



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:03 am GMT

PDB ID : 3EZ9  
Title : Partition Protein  
Authors : Schumacher, M.A.  
Deposited on : 2008-10-22  
Resolution : 2.80 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.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

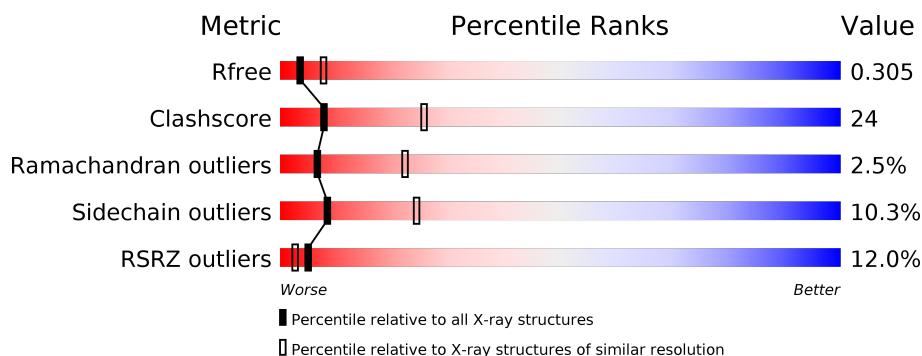
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	403	<div> <div>5%</div> <div>46%</div> <div>35%</div> <div>• •</div> <div>13%</div> </div>
1	B	403	<div> <div>15%</div> <div>45%</div> <div>35%</div> <div>6% •</div> <div>13%</div> </div>

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	MG	A	402	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5670 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 ParA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2802	1772	491	532	7			
1	B	350	Total	C	N	O	S	0	0	0
			2792	1763	491	531	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP B4ABW6
A	0	MET	-	EXPRESSION TAG	UNP B4ABW6
A	21	ALA	SER	CONFLICT	UNP B4ABW6
A	28	ASP	GLU	CONFLICT	UNP B4ABW6
A	35	GLN	LEU	CONFLICT	UNP B4ABW6
A	59	ASP	GLU	CONFLICT	UNP B4ABW6
A	67	GLU	ASP	CONFLICT	UNP B4ABW6
A	68	ASP	GLY	CONFLICT	UNP B4ABW6
A	71	GLN	GLU	CONFLICT	UNP B4ABW6
A	182	ASN	ASP	CONFLICT	UNP B4ABW6
A	198	VAL	ILE	CONFLICT	UNP B4ABW6
A	218	ARG	GLU	CONFLICT	UNP B4ABW6
A	219	GLU	ASP	CONFLICT	UNP B4ABW6
A	222	GLU	LYS	CONFLICT	UNP B4ABW6
A	228	GLN	MET	CONFLICT	UNP B4ABW6
A	229	ASN	LYS	CONFLICT	UNP B4ABW6
A	230	GLN	PRO	CONFLICT	UNP B4ABW6
A	231	TYR	SER	CONFLICT	UNP B4ABW6
A	233	ILE	VAL	CONFLICT	UNP B4ABW6
A	236	ARG	LYS	CONFLICT	UNP B4ABW6
A	237	ASN	LYS	CONFLICT	UNP B4ABW6
A	240	ASP	GLU	CONFLICT	UNP B4ABW6
A	360	VAL	ILE	CONFLICT	UNP B4ABW6
A	380	THR	ASN	CONFLICT	UNP B4ABW6
B	-1	MET	-	EXPRESSION TAG	UNP B4ABW6

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP B4ABW6
B	21	ALA	SER	CONFLICT	UNP B4ABW6
B	28	ASP	GLU	CONFLICT	UNP B4ABW6
B	35	GLN	LEU	CONFLICT	UNP B4ABW6
B	59	ASP	GLU	CONFLICT	UNP B4ABW6
B	67	GLU	ASP	CONFLICT	UNP B4ABW6
B	68	ASP	GLY	CONFLICT	UNP B4ABW6
B	71	GLN	GLU	CONFLICT	UNP B4ABW6
B	182	ASN	ASP	CONFLICT	UNP B4ABW6
B	198	VAL	ILE	CONFLICT	UNP B4ABW6
B	218	ARG	GLU	CONFLICT	UNP B4ABW6
B	219	GLU	ASP	CONFLICT	UNP B4ABW6
B	222	GLU	LYS	CONFLICT	UNP B4ABW6
B	228	GLN	MET	CONFLICT	UNP B4ABW6
B	229	ASN	LYS	CONFLICT	UNP B4ABW6
B	230	GLN	PRO	CONFLICT	UNP B4ABW6
B	231	TYR	SER	CONFLICT	UNP B4ABW6
B	233	ILE	VAL	CONFLICT	UNP B4ABW6
B	236	ARG	LYS	CONFLICT	UNP B4ABW6
B	237	ASN	LYS	CONFLICT	UNP B4ABW6
B	240	ASP	GLU	CONFLICT	UNP B4ABW6
B	360	VAL	ILE	CONFLICT	UNP B4ABW6
B	380	THR	ASN	CONFLICT	UNP B4ABW6

