E:224:THR:HG21	1.72	0.53
1:E:242:LEU:CD1	1:E:243:ILE:H	2.22	0.53
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:B:314:ASN:CG	1:D:314:ASN:HD21	2.16	0.53
1:D:85:LEU:H	1:D:85:LEU:HD23	1.73	0.53
1:D:138:MET:HE3	1:D:140:GLN:HE21	1.74	0.53
1:F:128:SER:HB2	1:F:139:PHE:HB2	1.91	0.52
1:B:222:ARG:O	1:B:226:TRP:HB2	2.09	0.52
1:B:267:THR:HG23	1:D:219:VAL:HG11	1.91	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:A:138:MET:HE3	1:A:140:GLN:HE21	1.74	0.52
1:E:330:VAL:O	1:E:334:MET:HG2	2.09	0.52
1:D:240:PRO:O	1:D:242:LEU:HD23	2.11	0.51
1:F:231:VAL:HG12	1:F:232:LEU:HD12	1.93	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:A:130:ILE:HB	1:A:137:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:N	1:B:203:PRO:HD3	2.26	0.51
1:E:120:HIS:O	1:E:121:GLU:CB	2.59	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:B:295:THR:HG21	1:D:290:VAL:HG13	1.94	0.49
1:D:327:TYR:HB3	1:D:328:PRO:HD3	1.93	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: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:H	1:A:85:LEU:HD23	1.78	0.49
1:A:222:ARG:O	1:A:226:TRP:HB2	2.12	0.49
1:A:333:VAL:O	1:A:337:ILE:HG13	2.12	0.48
1:D:331:LEU:HA	1:D:334:MET:HB2	1.94	0.48
1:F:255:TYR:O	1:F:258:THR:HG22	2.14	0.48
1:B:171:TYR:HB3	1:B:250:TYR:CE2	2.49	0.48
1:F:327:TYR:H	1:F:328:PRO:CD	2.27	0.48
1:A:236:TYR:HB2	1:A:251:PHE:CZ	2.49	0.48
1:A:240:PRO:HB2	1:A:241:PRO:CD	2.42	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:A:302:MET:N	1:A:303:PRO:CD	2.78	0.47
1:E:77:GLY:HA2	1:E:82:ILE:CD1	2.38	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:61:TRP:HZ2	1:A:138:MET:HE1	1.78	0.47
1:A:297:ILE:CD1	1:E:299:THR:HG23	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:VAL:O	1:B:340:ILE:HG13	2.14	0.47
1:E:99:VAL:CG2	1:E:231:VAL:HG13	2.44	0.47
1:D:295:THR:HA	1:F:294:LEU:HD13	1.96	0.47
1:F:130:ILE:HB	1:F:137:LEU:HB2	1.95	0.47
1:A:65:THR:HG21	1:A:143:ILE:HD13	1.97	0.46
1:B:31:VAL:HG22	1:B:62:ILE:HG23	1.97	0.46
1:F:185:LEU:HD21	1:F:265:VAL:HG22	1.96	0.46
1:A:255:TYR:HA	1:A:258:THR:HG22	1.98	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:D:244:GLU:C	1:D:246:GLU:H	2.23	0.46
1:E:138:MET:HE3	1:E:140:GLN:HE21	1.81	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:E:283:VAL:HG11	1:F:284:SER:HB3	1.98	0.45
1:F:86:VAL:O	1:F:90:ILE:HG13	2.16	0.45
1:E:255:TYR:HA	1:E:258:THR:HG22	1.97	0.45
1:E:298:ALA:O	1:E:302:MET:CB	2.64	0.45
1:A:218:LEU:HD21	1:A:268:PHE:HB3	1.99	0.45
1:E:120:HIS:HD2	1:E:210:ARG:HE	1.63	0.45
1:D:244:GLU:HG3	1:D:245:LYS:H	1.81	0.45
1:A:67:ILE:HG21	1:A:139:PHE:HB3	1.99	0.45
1:A:99:VAL:CG2	1:A:231:VAL:HG13	2.46	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:D:35:SER:OG	1:D:38:GLU:HG2	2.16	0.45
1:D:327:TYR:N	1:D:328:PRO:CD	2.79	0.45
1:E:100:GLU:HB2	1:E:107:PHE:HB3	1.99	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:F:299:THR:HG21	1:F:345:PHE:HE1	1.80	0.45
1:A:261:ILE:O	1:A:265:VAL:HG23	2.17	0.45
