Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 02:28 PM EDT

PDB ID	:	2IJD
Title	:	Crystal Structure of the Poliovirus Precursor Protein 3CD
Authors	:	Marcotte, L.L.; Gohara, D.W.; Filman, D.J.; Hogle, J.M.
Deposited on	:	2006-09-29
Resolution	:	3.40 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

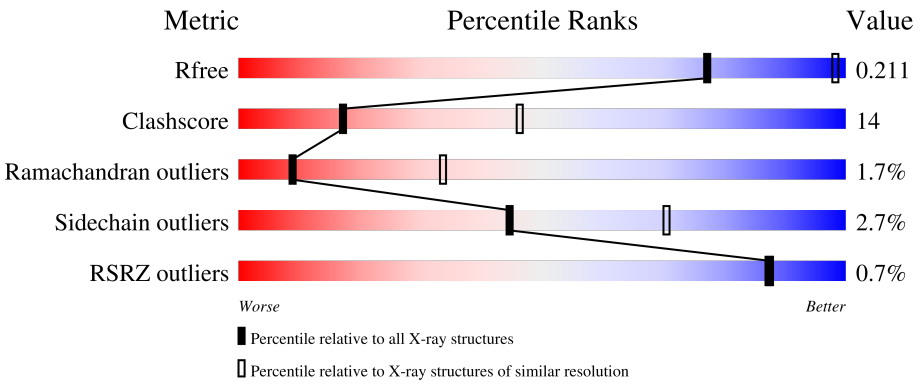
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 >=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 <=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	1	644	73% 25% •
1	2	644	% 73% 25% •

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
3	SO4	1	648	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10170 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 Picornain 3C, RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	644	5060	3226	850	956	28	0	0	0
1	2	644	5060	3226	850	956	28	0	0	0

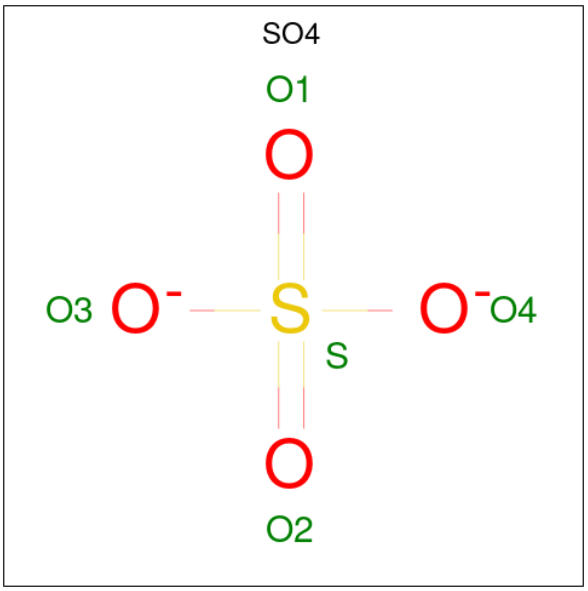
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	55	ALA	GLU	engineered mutation	UNP P03300
1	58	ALA	ASP	engineered mutation	UNP P03300
1	63	ALA	GLU	engineered mutation	UNP P03300
1	147	ALA	CYS	engineered mutation	UNP P03300
1	629	ASP	LEU	engineered mutation	UNP P03300
1	638	ASP	ARG	engineered mutation	UNP P03300
2	55	ALA	GLU	engineered mutation	UNP P03300
2	58	ALA	ASP	engineered mutation	UNP P03300
2	63	ALA	GLU	engineered mutation	UNP P03300
2	147	ALA	CYS	engineered mutation	UNP P03300
2	629	ASP	LEU	engineered mutation	UNP P03300
2	638	ASP	ARG	engineered mutation	UNP P03300

