



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:51 AM UTC

PDB ID : 2CA6 / pdb\_00002ca6  
Title : MIRAS structure determination from hemihedrally twinned crystals  
Authors : Hillig, R.C.; Renault, L.  
Deposited on : 2005-12-17  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (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

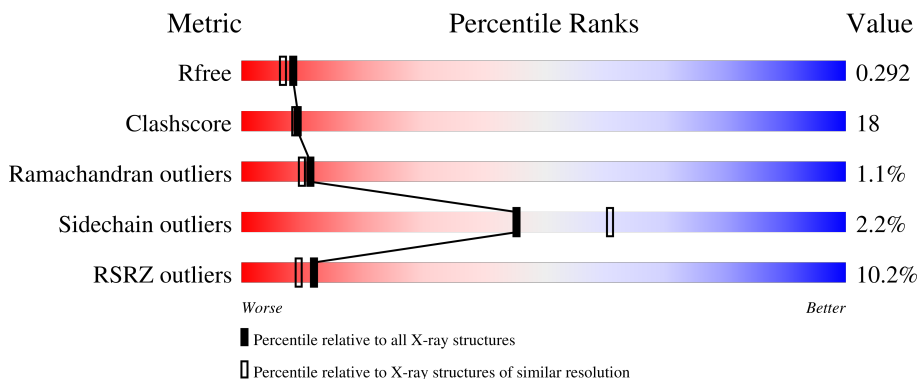
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	386	
1	B	386	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5673 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 RAN GTPASE-ACTIVATING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	344	2690	1694	469	519	8	0	0	1
1	B	344	2690	1694	469	519	8	0	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	conflict	UNP P41391
B	2	ALA	SER	conflict	UNP P41391

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	B	1	5	4	1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total	O	0	0
			148	148		
3	B	125	Total	O	0	0
			125	125		



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.21Å 175.21Å 55.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.00 – 2.20 31.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (31.00-2.20) 97.3 (31.00-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.00Å)	Xtrriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.165 , 0.218 (Not available) , 0.292	Depositor DCC
$R_{free}$ test set	4632 reflections (8.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtrriage
Anisotropy	0.559	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.375 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	5673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.41	1/2729 (0.0%)	0.97	10/3687 (0.3%)
1	B	0.39	1/2729 (0.0%)	1.00	11/3687 (0.3%)
All	All	0.40	2/5458 (0.0%)	0.99	21/7374 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	GLU	C-N	-5.65	1.25	1.33
1	B	344	GLU	C-N	-5.62	1.25	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	CYS	CA-C-N	8.11	128.20	119.28
1	A	93	CYS	C-N-CA	8.11	128.20	119.28
1	B	93	CYS	CA-C-N	8.06	128.14	119.28
1	B	93	CYS	C-N-CA	8.06	128.14	119.28
1	B	14	ASP	N-CA-C	-7.68	104.05	113.50
1	A	14	ASP	N-CA-C	-6.62	104.68	112.89
1	B	33	SER	N-CA-C	-6.33	105.56	113.28
1	A	174	GLY	N-CA-C	6.18	121.26	114.40
1	B	209	LEU	N-CA-C	6.12	117.95	111.28
1	B	227	THR	N-CA-C	6.12	118.26	108.41
1	B	226	ASN	N-CA-C	-6.11	99.75	109.23
1	A	301	LYS	N-CA-C	6.10	121.47	113.30
1	B	302	MET	CA-C-N	6.02	125.64	119.56
1	B	302	MET	C-N-CA	6.02	125.64	119.56
1	A	328	VAL	N-CA-C	-5.21	105.45	110.72
1	A	44	ILE	N-CA-C	5.21	115.86	107.73
1	B	288	LEU	N-CA-C	5.20	117.03	111.36

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ASP	N-CA-C	-5.20	106.20	112.54
1	A	314	ARG	N-CA-C	5.11	119.67	112.72
1	A	46	THR	N-CA-C	5.09	116.52	110.97
1	B	161	LEU	N-CA-C	-5.07	102.77	110.28

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	2690	0	2727	86	0
1	B	2690	0	2727	110	0
2	B	20	0	0	0	0
3	A	148	0	0	9	0
3	B	125	0	0	9	0
All	All	5673	0	5454	196	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 18.