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

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

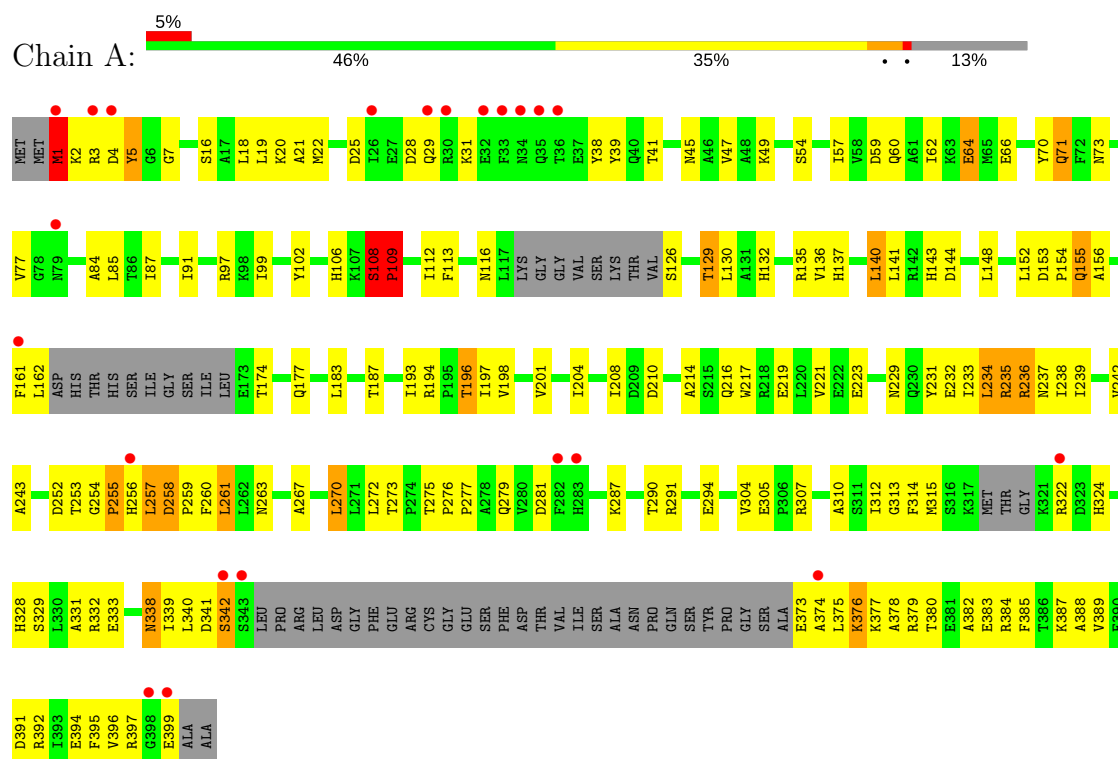
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	44	Total O 44 44	0	0
3	B	31	Total O 31 31	0	0

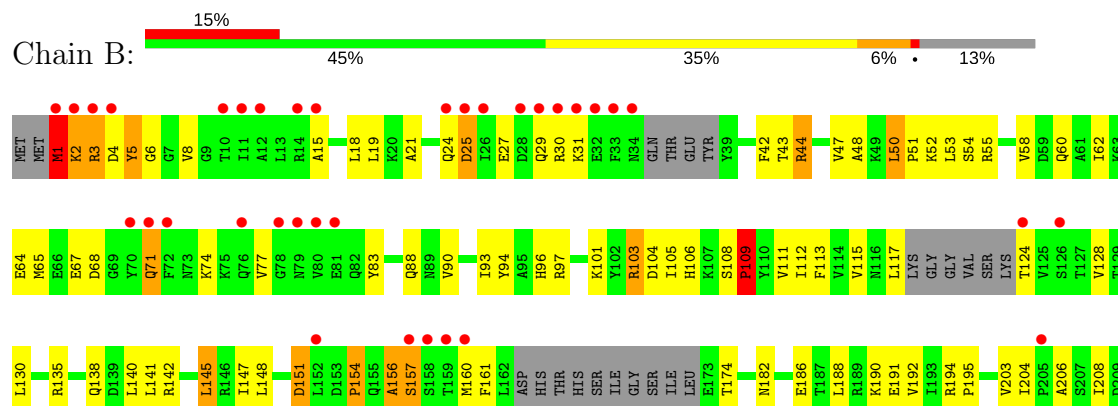
### 3 Residue-property plots

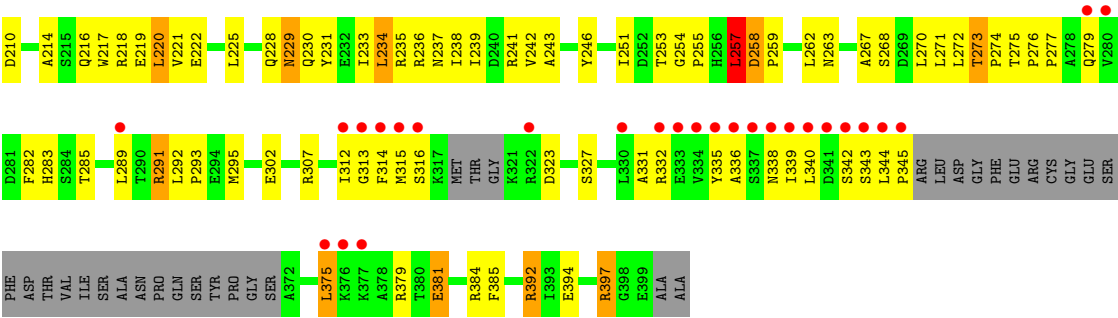
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Para



