



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:01 AM GMT

PDB ID : 2EVX  
Title : Crystal structure of pumpkin seed globulin  
Authors : Itoh, T.; Fukuda, T.; Mikami, B.; Utsumi, S.  
Deposited on : 2005-11-01  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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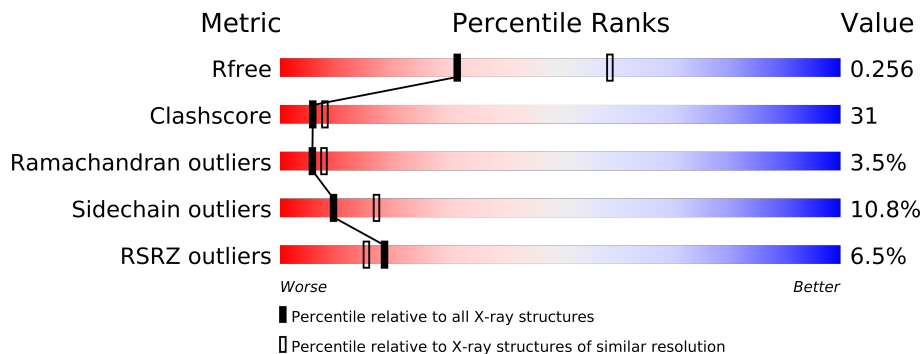
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

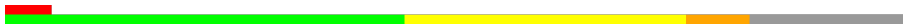
The reported resolution of this entry is 2.60 Å.

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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	459	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	501	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3147 atoms, of which 0 are hydrogen and 0 are deuterium.

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 11S globulin beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	7	0
			3090	1938	571	567	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	GLY	ILE	SEE REMARK 999	UNP P13744
A	294	GLU	VAL	SEE REMARK 999	UNP P13744

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.29Å 189.29Å 189.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.60 43.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (14.97-2.60) 100.0 (43.43-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.73 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.255 0.204 , 0.256	Depositor DCC
$R_{free}$ test set	1700 reflections (9.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.0	EDS
Estimated twinning fraction	0.047 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 17371 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.42	0/3172	0.66	0/4273

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3090	0	3053	193	0
2	A	2	0	0	0	0
3	A	55	0	0	1	0
All	All	3147	0	3053	193	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (193) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:433:ARG:H	1:A:433:ARG:HD3	1.10	1.17