All (196) 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:259:ARG:H	1:B:259:ARG:HD2	1.03	1.14
1:B:75:VAL:HG22	1:B:78:GLU:HG3	1.34	1.09
1:A:195:VAL:HG22	1:A:196:GLN:HG3	1.41	1.02
1:A:17:THR:HG22	1:A:18:THR:H	1.26	0.99
1:B:176:MET:HE2	1:B:207:LEU:HD13	1.47	0.94
1:B:259:ARG:HD2	1:B:259:ARG:N	1.83	0.92
1:B:259:ARG:H	1:B:259:ARG:CD	1.78	0.89
1:A:195:VAL:HG23	1:A:224:GLN:HB3	1.65	0.79
1:A:157:ASN:HA	3:A:2059:HOH:O	1.83	0.78
1:B:258:ALA:H	1:B:259:ARG:HH21	1.31	0.76
1:B:258:ALA:H	1:B:259:ARG:NH2	1.84	0.75

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:CG2	1:A:224:GLN:HB3	2.17	0.74
1:B:22:LYS:HE2	1:B:29:LEU:HD13	1.70	0.74
1:A:63:GLU:HA	1:A:96:LEU:HA	1.70	0.74
1:B:16:ILE:HD12	1:B:51:TRP:CE3	2.25	0.72
1:B:20:ASP:HA	1:B:23:SER:OG	1.91	0.71
1:A:308:LEU:HD23	1:A:337:LEU:HD13	1.73	0.71
1:A:66:GLU:OE1	1:A:100:ARG:HD2	1.91	0.70
1:A:200:ARG:HB3	1:A:201:PRO:HD2	1.72	0.70
1:A:224:GLN:NE2	1:A:225:ASP:HB2	2.06	0.69
1:B:112:GLU:HB3	1:B:113:PRO:HD3	1.74	0.69
1:B:176:MET:HE3	1:B:176:MET:HA	1.75	0.69
1:B:200:ARG:HB3	1:B:201:PRO:HD2	1.75	0.69
1:A:115:ILE:HG23	1:A:145:ALA:HB2	1.76	0.68
1:B:84:ARG:O	1:B:88:GLN:HG3	1.93	0.67
1:A:177:LYS:HA	1:A:206:HIS:HE1	1.60	0.66
1:B:258:ALA:N	1:B:259:ARG:HH21	1.93	0.66
1:B:200:ARG:HB3	1:B:200:ARG:HH11	1.60	0.65
1:A:177:LYS:HA	1:A:206:HIS:CE1	2.32	0.64
1:B:241:LYS:HD2	3:B:2083:HOH:O	1.97	0.64
1:A:17:THR:HG22	1:A:18:THR:N	2.07	0.64
1:A:28:LEU:O	1:A:28:LEU:HD13	1.98	0.63
1:A:195:VAL:HG12	3:A:2074:HOH:O	1.98	0.63
1:A:17:THR:HB	1:A:20:ASP:HB3	1.79	0.63
1:B:6:ILE:HG13	1:B:42:ASN:ND2	2.13	0.63
1:B:304:ASP:HB3	3:B:2105:HOH:O	1.99	0.62
1:A:320:ASP:O	1:A:324:GLU:HG3	1.99	0.61
1:B:46:THR:HG23	1:B:81:GLU:HG2	1.83	0.61
1:A:248:GLU:HG3	1:A:278:THR:HB	1.83	0.61
1:B:280:ARG:HA	1:B:309:GLU:HB2	1.83	0.60
1:B:215:CYS:HB3	3:B:2060:HOH:O	1.99	0.60
1:B:295:LYS:HG2	1:B:325:ILE:HG12	1.84	0.60
1:B:74:ARG:HH11	1:B:74:ARG:HG3	1.68	0.58
1:A:79:ILE:N	1:A:80:PRO:CD	2.67	0.58
1:A:177:LYS:HG2	3:A:2062:HOH:O	2.04	0.57
1:A:201:PRO:HD3	1:A:227:THR:HB	1.85	0.57
1:B:7:GLU:HA	1:B:40:SER:O	2.04	0.57
1:B:321:VAL:HA	1:B:324:GLU:OE1	2.05	0.57
1:A:272:GLU:HB3	3:A:2103:HOH:O	2.05	0.57
1:B:200:ARG:HB3	1:B:201:PRO:CD	2.35	0.57