#### • Molecule 1: Para





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.95Å 267.41Å 154.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.85 – 2.80 66.85 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.3 (66.85-2.80) 99.3 (66.85-2.67)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.65Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.254 , 0.294 0.267 , 0.305	Depositor DCC
$R_{free}$ test set	2015 reflections (6.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.3	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 70.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.62	2/2850 (0.1%)	0.94	11/3853 (0.3%)
1	B	0.47	1/2838 (0.0%)	0.82	4/3837 (0.1%)
All	All	0.55	3/5688 (0.1%)	0.88	15/7690 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLN	CB-CG	-12.98	1.17	1.52
1	B	1	MET	N-CA	6.89	1.60	1.46
1	A	109	PRO	N-CA	6.31	1.57	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	PRO	CA-N-CD	-24.64	77.00	111.50
1	A	109	PRO	CA-N-CD	-23.71	78.30	111.50
1	A	108	SER	C-N-CD	-8.96	100.89	120.60
1	A	109	PRO	N-CA-CB	8.45	113.44	103.30
1	A	1	MET	N-CA-C	8.09	132.84	111.00
1	B	1	MET	N-CA-C	7.62	131.58	111.00
1	A	1	MET	CA-C-N	6.47	131.43	117.20
1	B	1	MET	CA-C-N	6.41	131.30	117.20
1	A	109	PRO	CB-CA-C	-6.36	96.11	112.00
1	A	156	ALA	N-CA-C	6.06	127.37	111.00
1	A	39	TYR	N-CA-C	-5.99	94.82	111.00
1	A	108	SER	C-N-CA	5.86	146.62	122.00
1	A	109	PRO	CB-CG-CD	-5.20	86.21	106.50
1	A	261	LEU	CA-CB-CG	5.12	127.09	115.30
1	B	109	PRO	CA-CB-CG	-5.07	94.37	104.00

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	2802	0	2798	131	1
1	B	2792	0	2791	139	0
2	A	1	0	0	0	0
3	A	44	0	0	1	0
3	B	31	0	0	3	0
All	All	5670	0	5589	270	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 24.