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	1	1	1	1	0	0
2	2	1	1	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1	1	Total O S 5 4 1	0	0
3	1	1	Total O S 5 4 1	0	0
3	1	1	Total O S 5 4 1	0	0
3	1	1	Total O S 5 4 1	0	0
3	2	1	Total O S 5 4 1	0	0
3	2	1	Total O S 5 4 1	0	0
3	2	1	Total O S 5 4 1	0	0
3	2	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

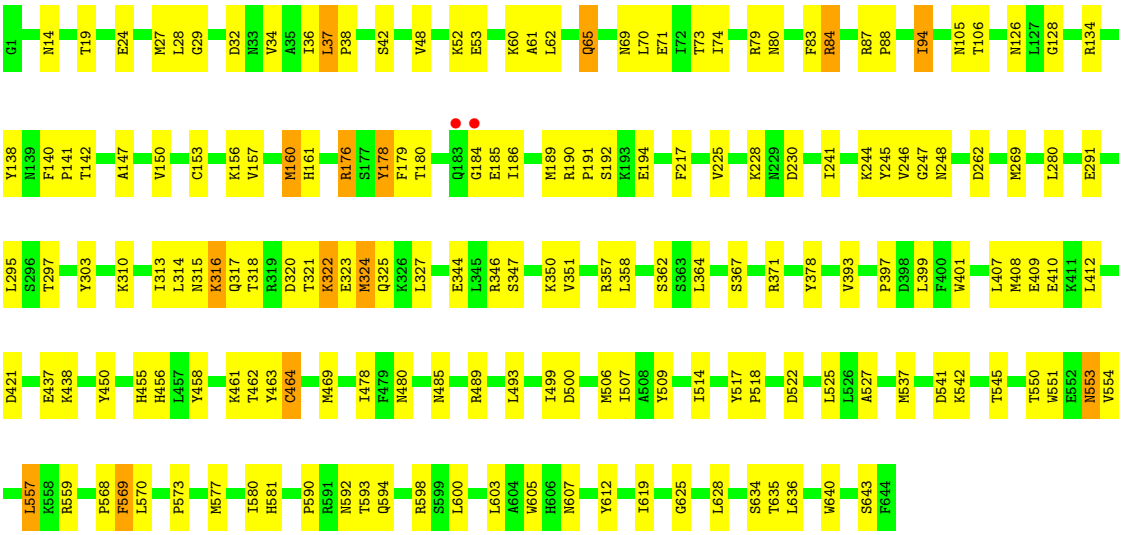
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1	4	Total O 4 4	0	0
4	2	4	Total O 4 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

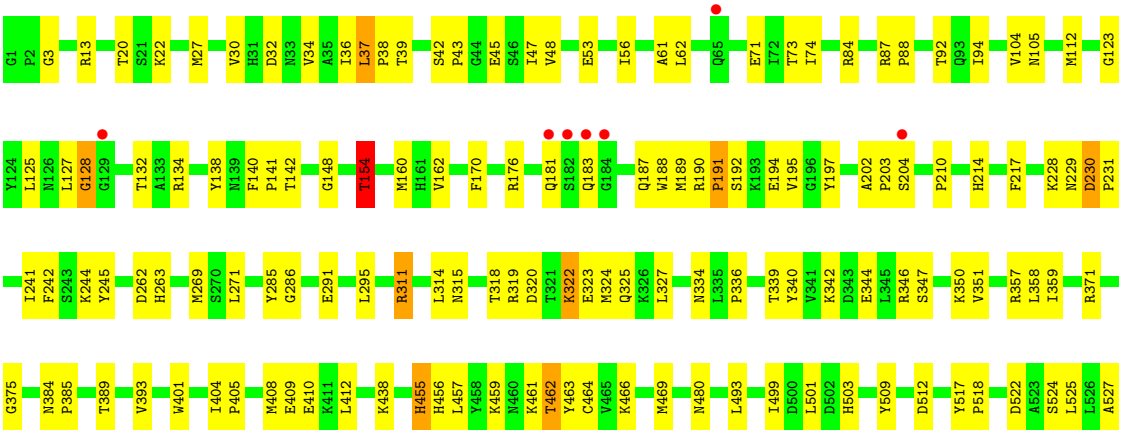
• Molecule 1: Picornain 3C, RNA-directed RNA polymerase