1:A:36:ILE:HG23	1:A:37:GLU:HG3	1.99	0.45
1:A:302:MET:H	1:A:303:PRO:HD2	1.82	0.45
1:D:270:ASP:CG	1:F:269:ARG:HH12	2.25	0.45
1:F:330:VAL:O	1:F:333:VAL:HG12	2.17	0.45
1:D:291:MET:HE3	1:F:290:VAL:HG12	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:132:THR:O	1:F:133:LYS:C	2.61	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:B:115:TYR:OH	1:B:120:HIS:ND1	2.50	0.44
1:B:302:MET:HE1	1:D:302:MET:SD	2.58	0.44
1:D:338:ALA:O	1:D:342:VAL:HG23	2.17	0.44
1:B:327:TYR:O	1:B:331:LEU:HB2	2.18	0.44
1:B:239:VAL:HG11	1:B:248:VAL:HG22	2.00	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: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:A:244:GLU:C	1:A:246:GLU:H	2.25	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:B:65:THR:HG21	1:B:143:ILE:HD13	2.01	0.43
1:B:202:ARG:HE	1:B:202:ARG:HA	1.83	0.43
1:E:222:ARG:HG3	1:E:223:LYS:N	2.33	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:B:36:ILE:HG23	1:B:37:GLU:HG3	2.00	0.42
1:D:244:GLU:O	1:D:246:GLU:N	2.51	0.42
1:A:243:ILE:HG13	1:A:243:ILE:O	2.20	0.42
1:B:230:GLU:HA	1:B:233:SER:HB2	2.02	0.42
1:E:272:VAL:HA	1:E:275:LEU:HB2	2.01	0.42
1:D:171:TYR:HE1	1:D:251:PHE:HD1	1.68	0.42
1:E:244:GLU:C	1:E:246:GLU:H	2.27	0.42
1:A:336:VAL:O	1:A:340:ILE:HG13	2.19	0.42
1:B:87:LEU:HA	1:B:90:ILE:HD12	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:MET:HE3	1:F:290:VAL:CG1	2.50	0.42
1:A:24:ARG:HA	1:A:68:HIS:CG	2.55	0.41
1:B:302:MET:H	1:B:303:PRO:HD2	1.85	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:A:148:ASP:N	1:A:149:PRO:CD	2.84	0.41
1:A:311:TYR:HE2	1:A:330:VAL:HG21	1.86	0.41
1:F:227:PRO:O	1:F:231:VAL:N	2.53	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: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:B:291:MET:HE3	1:D:290:VAL:HG12	2.02	0.41
1:E:51:LEU:N	1:E:52:PRO:CD	2.83	0.41
1:E:302:MET:HA	1:E:305:THR:HG22	2.02	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:B:204:GLU:HB3	1:B:205:LYS:H	1.62	0.41
1:E:165:ARG:HB3	1:E:166:ALA:H	1.72	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:D:122:LEU:HD23	1:D:122:LEU:H	1.86	0.41
1:D:299:THR:HG23	1:F:297:ILE:CD1	2.50	0.41
1:E:292:LYS:O	1:E:296:ILE:HG13	2.20	0.41
1:E:171:TYR:HE1	1:E:251:PHE:HD1	1.69	0.41
1:A:150:VAL:HG21	1:A:173:LEU:HD23	2.03	0.40
1:A:231:VAL:HG12	1:A:232:LEU:HD12	2.03	0.40
1:A:302:MET:HA	1:A:305:THR:HG22	2.04	0.40
1:B:324:LYS:O	1:B:325:TRP:HB2	2.20	0.40
1:F:171:TYR:CE1	1:F:251:PHE:HB2	2.57	0.40
1:A:122:LEU:H	1:A:122:LEU:HD23	1.86	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: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:F:77:GLY:HA3	1:F:87:LEU:HD21	2.03	0.40
1:A:226:TRP:N	1:A:227:PRO:HD2	2.37	0.40
1:D:130:ILE:HB	1:D:137:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:THR:HG21	1:E:345:PHE:HE1	1.87	0.40
1:F:96:ARG:O	1:F:97:PRO:C	2.64	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
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