All (270) 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:B:279:GLN:HA	1:B:282:PHE:HB3	1.46	0.97
1:B:182:ASN:OD1	1:B:241:ARG:NH2	1.99	0.95
1:B:335:TYR:HB2	1:B:339:ILE:HG12	1.52	0.92
1:A:47:VAL:HG21	1:A:85:LEU:HD12	1.53	0.90
1:A:236:ARG:HE	1:A:237:ASN:HD21	1.19	0.89
1:A:196:THR:HG23	1:A:198:VAL:H	1.37	0.88
1:B:342:SER:HG	1:B:385:PHE:HD1	0.90	0.85
1:B:342:SER:OG	1:B:385:PHE:HD1	1.60	0.85
1:B:21:ALA:HA	1:B:24:GLN:HG2	1.60	0.82
1:B:270:LEU:HD21	1:B:312:ILE:HG12	1.60	0.82
1:A:307:ARG:HD2	3:A:415:HOH:O	1.80	0.82
1:A:340:LEU:HD11	1:A:392:ARG:HG3	1.62	0.82
1:A:287:LYS:O	1:A:290:THR:HG22	1.79	0.81
1:A:374:ALA:O	1:A:378:ALA:HB3	1.80	0.80
1:A:183:LEU:HD22	1:A:187:THR:HG21	1.65	0.79
1:A:109:PRO:HD2	1:A:243:ALA:O	1.86	0.76
1:B:275:THR:HB	1:B:315:MET:HA	1.66	0.76
1:B:42:PHE:HE2	1:B:138:GLN:HE21	1.32	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASP:HB3	1:B:29:GLN:HE21	1.51	0.74
1:B:195:PRO:HD3	3:B:427:HOH:O	1.86	0.74
1:B:229:ASN:HD22	1:B:231:TYR:H	1.37	0.73
1:B:307:ARG:HD2	3:B:421:HOH:O	1.89	0.72
1:A:174:THR:HG23	1:A:177:GLN:H	1.54	0.71
1:B:218:ARG:O	1:B:222:GLU:HG3	1.91	0.71
1:A:375:LEU:O	1:A:379:ARG:HB2	1.91	0.70
1:A:279:GLN:NE2	1:A:322:ARG:HH12	1.89	0.69
1:A:174:THR:HG22	1:A:177:GLN:HE21	1.57	0.69
1:A:57:ILE:HD12	1:A:97:ARG:HE	1.58	0.69
1:B:228:GLN:NE2	1:B:236:ARG:HE	1.89	0.69
1:B:108:SER:HB3	1:B:243:ALA:O	1.93	0.68
1:A:310:ALA:HB1	1:A:396:VAL:HG11	1.75	0.68
1:A:137:HIS:HB3	1:A:140:LEU:HB2	1.76	0.67
1:A:392:ARG:O	1:A:396:VAL:HG23	1.93	0.67
1:B:314:PHE:HB3	1:B:340:LEU:HB2	1.75	0.67
1:A:216:GLN:HG2	1:A:219:GLU:HB3	1.78	0.66
1:A:380:THR:O	1:A:384:ARG:HG3	1.95	0.65
1:A:41:THR:HG23	1:A:84:ALA:HB1	1.78	0.65
1:B:270:LEU:HD22	1:B:271:LEU:H	1.61	0.65
1:B:274:PRO:HB3	1:B:314:PHE:CZ	2.31	0.65
1:A:236:ARG:HE	1:A:237:ASN:ND2	1.92	0.65
1:B:339:ILE:N	1:B:392:ARG:HH22	1.95	0.65
1:B:58:VAL:O	1:B:62:ILE:HG12	1.97	0.65
1:B:258:ASP:H	1:B:259:PRO:HD2	1.60	0.64
1:B:340:LEU:HD21	1:B:392:ARG:HG3	1.80	0.64
1:B:4:ASP:O	1:B:8:VAL:HG23	1.97	0.64
1:A:174:THR:HG21	1:A:210:ASP:OD1	1.97	0.64
1:A:214:ALA:HB1	1:A:257:LEU:HD11	1.80	0.64
1:A:112:ILE:HG23	1:A:270:LEU:HD23	1.81	0.63
1:B:228:GLN:CD	1:B:236:ARG:HE	2.01	0.63
1:B:62:ILE:HD13	1:B:93:ILE:HD11	1.79	0.62
1:A:2:LYS:HB2	1:A:5:TYR:CD2	2.34	0.62
1:A:258:ASP:H	1:A:259:PRO:HD2	1.63	0.62
1:A:229:ASN:ND2	1:A:231:TYR:H	1.98	0.61
1:A:1:MET:SD	1:A:1:MET:N	2.70	0.61
1:B:103:ARG:HB3	1:B:103:ARG:HH11	1.66	0.61
1:B:339:ILE:H	1:B:392:ARG:HH22	1.48	0.61
1:A:132:HIS:O	1:A:136:VAL:HG22	2.01	0.61
1:A:255:PRO:HD2	1:A:256:HIS:ND1	2.16	0.61
1:B:47:VAL:HA	1:B:50:LEU:HD22	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ARG:NE	1:B:3:ARG:HA	2.16	0.60
1:B:65:MET:HG3	1:B:96:HIS:ND1	2.17	0.60
1:B:332:ARG:HA	1:B:339:ILE:HD13	1.83	0.60
1:A:229:ASN:HD22	1:A:231:TYR:H	1.48	0.60
1:A:62:ILE:O	1:A:66:GLU:HB2	2.01	0.60
1:B:1:MET:N	1:B:1:MET:SD	2.70	0.60
1:A:19:LEU:O	1:A:22:MET:HB2	2.01	0.59
1:B:312:ILE:HD12	1:B:392:ARG:HH11	1.67	0.59