1:B:18:THR:O	1:B:21:GLU:HG2	2.05	0.56
1:B:32:ASP:HA	1:B:59:LYS:HD2	1.85	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:HB3	1:A:201:PRO:CD	2.34	0.56
1:B:248:GLU:HG3	1:B:278:THR:HB	1.86	0.56
1:A:42:ASN:O	1:A:70:ILE:HA	2.06	0.55
1:B:26:ALA:HB3	3:B:2001:HOH:O	2.07	0.55
1:B:31:ASP:O	1:B:34:VAL:HG23	2.06	0.55
1:B:280:ARG:HG2	1:B:309:GLU:OE2	2.06	0.55
1:A:280:ARG:NH1	1:A:309:GLU:OE2	2.40	0.55
1:B:281:LEU:HB2	1:B:310:LEU:HD23	1.89	0.55
1:A:16:ILE:HG13	1:A:51:TRP:CE3	2.42	0.55
1:B:321:VAL:O	1:B:325:ILE:HG13	2.07	0.54
1:B:298:ILE:HA	1:B:302:MET:HB2	1.89	0.54
1:B:320:ASP:O	1:B:324:GLU:HG3	2.08	0.54
1:B:287:GLU:O	1:B:291:VAL:HG23	2.08	0.54
1:B:15:ALA:HB2	1:B:47:GLU:HB2	1.90	0.53
1:A:282:GLN:HG3	1:A:309:GLU:HB3	1.88	0.53
1:B:183:PHE:CE2	1:B:207:LEU:HD11	2.43	0.53
1:B:334:ARG:HB2	1:B:334:ARG:NH1	2.23	0.53
1:A:131:ASN:HA	1:A:168:ARG:O	2.09	0.53
1:B:200:ARG:HB3	1:B:200:ARG:NH1	2.24	0.53
1:A:195:VAL:HG23	1:A:224:GLN:O	2.08	0.53
1:B:45:GLY:HA2	1:B:74:ARG:NH1	2.24	0.52
1:B:245:ASN:HB3	3:B:2089:HOH:O	2.10	0.52
1:B:74:ARG:HG3	1:B:74:ARG:NH1	2.26	0.51
1:B:164:ILE:C	1:B:165:ILE:HD12	2.35	0.51
1:A:46:THR:HG23	1:A:81:GLU:HG2	1.93	0.51
1:A:111:GLN:O	1:A:115:ILE:HG13	2.11	0.51
1:B:202:GLU:HG3	3:B:2068:HOH:O	2.09	0.51
1:A:74:ARG:HH11	1:A:74:ARG:HG3	1.76	0.51
1:B:256:LEU:O	1:B:257:SER:CB	2.59	0.51
1:B:138:ALA:O	1:B:142:ILE:HG12	2.11	0.50
1:A:130:HIS:CE1	1:A:168:ARG:HD3	2.46	0.50
1:A:166:CYS:O	1:A:194:MET:HA	2.12	0.49
1:A:261:ALA:O	1:A:265:VAL:HG23	2.11	0.49
1:B:183:PHE:HE2	1:B:207:LEU:HD11	1.77	0.49
1:B:3:ARG:HG2	1:B:4:PHE:N	2.27	0.49
1:A:25:PHE:HB2	1:A:51:TRP:CH2	2.47	0.49
1:B:54:GLU:HB3	3:B:2006:HOH:O	2.11	0.49
1:B:63:GLU:HA	1:B:95:LYS:O	2.13	0.49
1:B:166:CYS:O	1:B:194:MET:HA	2.11	0.49
1:B:21:GLU:HG3	1:B:22:LYS:N	2.27	0.49
1:B:296:THR:HG22	1:B:300:GLU:OE1	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASP:HA	1:B:59:LYS:CD	2.43	0.48
1:B:311:ASN:HB2	1:B:338:ASP:OD2	2.13	0.48
1:B:312:GLY:HA2	1:B:342:ASP:O	2.13	0.48
1:A:206:HIS:CD2	1:A:210:GLU:HG3	2.47	0.48
1:B:171:LEU:HB2	1:B:197:ASN:HB3	1.94	0.48
1:A:121:HIS:NE2	1:A:123:PRO:HG2	2.29	0.48
1:B:74:ARG:NH2	3:B:2015:HOH:O	2.47	0.48
1:A:17:THR:CB	1:A:20:ASP:HB3	2.43	0.48