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%)	3	26
1	B	330/354 (93%)	289 (88%)	32 (10%)	9 (3%)	4	28
1	D	330/354 (93%)	292 (88%)	30 (9%)	8 (2%)	4	29
1	E	330/354 (93%)	291 (88%)	30 (9%)	9 (3%)	4	28
1	F	330/354 (93%)	290 (88%)	32 (10%)	8 (2%)	4	29
All	All	1650/1770 (93%)	1455 (88%)	151 (9%)	44 (3%)	4	28

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

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Mol	Chain	Res	Type
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
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%)	307 (98%)	5 (2%)	55	69
1	B	312/332 (94%)	305 (98%)	7 (2%)	45	64
1	D	312/332 (94%)	305 (98%)	7 (2%)	45	64
1	E	312/332 (94%)	308 (99%)	4 (1%)	61	71
1	F	312/332 (94%)	307 (98%)	5 (2%)	55	69
All	All	1560/1660 (94%)	1532 (98%)	28 (2%)	51	67

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
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
1	B	285	ASN
1	B	311	TYR
1	D	9	LYS
1	D	85	LEU
1	D	95	GLN
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	222	ARG
1	E	311	TYR
1	F	9	LYS
1	F	196	GLU
1	F	222	ARG
1	F	231	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	269	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	33	ASN
1	A	92	ASN
1	A	94	HIS
1	A	95	GLN
1	A	217	ASN
1	A	285	ASN
1	B	33	ASN
1	B	104	ASN
1	B	126	GLN
1	B	134	ASN
1	B	285	ASN
1	D	33	ASN
1	D	63	ASN
1	D	83	HIS
1	D	95	GLN
1	D	104	ASN
1	D	126	GLN
1	D	140	GLN
1	D	285	ASN
1	D	314	ASN
1	E	33	ASN
1	E	95	GLN
1	E	217	ASN
1	E	285	ASN
1	E	314	ASN
1	F	63	ASN
1	F	95	GLN
1	F	104	ASN
1	F	126	GLN
1	F	140	GLN
1	F	217	ASN
1	F	285	ASN
1	F	314	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](#)

There are no ligands in this entry.

### 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, 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%)	0.27	7 (2%) 63 44	157, 163, 169, 171	0
1	B	334/354 (94%)	0.27	5 (1%) 72 50	157, 163, 169, 563	0
1	D	334/354 (94%)	0.26	6 (1%) 67 47	157, 163, 169, 172	0
1	E	334/354 (94%)	0.20	4 (1%) 76 55	157, 163, 169, 172	0
1	F	334/354 (94%)	0.10	3 (0%) 81 62	157, 163, 169, 172	0
All	All	1670/1770 (94%)	0.22	25 (1%) 72 50	157, 163, 169, 563	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	ILE	4.3
1	A	256	ASP	3.5
1	A	194	VAL	3.4
1	E	305	THR	3.2
1	D	313	MET	2.8
1	E	251	PHE	2.8
1	A	348	LYS	2.8
1	D	171	TYR	2.7
1	D	96	ARG	2.7
1	E	328	PRO	2.6
1	D	275	LEU	2.6
1	A	255	TYR	2.5
1	A	25	GLU	2.5
1	F	286	LYS	2.3
1	A	191	GLU	2.3
1	A	210	ARG	2.3
1	D	135	CYS	2.2
1	F	305	THR	2.1
1	D	26	ASP	2.1
1	E	308	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	312	GLY	2.0
1	B	96	ARG	2.0
1	B	343	VAL	2.0
1	B	304	LEU	2.0
1	F	308	ALA	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.