1:A:313:GLY:O	1:A:339:ILE:HA	2.03	0.59
1:B:314:PHE:CB	1:B:340:LEU:HB2	2.32	0.59
1:B:214:ALA:HB1	1:B:257:LEU:HD11	1.85	0.58
1:A:385:PHE:O	1:A:388:ALA:HB3	2.03	0.58
1:A:45:ASN:O	1:A:49:LYS:HG3	2.04	0.58
1:B:186:GLU:H	1:B:186:GLU:CD	2.06	0.58
1:B:292:LEU:O	1:B:295:MET:HB2	2.04	0.57
1:B:97:ARG:HH11	1:B:97:ARG:HG3	1.68	0.57
1:A:113:PHE:HZ	1:A:261:LEU:HD22	1.69	0.57
1:B:111:VAL:HB	1:B:268:SER:HA	1.86	0.57
1:B:30:ARG:HH12	1:B:31:LYS:HE3	1.70	0.57
1:A:174:THR:HG22	1:A:177:GLN:HG3	1.87	0.57
1:B:229:ASN:ND2	1:B:231:TYR:H	2.02	0.57
1:A:109:PRO:CD	1:A:243:ALA:O	2.54	0.56
1:B:27:GLU:HA	1:B:30:ARG:NH2	2.21	0.55
1:A:254:GLY:HA3	1:A:256:HIS:CE1	2.41	0.55
1:A:387:LYS:HD3	1:A:391:ASP:OD2	2.06	0.55
1:A:57:ILE:HD12	1:A:97:ARG:NE	2.20	0.55
1:A:310:ALA:CB	1:A:396:VAL:HG11	2.36	0.55
1:B:216:GLN:O	1:B:220:LEU:HB2	2.07	0.55
1:A:18:LEU:HD23	1:A:18:LEU:O	2.06	0.55
1:A:196:THR:HG23	1:A:198:VAL:N	2.17	0.54
1:A:54:SER:OG	1:A:57:ILE:HG12	2.07	0.54
1:B:154:PRO:HB3	1:B:208:ILE:HA	1.89	0.54
1:A:315:MET:CE	1:A:328:HIS:HA	2.37	0.54
1:A:257:LEU:HD13	1:A:258:ASP:H	1.71	0.54
1:B:151:ASP:HB3	1:B:206:ALA:HB2	1.90	0.54
1:B:190:LYS:HG3	1:B:191:GLU:HG3	1.90	0.54
1:B:25:ASP:HB3	1:B:29:GLN:NE2	2.22	0.54
1:B:235:ARG:HG2	1:B:267:ALA:CB	2.38	0.54
1:B:74:LYS:HG3	1:B:83:TYR:HA	1.89	0.53
1:B:231:TYR:CZ	1:B:262:LEU:HD13	2.44	0.53
1:B:314:PHE:HB3	1:B:340:LEU:HD12	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:HG2	1:B:237:ASN:OD1	2.08	0.53
1:A:290:THR:HG23	1:A:291:ARG:HH11	1.74	0.53
1:A:385:PHE:O	1:A:389:VAL:HG23	2.09	0.53
1:B:51:PRO:C	1:B:53:LEU:H	2.12	0.52
1:A:132:HIS:NE2	1:A:196:THR:HG21	2.24	0.52
1:B:128:VAL:HG11	1:B:160:MET:HG2	1.92	0.52
1:A:197:ILE:HG13	1:A:198:VAL:HG23	1.90	0.52
1:A:256:HIS:CD2	1:A:257:LEU:N	2.77	0.52
1:A:20:LYS:C	1:A:22:MET:H	2.13	0.52
1:B:47:VAL:O	1:B:50:LEU:HB2	2.10	0.52
1:B:65:MET:SD	1:B:93:ILE:HD13	2.49	0.52
1:B:231:TYR:CE1	1:B:302:GLU:HG3	2.45	0.52
1:B:336:ALA:C	1:B:338:ASN:H	2.13	0.52
1:B:43:THR:O	1:B:47:VAL:HG23	2.10	0.52
1:A:196:THR:HG23	1:A:197:ILE:N	2.24	0.51
1:A:18:LEU:O	1:A:21:ALA:HB3	2.11	0.51
1:B:313:GLY:HA3	1:B:335:TYR:CD1	2.44	0.51
1:A:87:ILE:HG23	1:A:141:LEU:HD22	1.93	0.51
1:B:147:ILE:HG22	1:B:148:LEU:N	2.25	0.51
1:B:375:LEU:O	1:B:379:ARG:HB2	2.11	0.51
1:A:313:GLY:O	1:A:339:ILE:HD12	2.11	0.51
1:A:154:PRO:O	1:A:155:GLN:HG3	2.11	0.51
1:A:341:ASP:O	1:A:342:SER:HB3	2.10	0.51
1:A:60:GLN:O	1:A:64:GLU:HB2	2.10	0.51
1:A:73:ASN:HB3	1:A:84:ALA:O	2.11	0.50
1:A:116:ASN:HD22	1:A:254:GLY:HA2	1.76	0.50
1:A:22:MET:HA	1:A:25:ASP:OD1	2.11	0.50
1:B:124:THR:HG22	1:B:160:MET:HE2	1.93	0.50
1:B:292:LEU:O	1:B:295:MET:N	2.45	0.50
1:B:338:ASN:HA	1:B:392:ARG:NH2	2.27	0.50
1:B:315:MET:O	1:B:343:SER:HA	2.12	0.49
1:B:124:THR:CG2	1:B:156:ALA:HB1	2.42	0.49
1:B:225:LEU:HD13	1:B:233:ILE:HD12	1.94	0.49
1:B:64:GLU:HB3	1:B:96:HIS:HE1	1.77	0.49
1:A:256:HIS:CG	1:A:257:LEU:N	2.81	0.49
1:A:102:TYR:HB2	1:A:143:HIS:HB3	1.94	0.49