1:A:20:ASP:O	1:A:24:VAL:HB	2.14	0.48
1:A:120:LYS:HE3	3:A:2042:HOH:O	2.14	0.48
1:B:274:ILE:HB	1:B:301:LYS:O	2.14	0.47
1:B:208:LEU:HD13	1:B:236:LEU:HA	1.95	0.47
1:A:290:ALA:HA	3:A:2111:HOH:O	2.14	0.47
1:B:112:GLU:O	1:B:116:ASP:HB2	2.14	0.47
1:B:167:GLY:HA2	1:B:197:ASN:HD21	1.79	0.47
1:B:240:LEU:HD23	1:B:243:TRP:CZ3	2.49	0.47
1:B:67:PHE:HB2	1:B:101:LEU:HD23	1.97	0.47
1:A:195:VAL:HG22	1:A:196:GLN:N	2.29	0.47
1:B:6:ILE:HG13	1:B:42:ASN:HD21	1.79	0.47
1:B:165:ILE:HD12	1:B:165:ILE:N	2.30	0.47
1:A:245:ASN:HD22	1:A:245:ASN:N	2.11	0.47
1:B:200:ARG:HH11	1:B:200:ARG:CB	2.27	0.47
1:A:122:THR:N	1:A:123:PRO:HD2	2.30	0.46
1:A:130:HIS:HE1	1:A:168:ARG:HD3	1.79	0.46
1:B:228:PHE:O	1:B:229:THR:OG1	2.30	0.46
1:B:79:ILE:N	1:B:80:PRO:CD	2.77	0.46
1:B:136:PRO:HG3	1:B:172:GLU:HB2	1.97	0.46
1:B:277:GLN:HA	1:B:305:LEU:HA	1.96	0.46
1:B:176:MET:HG2	1:B:203:GLY:O	2.15	0.46
1:A:176:MET:HA	1:A:176:MET:HE2	1.98	0.46
1:A:228:PHE:HB2	1:A:254:CYS:O	2.16	0.46
1:B:177:LYS:HA	1:B:206:HIS:CE1	2.51	0.46
1:B:327:GLU:HA	1:B:330:SER:HB2	1.98	0.45
1:A:195:VAL:HG23	1:A:224:GLN:C	2.42	0.45
1:A:195:VAL:HG21	1:A:224:GLN:OE1	2.17	0.45
1:A:306:LEU:HD23	1:A:334:ARG:HG3	1.98	0.45
1:B:143:ALA:HB1	1:B:182:THR:OG1	2.16	0.45
1:B:91:LEU:HD13	1:B:117:PHE:CD1	2.51	0.45
1:A:121:HIS:C	1:A:123:PRO:HD2	2.42	0.45
1:A:66:GLU:C	1:A:67:PHE:HD1	2.24	0.44
1:A:25:PHE:HB2	1:A:51:TRP:HH2	1.82	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HG22	1:A:21:GLU:HB2	1.98	0.44
1:A:122:THR:N	1:A:123:PRO:CD	2.81	0.44
1:A:174:GLY:HA3	3:A:2015:HOH:O	2.17	0.44
1:A:21:GLU:HG3	1:A:51:TRP:CZ2	2.52	0.44
1:B:38:VAL:HG13	1:B:66:GLU:HB3	2.00	0.44
1:A:63:GLU:HB3	1:A:97:HIS:CD2	2.53	0.44
1:A:244:PRO:C	1:A:245:ASN:HD22	2.26	0.44
1:B:267:ALA:O	1:B:271:LEU:HG	2.18	0.44
1:B:110:ALA:C	1:B:113:PRO:HD2	2.43	0.44
1:B:9:LYS:O	1:B:10:SER:C	2.61	0.43
1:B:256:LEU:HG	1:B:284:ASN:OD1	2.18	0.43
1:A:17:THR:HB	1:A:20:ASP:CB	2.44	0.43
1:A:16:ILE:HD12	1:A:25:PHE:CE1	2.53	0.43
1:A:115:ILE:HD11	1:A:141:LYS:HB3	2.01	0.43
1:B:125:GLU:O	1:B:161:LEU:HD12	2.18	0.43
1:A:17:THR:CG2	1:A:18:THR:H	2.07	0.43
1:A:156:LYS:O	1:A:157:ASN:HB2	2.18	0.43
1:A:48:ALA:O	1:A:52:LEU:HG	2.19	0.43
1:A:245:ASN:N	1:A:245:ASN:ND2	2.66	0.43