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:185:GLN:H	1:A:185:GLN:HE21	1.06	1.00
1:A:174:LEU:H	1:A:188:ARG:NH1	1.61	0.98
1:A:82:ASN:H	1:A:82:ASN:HD22	1.14	0.90
1:A:112:ARG:HB2	1:A:122:LYS:HB3	1.55	0.89
1:A:433:ARG:N	1:A:433:ARG:HD3	1.89	0.88
1:A:55:ASN:HD22	1:A:58:PHE:H	1.18	0.87
1:A:173[B]:TYR:CD1	1:A:188:ARG:HG2	2.11	0.86
1:A:176:LYS:HB2	1:A:187[B]:GLU:OE2	1.77	0.85
1:A:173[B]:TYR:HD1	1:A:188:ARG:HG2	1.43	0.83
1:A:280:THR:O	1:A:283:THR:HG22	1.78	0.82
1:A:444:GLN:HE21	1:A:444:GLN:HA	1.47	0.79
1:A:185:GLN:N	1:A:185:GLN:HE21	1.80	0.79
1:A:342:ASN:HD21	1:A:406:ILE:H	1.31	0.78
1:A:55:ASN:ND2	1:A:58:PHE:H	1.81	0.78
1:A:182:ARG:NH1	1:A:238:GLU:HG3	1.99	0.78
1:A:53:GLN:HG3	1:A:188:ARG:NE	2.00	0.77
1:A:76:LEU:HD23	1:A:147[A]:MET:SD	2.23	0.77
1:A:347:MET:HE1	1:A:387:LYS:NZ	1.99	0.77
1:A:342:ASN:H	1:A:342:ASN:HD22	1.32	0.75
1:A:433:ARG:CD	1:A:433:ARG:H	1.95	0.74
1:A:76:LEU:HB3	1:A:147[A]:MET:HG2	1.71	0.73
1:A:38:VAL:HG12	1:A:39:ARG:HG3	1.69	0.72
1:A:185:GLN:H	1:A:185:GLN:NE2	1.84	0.71
1:A:247:GLU:HG3	1:A:248:ASP:OD1	1.90	0.71
1:A:27:CYS:HB3	1:A:29:LEU:HD21	1.72	0.71
1:A:82:ASN:HD22	1:A:82:ASN:N	1.89	0.71
1:A:432:SER:OG	1:A:435:GLU:HG3	1.90	0.71
1:A:112:ARG:CB	1:A:122:LYS:HB3	2.21	0.70
1:A:173[A]:TYR:HD2	1:A:188:ARG:HG2	1.54	0.70
1:A:82:ASN:O	1:A:168:ASN:HB2	1.92	0.70
1:A:55:ASN:HD21	1:A:57:GLU:HB2	1.55	0.70
1:A:171:ASP:HB2	1:A:172:PRO:HD2	1.72	0.70
1:A:64:ASN:HD21	1:A:188:ARG:NH1	1.89	0.69
1:A:40[B]:ARG:HG2	1:A:49:GLU:HG2	1.72	0.69
1:A:414:VAL:HG22	1:A:446:MET:SD	2.33	0.69
1:A:321:ARG:HH21	1:A:321:ARG:HG2	1.56	0.69
1:A:38:VAL:CG1	1:A:39:ARG:HG3	2.23	0.68
1:A:314:LEU:HG	1:A:316:ILE:HG22	1.76	0.68
1:A:321:ARG:CG	1:A:321:ARG:HH21	2.07	0.68
1:A:111:LEU:H	1:A:112:ARG:HH21	1.43	0.67
1:A:329:LEU:HD11	1:A:335:VAL:HG23	1.77	0.67
1:A:182:ARG:HH11	1:A:238:GLU:HG3	1.60	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:298:VAL:O	1:A:305:ARG:HB2	1.95	0.66
1:A:173[A]:TYR:CD2	1:A:188:ARG:HG2	2.31	0.65
1:A:215:ASP:O	1:A:219:GLU:HG3	1.96	0.65
1:A:82:ASN:H	1:A:82:ASN:ND2	1.92	0.65
1:A:342:ASN:ND2	1:A:406:ILE:H	1.93	0.65
1:A:176:LYS:HD2	1:A:178:TYR:CE1	2.32	0.65
1:A:356:VAL:HG22	1:A:387:LYS:HG2	1.79	0.63
1:A:106:THR:HG23	1:A:124:GLN:HG2	1.80	0.63
1:A:402:ASN:HD22	1:A:403:ASP:N	1.96	0.62
1:A:332:ASN:HD22	1:A:332:ASN:N	1.97	0.62
1:A:347:MET:CE	1:A:387:LYS:NZ	2.62	0.61
1:A:185:GLN:N	1:A:185:GLN:NE2	2.45	0.61
1:A:445:GLU:OE2	1:A:449:LEU:HA	1.99	0.61
1:A:82:ASN:HD21	1:A:175:ARG:H	1.49	0.61
1:A:27:CYS:HB3	1:A:29:LEU:CD2	2.31	0.61
1:A:413:ARG:HG3	1:A:444:GLN:O	2.00	0.61
1:A:37:PRO:HG3	1:A:51:TRP:CH2	2.35	0.60