1:A:294:GLU:CD	1:A:294:GLU:H	2.16	0.49
1:A:87:ILE:O	1:A:91:ILE:HG13	2.13	0.49
1:B:111:VAL:HG21	1:B:239:ILE:HD13	1.95	0.49
1:B:112:ILE:HG23	1:B:270:LEU:HD12	1.95	0.49
1:B:270:LEU:HD22	1:B:271:LEU:N	2.26	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PHE:HB3	1:B:271:LEU:HD12	1.93	0.49
1:B:188:LEU:HD23	1:B:192:VAL:HG21	1.95	0.49
1:B:327:SER:O	1:B:331:ALA:HB2	2.13	0.48
1:A:174:THR:HG22	1:A:177:GLN:NE2	2.27	0.48
1:B:381:GLU:O	1:B:384:ARG:HB3	2.14	0.48
1:B:71:GLN:NE2	1:B:71:GLN:H	2.11	0.48
1:B:228:GLN:HE22	1:B:237:ASN:HD21	1.62	0.48
1:A:396:VAL:O	1:A:396:VAL:HG12	2.14	0.48
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.79	0.48
1:B:105:ILE:HG23	1:B:106:HIS:CD2	2.48	0.48
1:B:229:ASN:C	1:B:229:ASN:HD22	2.17	0.48
1:A:395:PHE:CD1	1:A:399:GLU:OE1	2.67	0.48
1:A:152:LEU:HB2	1:A:253:THR:HG22	1.96	0.48
1:A:232:GLU:O	1:A:236:ARG:HB2	2.14	0.47
1:A:235:ARG:HG2	1:A:267:ALA:CB	2.44	0.47
1:B:344:LEU:HD22	1:B:345:PRO:HD2	1.95	0.47
1:A:276:PRO:HB2	1:A:281:ASP:HB2	1.97	0.47
1:A:270:LEU:HD11	1:A:312:ILE:HG12	1.96	0.47
1:A:342:SER:HB3	1:A:385:PHE:CD1	2.49	0.47
1:B:15:ALA:O	1:B:19:LEU:HG	2.13	0.47
1:B:234:LEU:HB2	1:B:263:ASN:HB3	1.96	0.47
1:A:273:THR:O	1:A:313:GLY:HA2	2.15	0.47
1:B:214:ALA:O	1:B:259:PRO:HG3	2.15	0.47
1:A:373:GLU:O	1:A:377:LYS:HB2	2.15	0.47
1:A:238:ILE:O	1:A:242:VAL:HG22	2.15	0.47
1:A:315:MET:HE1	1:A:331:ALA:CB	2.45	0.47
1:B:233:ILE:HG23	1:B:237:ASN:HD22	1.80	0.47
1:B:239:ILE:HD12	1:B:267:ALA:HB1	1.97	0.47
1:A:25:ASP:O	1:A:28:ASP:HB3	2.15	0.47
1:B:145:LEU:CD2	1:B:145:LEU:H	2.27	0.47
1:B:50:LEU:O	1:B:53:LEU:HB2	2.14	0.47
1:A:234:LEU:HB2	1:A:263:ASN:HB3	1.97	0.46
1:A:277:PRO:HB2	1:A:324:HIS:CG	2.50	0.46
1:A:106:HIS:NE2	1:A:394:GLU:OE1	2.49	0.46
1:B:109:PRO:HG3	1:B:243:ALA:HA	1.98	0.46
1:B:276:PRO:HB2	1:B:282:PHE:HA	1.98	0.46
1:A:235:ARG:NE	1:A:239:ILE:HG21	2.31	0.45
1:B:194:ARG:HA	1:B:194:ARG:HD3	1.67	0.45
1:B:77:VAL:O	1:B:77:VAL:HG23	2.16	0.45
1:B:219:GLU:CD	1:B:219:GLU:H	2.18	0.45
1:A:174:THR:CG2	1:A:177:GLN:H	2.27	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASN:HA	1:A:392:ARG:NH2	2.32	0.45
1:A:41:THR:HG23	1:A:84:ALA:CB	2.46	0.45
1:B:115:VAL:HG21	1:B:273:THR:HG23	1.98	0.45
1:B:335:TYR:CB	1:B:339:ILE:HG12	2.37	0.45
1:B:148:LEU:HD13	1:B:246:TYR:CZ	2.52	0.45
1:B:52:LYS:HG3	1:B:142:ARG:HD2	1.98	0.45
1:A:148:LEU:HD11	1:A:204:ILE:HG13	1.99	0.45
1:B:233:ILE:HG23	1:B:237:ASN:ND2	2.33	0.44
1:A:196:THR:HG21	1:A:201:VAL:HB	1.99	0.44
1:A:329:SER:HA	1:A:332:ARG:HH11	1.82	0.44
1:B:25:ASP:O	1:B:29:GLN:HG3	2.17	0.44
1:A:229:ASN:O	1:A:233:ILE:HG13	2.17	0.44
1:A:174:THR:HG22	1:A:177:GLN:CG	2.46	0.44
1:A:378:ALA:O	1:A:379:ARG:C	2.56	0.44
1:A:196:THR:HG22	1:A:198:VAL:O	2.18	0.44
1:B:214:ALA:CB	1:B:257:LEU:HD11	2.46	0.44
1:B:124:THR:CG2	1:B:157:SER:H	2.31	0.44
1:B:251:ILE:HD12	1:B:268:SER:OG	2.17	0.44
1:B:186:GLU:N	1:B:186:GLU:CD	2.71	0.44
1:B:1:MET:HE1	3:B:402:HOH:O	2.16	0.44
1:B:109:PRO:HD2	1:B:246:TYR:O	2.18	0.44