1:B:240:LEU:HD23	1:B:243:TRP:HZ3	1.83	0.43
1:A:100:ARG:HG2	1:A:128:TYR:CD1	2.53	0.43
1:B:106:PHE:CD2	1:B:114:LEU:HD11	2.53	0.43
1:A:14:ASP:O	1:A:47:GLU:HB3	2.18	0.42
1:B:282:GLN:HG3	1:B:309:GLU:HB3	2.00	0.42
1:B:224:GLN:HG2	1:B:252:ASN:HB2	2.01	0.42
1:A:161:LEU:O	1:A:189:LEU:HD23	2.19	0.42
1:B:17:THR:OG1	1:B:18:THR:N	2.52	0.42
1:B:83:LEU:O	1:B:87:LEU:HG	2.20	0.42
1:B:208:LEU:HD13	1:B:236:LEU:CA	2.49	0.42
1:A:61:ASP:HB2	3:A:2008:HOH:O	2.20	0.42
1:A:291:VAL:HG21	1:A:315:PHE:CD2	2.55	0.42
1:B:100:ARG:HA	1:B:128:TYR:HB2	2.01	0.42
1:B:169:ASN:O	1:B:170:ARG:C	2.62	0.42
1:A:212:LEU:HB3	1:A:243:TRP:HZ2	1.85	0.42
1:B:279:LEU:HG	1:B:281:LEU:HG	2.02	0.42
1:A:334:ARG:HB2	1:A:334:ARG:NH1	2.35	0.42
1:A:336:GLU:HA	3:A:2140:HOH:O	2.19	0.41
1:B:16:ILE:O	1:B:17:THR:O	2.37	0.41
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.91	0.41
1:B:191:THR:HG23	1:B:220:VAL:HB	2.02	0.41
1:B:195:VAL:HB	1:B:224:GLN:HB3	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLY:HA2	1:A:342:ASP:O	2.20	0.41
1:A:164:ILE:C	1:A:165:ILE:HD13	2.45	0.41
1:B:122:THR:N	1:B:123:PRO:CD	2.83	0.41
1:B:257:SER:HB2	1:B:259:ARG:NH2	2.36	0.41
1:B:280:ARG:NH1	1:B:309:GLU:OE2	2.53	0.41
1:A:63:GLU:O	1:A:96:LEU:HD12	2.21	0.41
1:A:254:CYS:O	1:A:255:LEU:C	2.64	0.41
1:A:306:LEU:HA	1:A:335:GLY:HA2	2.02	0.41
1:B:176:MET:HE3	1:B:179:TRP:HB2	2.03	0.41
1:B:225:ASP:HA	1:B:253:ASP:O	2.21	0.41
1:A:2:ALA:HB3	1:A:34:VAL:HA	2.03	0.41
1:A:3:ARG:NH2	1:A:38:VAL:HG21	2.36	0.41
1:B:155:ALA:HA	3:B:2045:HOH:O	2.20	0.41
1:B:306:LEU:HA	1:B:335:GLY:HA2	2.02	0.41
1:B:236:LEU:HD21	1:B:251:LEU:HD11	2.03	0.40
1:A:308:LEU:HD23	1:A:337:LEU:CD1	2.49	0.40
1:B:17:THR:OG1	1:B:20:ASP:OD2	2.36	0.40
1:B:325:ILE:HG22	1:B:329:PHE:CE2	2.57	0.40
1:B:44:ILE:O	1:B:74:ARG:NH1	2.54	0.40
1:B:317:GLU:HG2	1:B:340:LEU:HD12	2.03	0.40
1:A:227:THR:HG22	1:A:229:THR:HG23	2.04	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	342/386 (89%)	310 (91%)	29 (8%)	3 (1%)	14	14
1	B	294/386 (76%)	268 (91%)	22 (8%)	4 (1%)	9	7
All	All	636/772 (82%)	578 (91%)	51 (8%)	7 (1%)	11	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	172	GLU
1	B	17	THR
1	A	257	SER
1	B	257	SER
1	B	172	GLU
1	B	6	ILE