1:A:186:VAL:C	1:A:188:ARG:H	2.05	0.60
1:A:298:VAL:CG1	1:A:306:ILE:HB	2.31	0.60
1:A:48:THR:HG23	1:A:68:HIS:CD2	2.36	0.60
1:A:357:GLN:HE21	1:A:368:ASP:CG	2.05	0.59
1:A:240:ASP:OD1	1:A:241:ARG:HD2	2.02	0.59
1:A:281:ILE:HA	1:A:284:LEU:HD21	1.84	0.59
1:A:160:PHE:HE2	1:A:346:VAL:HG21	1.67	0.59
1:A:112:ARG:HD3	1:A:122:LYS:HA	1.85	0.58
1:A:347:MET:HE1	1:A:387:LYS:HZ2	1.67	0.58
1:A:412:GLY:N	1:A:415:SER:OG	2.35	0.58
1:A:342:ASN:N	1:A:342:ASN:HD22	1.97	0.58
1:A:112:ARG:HB3	1:A:121:PHE:O	2.04	0.57
1:A:347:MET:HE1	1:A:387:LYS:CD	2.34	0.57
1:A:414:VAL:O	1:A:414:VAL:HG23	2.04	0.57
1:A:96:ARG:HG2	1:A:131:PHE:CD2	2.40	0.57
1:A:247:GLU:HG3	1:A:248:ASP:H	1.70	0.56
1:A:94:GLY:HA2	1:A:150:ARG:HG2	1.86	0.56
1:A:378:MET:O	1:A:380:PRO:HD3	2.05	0.56
1:A:321:ARG:CG	1:A:321:ARG:NH2	2.69	0.55
1:A:82:ASN:ND2	1:A:175:ARG:H	2.04	0.55
1:A:186:VAL:C	1:A:188:ARG:N	2.59	0.55
1:A:110:ASP:C	1:A:112:ARG:H	2.09	0.55
1:A:53:GLN:HG3	1:A:188:ARG:HE	1.70	0.55
1:A:109:THR:OG1	1:A:112:ARG:HD2	2.06	0.55
1:A:397:ILE:O	1:A:397:ILE:HG23	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:342:ASN:HD21	1:A:405:ALA:HA	1.72	0.55
1:A:298:VAL:HG13	1:A:306:ILE:HB	1.88	0.55
1:A:185:GLN:O	1:A:185:GLN:HG2	2.07	0.55
1:A:78:PRO:HA	1:A:145:HIS:O	2.07	0.54
1:A:105:GLU:O	1:A:107:TYR:HD2	1.91	0.53
1:A:337:PRO:HA	1:A:385:VAL:O	2.08	0.53
1:A:292:ARG:HG3	1:A:293:SER:N	2.23	0.53
1:A:347:MET:HE2	1:A:396:TRP:CG	2.43	0.53
1:A:429:TYR:O	1:A:431:ILE:HG23	2.08	0.53
1:A:444:GLN:HE21	1:A:444:GLN:CA	2.14	0.52
1:A:342:ASN:ND2	1:A:342:ASN:H	2.04	0.52
1:A:76:LEU:HD23	1:A:147[A]:MET:CG	2.39	0.52
1:A:176:LYS:HD2	1:A:178:TYR:CZ	2.45	0.52
1:A:347:MET:CE	1:A:387:LYS:HZ2	2.21	0.52
1:A:109:THR:HG23	1:A:125:HIS:NE2	2.25	0.52
1:A:83:ALA:HB1	1:A:162:ASP:O	2.09	0.52
1:A:433:ARG:HH11	1:A:433:ARG:HG2	1.75	0.51
1:A:45:ALA:HB3	1:A:242:ILE:HG22	1.92	0.51
1:A:246:ASP:O	1:A:247:GLU:HG2	2.11	0.51
1:A:353:ASN:ND2	1:A:370:GLU:OE2	2.44	0.51
1:A:98:ILE:HD11	1:A:143:VAL:CG1	2.42	0.50
1:A:377:LEU:HD23	1:A:379:ILE:HD11	1.94	0.50
1:A:216:GLU:O	1:A:220[B]:GLU:HG3	2.12	0.50
1:A:444:GLN:NE2	1:A:444:GLN:HA	2.22	0.50
1:A:342:ASN:HD21	1:A:406:ILE:N	2.05	0.50
1:A:185:GLN:O	1:A:185:GLN:CG	2.60	0.49
1:A:50:VAL:HG12	1:A:66:ILE:HG12	1.94	0.49
1:A:247:GLU:HG3	1:A:248:ASP:N	2.27	0.49
1:A:72:PRO:O	1:A:73:LYS:HB2	2.12	0.49
1:A:110:ASP:O	1:A:112:ARG:N	2.45	0.49
1:A:91:GLN:O	1:A:155:LEU:HD23	2.11	0.49
1:A:174:LEU:H	1:A:188:ARG:HH12	1.51	0.49
1:A:434:GLU:O	1:A:437:GLN:HB3	2.12	0.49
1:A:298:VAL:HG13	1:A:306:ILE:O	2.12	0.48
1:A:381:GLN:O	1:A:382:ASN:HB2	2.13	0.48
1:A:298:VAL:HG11	1:A:306:ILE:HB	1.96	0.48
1:A:173[B]:TYR:CE1	1:A:188:ARG:HG2	2.49	0.48