1:A:126:SER:O	1:A:129:THR:HG22	2.18	0.44
1:A:217:TRP:O	1:A:221:VAL:HG23	2.18	0.44
1:B:2:LYS:H	1:B:6:GLY:CA	2.30	0.44
1:B:109:PRO:CG	1:B:243:ALA:HA	2.48	0.43
1:B:90:VAL:HB	1:B:141:LEU:HD23	1.99	0.43
1:B:128:VAL:HB	1:B:160:MET:HE2	2.00	0.43
1:A:20:LYS:C	1:A:22:MET:N	2.72	0.43
1:A:291:ARG:HA	1:A:294:GLU:OE2	2.17	0.43
1:A:237:ASN:ND2	1:A:237:ASN:N	2.63	0.43
1:B:101:LYS:O	1:B:104:ASP:HB2	2.17	0.43
1:A:153:ASP:O	1:A:155:GLN:N	2.48	0.43
1:A:235:ARG:HG2	1:A:267:ALA:HB1	2.00	0.43
1:B:229:ASN:HD22	1:B:230:GLN:N	2.17	0.43
1:B:235:ARG:HG2	1:B:267:ALA:HB1	1.99	0.43
1:B:257:LEU:HD13	1:B:258:ASP:H	1.82	0.43
1:B:5:TYR:CD1	1:B:5:TYR:O	2.72	0.43
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.84	0.42
1:A:257:LEU:HD12	1:A:260:PHE:HB2	2.02	0.42
1:A:2:LYS:HB2	1:A:5:TYR:HD2	1.82	0.42
1:A:237:ASN:N	1:A:237:ASN:HD22	2.18	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HD12	1:A:392:ARG:HE	1.85	0.42
1:B:292:LEU:N	1:B:293:PRO:HD2	2.34	0.42
1:B:30:ARG:HG3	1:B:30:ARG:HH11	1.85	0.42
1:B:44:ARG:NH1	1:B:44:ARG:HG3	2.35	0.42
1:A:97:ARG:HB3	1:A:99:ILE:CD1	2.48	0.42
1:B:381:GLU:OE1	1:B:384:ARG:HD2	2.20	0.42
1:A:340:LEU:HD11	1:A:392:ARG:CG	2.41	0.41
1:A:77:VAL:HG23	1:A:77:VAL:O	2.20	0.41
1:A:113:PHE:HZ	1:A:261:LEU:CD2	2.32	0.41
1:B:275:THR:O	1:B:316:SER:HB2	2.20	0.41
1:A:91:ILE:HD13	1:A:144:ASP:OD1	2.19	0.41
1:B:48:ALA:HB1	1:B:55:ARG:N	2.36	0.41
1:B:53:LEU:HG	1:B:94:TYR:CE2	2.56	0.41
1:A:382:ALA:O	1:A:385:PHE:HB3	2.20	0.41
1:B:174:THR:HG21	1:B:210:ASP:OD1	2.20	0.41
1:A:108:SER:HB3	1:A:243:ALA:O	2.19	0.41
1:A:373:GLU:HA	1:A:377:LYS:HG3	2.02	0.41
1:B:279:GLN:HA	1:B:282:PHE:CB	2.33	0.41
1:A:5:TYR:C	1:A:7:GLY:H	2.24	0.41
1:B:18:LEU:O	1:B:18:LEU:HD23	2.21	0.41
1:A:71:GLN:HE21	1:A:71:GLN:HB2	1.63	0.41
1:B:217:TRP:O	1:B:221:VAL:HG23	2.21	0.41
1:B:238:ILE:O	1:B:242:VAL:HG22	2.21	0.41
1:B:253:THR:HG22	1:B:254:GLY:O	2.21	0.41
1:B:203:VAL:HG12	1:B:204:ILE:N	2.36	0.41
1:A:28:ASP:HA	1:A:31:LYS:HE3	2.02	0.41
1:B:276:PRO:HA	1:B:277:PRO:HD2	1.97	0.41
1:B:285:THR:O	1:B:289:LEU:HG	2.20	0.41
1:A:270:LEU:HA	1:A:310:ALA:O	2.20	0.41
1:A:275:THR:HA	1:A:276:PRO:HD3	1.85	0.41
1:B:109:PRO:CD	1:B:246:TYR:O	2.69	0.41
1:A:314:PHE:HB3	1:A:340:LEU:HB2	2.03	0.40
1:A:54:SER:O	1:A:57:ILE:N	2.53	0.40
1:B:145:LEU:N	1:B:145:LEU:HD23	2.36	0.40
1:A:16:SER:HA	1:A:19:LEU:HD12	2.02	0.40
1:A:315:MET:HE1	1:A:331:ALA:HB2	2.04	0.40
1:A:379:ARG:O	1:A:383:GLU:HG3	2.21	0.40
1:B:291:ARG:HA	1:B:291:ARG:HD2	1.84	0.40
1:B:8:VAL:HG12	1:B:8:VAL:O	2.21	0.40
1:A:5:TYR:O	1:A:5:TYR:CD1	2.74	0.40
1:A:193:ILE:HD11	1:A:242:VAL:HG11	2.04	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD23	1:B:255:PRO:HG3	2.03	0.40
1:B:340:LEU:HD21	1:B:392:ARG:CG	2.49	0.40
1:B:344:LEU:HA	1:B:345:PRO:HD3	1.90	0.40
1:A:108:SER:HB3	1:A:109:PRO:HD2	2.04	0.40
1:A:196:THR:CG2	1:A:198:VAL:H	2.21	0.40
1:A:315:MET:HE1	1:A:328:HIS:HA	2.03	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:60:GLN:CG	1:A:399:GLU:OE2[8_565]	1.69	0.51