### 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	294/334 (88%)	290 (99%)	4 (1%)	59 75
1	B	294/334 (88%)	285 (97%)	9 (3%)	35 48
All	All	588/668 (88%)	575 (98%)	13 (2%)	45 61

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	201	PRO
1	A	212	LEU
1	A	289	ASP
1	B	21	GLU
1	B	32	ASP
1	B	66	GLU
1	B	75	VAL
1	B	116	ASP
1	B	162	ARG
1	B	176	MET
1	B	212	LEU
1	B	259	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	130	HIS
1	A	131	ASN
1	A	137	GLN
1	A	206	HIS
1	A	245	ASN
1	A	277	GLN
1	B	137	GLN
1	B	206	HIS

### 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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	B	1345	-	4,4,4	0.38	0	6,6,6	0.07	0
2	SO4	B	1348	-	4,4,4	0.42	0	6,6,6	0.08	0
2	SO4	B	1346	-	4,4,4	0.39	0	6,6,6	0.08	0
2	SO4	B	1347	-	4,4,4	0.38	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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	344/386 (89%)	0.60	28 (8%) 18 15	7, 17, 39, 73	0
1	B	344/386 (89%)	0.97	42 (12%) 8 6	6, 20, 63, 87	0
All	All	688/772 (89%)	0.79	70 (10%) 12 9	6, 18, 48, 87	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	LEU	6.7
1	B	16	ILE	6.1
1	B	13	LEU	5.7
1	A	345	GLU	5.7
1	B	15	ALA	5.5
1	B	29	LEU	5.4
1	B	17	THR	5.3
1	B	21	GLU	5.1
1	B	18	THR	5.0
1	B	27	VAL	5.0
1	A	20	ASP	4.9
1	A	24	VAL	4.8
1	A	334	ARG	4.6
1	A	17	THR	4.6
1	B	30	GLU	4.3
1	A	32	ASP	4.2
1	B	12	LYS	4.1
1	B	24	VAL	4.0
1	B	32	ASP	3.9
1	A	27	VAL	3.9
1	B	20	ASP	3.8
1	B	25	PHE	3.7
1	B	28	LEU	3.7
1	B	19	GLU	3.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	22	LYS	3.5
1	A	29	LEU	3.5
1	A	18	THR	3.3
1	B	31	ASP	3.3
1	B	345	GLU	3.3
1	B	136	PRO	3.2
1	B	72	THR	3.2
1	A	16	ILE	3.1
1	B	79	ILE	3.0
1	B	23	SER	3.0
1	B	14	ASP	3.0
1	B	75	VAL	3.0
1	B	57	ALA	3.0
1	A	61	ASP	2.9
1	A	344	GLU	2.9
1	B	4	PHE	2.9
1	B	22	LYS	2.9
1	B	2	ALA	2.8
1	A	23	SER	2.8
1	B	26	ALA	2.7
1	B	344	GLU	2.7
1	B	5	SER	2.7
1	A	19	GLU	2.6
1	A	12	LYS	2.6
1	A	15	ALA	2.6
1	B	10	SER	2.6
1	A	21	GLU	2.5
1	B	43	THR	2.5
1	B	6	ILE	2.5
1	B	34	VAL	2.5
1	A	25	PHE	2.4
1	A	30	GLU	2.4
1	B	65	ALA	2.4
1	A	107	GLY	2.4
1	A	14	ASP	2.3
1	B	60	LYS	2.3
1	B	137	GLN	2.2
1	B	33	SER	2.2
1	B	62	LEU	2.1
1	A	44	ILE	2.1
1	A	28	LEU	2.1
1	B	8	GLY	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	314	ARG	2.1
1	A	59	LYS	2.0
1	A	164	ILE	2.0
1	A	36	GLU	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](#)

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. 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	B-factors(Å <sup>2</sup> )	Q < 0.9
2	SO4	B	1346	5/5	0.59	0.24	75,75,81,83	0
2	SO4	B	1348	5/5	0.67	0.27	61,65,66,72	0
2	SO4	B	1345	5/5	0.76	0.19	60,63,66,66	0
2	SO4	B	1347	5/5	0.78	0.22	61,64,65,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.