1:A:96:ARG:HG3	1:A:129:ARG:O	2.13	0.47
1:A:152:GLN:HA	1:A:152:GLN:NE2	2.30	0.47
1:A:361:ASN:ND2	1:A:361:ASN:H	2.12	0.47
1:A:385:VAL:HG22	1:A:386:ILE:N	2.29	0.47
1:A:388:ARG:HH22	1:A:453:ARG:HB3	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:239:ARG:CZ	1:A:243:VAL:HG11	2.45	0.47
1:A:433:ARG:HG2	1:A:433:ARG:NH1	2.30	0.46
1:A:170:ILE:HG22	1:A:171:ASP:N	2.29	0.46
1:A:388:ARG:CZ	1:A:453:ARG:NH1	2.78	0.46
1:A:99:ALA:O	1:A:100:ILE:HB	2.14	0.46
1:A:445:GLU:OE1	1:A:450:SER:OG	2.26	0.46
1:A:437:GLN:HB2	1:A:437:GLN:HE21	1.61	0.46
1:A:107:TYR:O	1:A:124:GLN:HA	2.16	0.45
1:A:410:LEU:HD12	1:A:410:LEU:HA	1.82	0.45
1:A:106:THR:HG23	1:A:124:GLN:CG	2.45	0.45
1:A:420:LEU:HA	1:A:421:PRO:HD3	1.83	0.45
1:A:91:GLN:HA	1:A:133:GLU:HG2	1.99	0.45
1:A:351:ARG:HG2	1:A:352:GLY:N	2.31	0.45
1:A:112:ARG:CD	1:A:122:LYS:HA	2.46	0.45
1:A:347:MET:CE	1:A:387:LYS:HZ3	2.28	0.45
1:A:53:GLN:HG3	1:A:188:ARG:CD	2.46	0.44
1:A:304:GLY:HA3	1:A:328:VAL:O	2.18	0.44
1:A:241:ARG:HG2	1:A:242:ILE:HG13	1.98	0.44
1:A:222:PHE:O	1:A:223:GLN:HB2	2.18	0.44
1:A:347:MET:HE2	1:A:396:TRP:CD2	2.53	0.44
1:A:332:ASN:ND2	1:A:332:ASN:N	2.65	0.43
1:A:98:ILE:CD1	1:A:143:VAL:HG12	2.48	0.43
1:A:37:PRO:HG3	1:A:51:TRP:CZ2	2.54	0.43
1:A:388:ARG:NH2	1:A:453:ARG:HB3	2.33	0.43
1:A:385:VAL:CG2	1:A:386:ILE:N	2.81	0.43
1:A:377:LEU:CD2	1:A:379:ILE:HD11	2.49	0.43
1:A:174:LEU:HB3	1:A:188:ARG:HH11	1.83	0.43
1:A:351:ARG:HB3	1:A:395:GLU:HB2	2.00	0.43
1:A:71:ARG:C	1:A:149:ASN:HD22	2.22	0.43
1:A:372:ARG:NH2	1:A:372:ARG:HG2	2.33	0.43
1:A:414:VAL:CG2	1:A:446:MET:HE1	2.49	0.42
1:A:66:ILE:HB	1:A:159:VAL:HB	2.01	0.42
1:A:412:GLY:HA2	1:A:443:GLN:HG3	2.01	0.42
1:A:372:ARG:O	1:A:373:GLU:C	2.57	0.42
1:A:111:LEU:N	1:A:112:ARG:HH21	2.15	0.42
1:A:343:SER:HB3	1:A:402:ASN:HB2	2.02	0.42
1:A:284:LEU:N	1:A:284:LEU:HD23	2.34	0.42
1:A:84:PRO:HG2	1:A:165:ASN:CG	2.39	0.42
1:A:247:GLU:CG	1:A:248:ASP:H	2.32	0.41
1:A:329:LEU:HD22	1:A:333:ALA:CB	2.50	0.41
1:A:351:ARG:HD2	1:A:395:GLU:OE2	2.20	0.41
1:A:224:ILE:HD12	1:A:228:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:38:VAL:HG13	1:A:39:ARG:HG3	2.02	0.41
1:A:219:GLU:CG	1:A:229:VAL:HG21	2.50	0.41
1:A:55:ASN:ND2	1:A:57:GLU:HB2	2.29	0.41
1:A:328:VAL:HG22	1:A:395:GLU:HG2	2.02	0.41
1:A:187[A]:GLU:HG3	3:A:1017:HOH:O	2.20	0.41
1:A:361:ASN:HD22	1:A:361:ASN:H	1.67	0.41
1:A:100:ILE:HD11	1:A:286:LEU:HD11	2.03	0.41
1:A:245:VAL:HG11	1:A:249:PHE:CG	2.56	0.41
1:A:290:ILE:HG21	1:A:309:ALA:HB2	2.02	0.41
1:A:246:ASP:C	1:A:247:GLU:HG2	2.42	0.40
1:A:450:SER:O	1:A:451:PRO:C	2.60	0.40
1:A:225:ASP:OD2	1:A:228:LEU:HB2	2.21	0.40
1:A:372:ARG:HG2	1:A:372:ARG:HH21	1.85	0.40