## 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	339/403 (84%)	303 (89%)	30 (9%)	6 (2%)	10	32
1	B	338/403 (84%)	293 (87%)	34 (10%)	11 (3%)	4	15
All	All	677/806 (84%)	596 (88%)	64 (10%)	17 (2%)	6	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	PRO
1	B	109	PRO
1	B	161	PHE
1	A	342	SER
1	A	376	LYS
1	B	3	ARG
1	B	68	ASP

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	258	ASP
1	A	258	ASP
1	B	2	LYS
1	B	156	ALA
1	B	157	SER
1	B	397	ARG
1	A	70	TYR
1	A	255	PRO
1	B	154	PRO
1	B	257	LEU

### 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	305/350 (87%)	272 (89%)	33 (11%)	7	22
1	B	304/350 (87%)	274 (90%)	30 (10%)	9	26
All	All	609/700 (87%)	546 (90%)	63 (10%)	8	24

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ARG
1	A	4	ASP
1	A	5	TYR
1	A	38	TYR
1	A	59	ASP
1	A	64	GLU
1	A	71	GLN
1	A	108	SER
1	A	129	THR
1	A	130	LEU
1	A	135	ARG
1	A	140	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	155	GLN
1	A	161	PHE
1	A	162	LEU
1	A	194	ARG
1	A	196	THR
1	A	208	ILE
1	A	223	GLU
1	A	234	LEU
1	A	235	ARG
1	A	236	ARG
1	A	252	ASP
1	A	257	LEU
1	A	270	LEU
1	A	272	LEU
1	A	304	VAL
1	A	305	GLU
1	A	333	GLU
1	A	338	ASN
1	A	376	LYS
1	A	397	ARG
1	B	1	MET
1	B	5	TYR
1	B	25	ASP
1	B	44	ARG
1	B	50	LEU
1	B	54	SER
1	B	60	GLN
1	B	67	GLU
1	B	71	GLN
1	B	88	GLN
1	B	103	ARG
1	B	109	PRO
1	B	130	LEU
1	B	135	ARG
1	B	140	LEU
1	B	145	LEU
1	B	151	ASP
1	B	220	LEU
1	B	229	ASN
1	B	234	LEU
1	B	257	LEU
1	B	273	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	283	HIS
1	B	291	ARG
1	B	323	ASP
1	B	375	LEU
1	B	381	GLU
1	B	392	ARG
1	B	394	GLU
1	B	397	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	71	GLN
1	A	96	HIS
1	A	116	ASN
1	A	177	GLN
1	A	228	GLN
1	A	229	ASN
1	A	230	GLN
1	A	237	ASN
1	A	279	GLN
1	A	298	GLN
1	B	29	GLN
1	B	71	GLN
1	B	106	HIS
1	B	138	GLN
1	B	155	GLN
1	B	228	GLN
1	B	229	ASN
1	B	230	GLN
1	B	298	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	349/403 (86%)	0.28	22 (6%) 21 13	33, 65, 148, 167	0
1	B	350/403 (86%)	0.84	62 (17%) 2 1	45, 89, 163, 179	0
All	All	699/806 (86%)	0.56	84 (12%) 5 3	33, 76, 159, 179	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ARG	9.6
1	B	343	SER	9.5
1	B	342	SER	9.3
1	B	334	VAL	8.8
1	B	315	MET	8.6
1	B	340	LEU	8.4
1	A	30	ARG	7.6
1	B	339	ILE	7.4
1	B	345	PRO	7.2
1	B	33	PHE	6.8
1	B	314	PHE	6.4
1	B	280	VAL	6.2
1	A	3	ARG	6.1
1	A	399	GLU	6.0
1	B	337	SER	5.8
1	B	29	GLN	5.5
1	B	338	ASN	5.3
1	B	336	ALA	5.2
1	B	28	ASP	5.2
1	A	32	GLU	5.1
1	A	26	ILE	5.1
1	B	158	SER	4.9
1	B	322	ARG	4.7
1	A	398	GLY	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	316	SER	4.5
1	A	256	HIS	4.5
1	B	4	ASP	4.2
1	B	341	ASP	4.1
1	A	4	ASP	4.1
1	B	72	PHE	4.0
1	B	79	ASN	4.0
1	B	80	VAL	3.9
1	A	29	GLN	3.8
1	B	78	GLY	3.7
1	B	344	LEU	3.6
1	B	32	GLU	3.5
1	A	282	PHE	3.4
1	B	159	THR	3.4
1	B	14	ARG	3.4
1	B	279	GLN	3.2
1	B	333	GLU	3.2
1	A	35	GLN	3.1
1	B	376	LYS	3.1
1	B	11	ILE	3.0
1	B	70	TYR	3.0
1	B	2	LYS	3.0
1	B	377	LYS	2.9
1	A	33	PHE	2.9
1	B	34	ASN	2.9
1	A	322	ARG	2.8
1	B	10	THR	2.8
1	B	332	ARG	2.7
1	B	12	ALA	2.7
1	B	375	LEU	2.7
1	A	34	ASN	2.6
1	A	1	MET	2.6
1	B	205	PRO	2.6
1	B	312	ILE	2.5
1	A	36	THR	2.5
1	B	157	SER	2.4
1	B	124	THR	2.4
1	A	283	HIS	2.4
1	B	31	LYS	2.4
1	A	161	PHE	2.4
1	B	25	ASP	2.4
1	B	71	GLN	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	374	ALA	2.3
1	B	81	GLU	2.3
1	B	289	LEU	2.3
1	B	160	MET	2.3
1	A	79	ASN	2.3
1	B	76	GLN	2.3
1	B	15	ALA	2.3
1	B	313	GLY	2.3
1	B	24	GLN	2.3
1	B	30	ARG	2.3
1	B	1	MET	2.3
1	B	126	SER	2.2
1	B	26	ILE	2.2
1	B	335	TYR	2.2
1	B	330	LEU	2.1
1	B	152	LEU	2.1
1	A	343	SER	2.1
1	A	342	SER	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](#)

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	MG	A	402	1/1	0.71	0.53	14.06	33,33,33,33	1



## 6.5 Other polymers [i](#)

There are no such residues in this entry.