There are no symmetry-related clashes.

## 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	381/459 (83%)	340 (89%)	28 (7%)	13 (3%)	6 8

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	247	GLU
1	A	99	ALA
1	A	111	LEU
1	A	451	PRO
1	A	188	ARG
1	A	100	ILE
1	A	240	ASP
1	A	252	LEU
1	A	170	ILE

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Mol	Chain	Res	Type
1	A	109	THR
1	A	172	PRO
1	A	189	GLY

### 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	330/391 (84%)	290 (88%)	40 (12%)	<b>7</b> <b>13</b>

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	31	ASN
1	A	38	VAL
1	A	40[A]	ARG
1	A	40[B]	ARG
1	A	82	ASN
1	A	96	ARG
1	A	109	THR
1	A	112	ARG
1	A	147[A]	MET
1	A	147[B]	MET
1	A	155	LEU
1	A	173[A]	TYR
1	A	173[B]	TYR
1	A	176	LYS
1	A	185	GLN
1	A	187[A]	GLU
1	A	187[B]	GLU
1	A	235[A]	GLU
1	A	235[B]	GLU
1	A	241	ARG
1	A	249	PHE
1	A	250	GLU
1	A	252	LEU
1	A	281	ILE

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Mol	Chain	Res	Type
1	A	284	LEU
1	A	297	ASP
1	A	298	VAL
1	A	305	ARG
1	A	326	ARG
1	A	332	ASN
1	A	342	ASN
1	A	402	ASN
1	A	407	THR
1	A	410	LEU
1	A	433	ARG
1	A	439	LEU
1	A	444	GLN
1	A	447	ARG
1	A	451	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	55	ASN
1	A	64	ASN
1	A	68	HIS
1	A	82	ASN
1	A	91	GLN
1	A	108	GLN
1	A	124	GLN
1	A	149	ASN
1	A	152	GLN
1	A	185	GLN
1	A	289	ASN
1	A	312	HIS
1	A	332	ASN
1	A	342	ASN
1	A	357	GLN
1	A	361	ASN
1	A	381	GLN
1	A	402	ASN
1	A	408	ASN
1	A	416	GLN
1	A	437	GLN
1	A	444	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are 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.

## 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	382/459 (83%)	-0.08	25 (6%) 18 15	24, 42, 85, 108	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	LEU	6.0
1	A	190	VAL	5.2
1	A	110	ASP	4.6
1	A	186	VAL	3.9
1	A	189	GLY	3.9
1	A	235[A]	GLU	3.6
1	A	111	LEU	3.5
1	A	122	LYS	3.4
1	A	204	GLU	3.4
1	A	453	ARG	3.4
1	A	250	GLU	3.4
1	A	281	ILE	3.3
1	A	279	GLU	3.3
1	A	173[A]	TYR	3.3
1	A	252	LEU	3.1
1	A	112	ARG	2.9
1	A	121	PHE	2.8
1	A	40[A]	ARG	2.7
1	A	280	THR	2.5
1	A	251	VAL	2.3
1	A	185	GLN	2.2
1	A	187[A]	GLU	2.1
1	A	433	ARG	2.1
1	A	109	THR	2.0
1	A	147[A]	MET	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	501	1/1	0.29	6.65	47,47,47,47	0
2	MG	A	502	1/1	0.15	0.48	28,28,28,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.