Chain 1:



• Molecule 1: Picornain 3C, RNA-directed RNA polymerase

Chain 2:



M537
T545
T550
W551
E552
N553
V554
T555
F556
L557
K558
R559
F560
F561
R562
Y567
P568
F569
L570
P573
M577
H581
R598
W605
Y612
F615
L616
I619
I624
G625
R626
A627
L628
S634
T635
L636
F644

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	208.54Å 230.44Å 151.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 3.40 19.90 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.90-3.40) 98.1 (19.90-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.90 (at 3.44Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.231 0.177 , 0.211	Depositor DCC
R_{free} test set	2510 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	94.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 63.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10170	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, ZN

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	1	0.65	0/5175	0.93	11/7006 (0.2%)
1	2	0.65	1/5175 (0.0%)	0.92	9/7006 (0.1%)
All	All	0.65	1/10350 (0.0%)	0.92	20/14012 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	340	TYR	CE1-CZ	5.65	1.45	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	557	LEU	CA-CB-CG	-7.51	98.03	115.30
1	1	557	LEU	CA-CB-CG	-6.87	99.50	115.30
1	1	557	LEU	CB-CA-C	6.37	122.30	110.20
1	2	37	LEU	CA-CB-CG	6.36	129.93	115.30
1	2	84	ARG	CA-CB-CG	6.35	127.36	113.40
1	2	84	ARG	CB-CA-C	-6.17	98.07	110.40
1	1	557	LEU	N-CA-C	-5.75	95.48	111.00
1	1	84	ARG	CB-CG-CD	-5.50	97.31	111.60
1	1	269	MET	CA-CB-CG	-5.49	103.97	113.30
1	1	603	LEU	CA-CB-CG	5.47	127.88	115.30
1	1	84	ARG	CB-CA-C	-5.38	99.63	110.40
1	2	557	LEU	CB-CA-C	5.37	120.40	110.20
1	2	558	LYS	CD-CE-NZ	5.36	124.04	111.70
1	1	84	ARG	CA-CB-CG	5.34	125.16	113.40
1	2	557	LEU	C-N-CA	-5.31	108.43	121.70
1	1	184	GLY	N-CA-C	-5.23	100.03	113.10
1	1	160	MET	CG-SD-CE	-5.17	91.92	100.20
1	2	269	MET	CA-CB-CG	-5.14	104.56	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	84	ARG	N-CA-CB	5.11	119.80	110.60
1	1	437	GLU	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	5060	0	5028	139	0
1	2	5060	0	5028	143	0
2	1	1	0	0	0	0
2	2	1	0	0	0	0
3	1	20	0	0	1	0
3	2	20	0	0	2	0
4	1	4	0	0	0	0
4	2	4	0	0	0	0
All	All	10170	0	10056	281	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 14.

All (281) 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)
1:1:228:LYS:H	1:1:228:LYS:HD2	1.10	1.16
1:1:485:ASN:HA	1:1:506:MET:HE3	1.28	1.15
1:2:39:THR:HG22	1:2:73:THR:HG23	1.27	1.12
1:2:228:LYS:H	1:2:228:LYS:HD2	0.96	1.07
1:2:409:GLU:HG3	1:2:410:GLU:H	1.20	1.02
1:2:455:HIS:HB3	1:2:464:CYS:HA	1.41	1.02
1:1:409:GLU:HG3	1:1:410:GLU:H	1.27	0.99
1:2:228:LYS:HD2	1:2:228:LYS:N	1.79	0.96
1:2:228:LYS:H	1:2:228:LYS:CD	1.76	0.94
1:2:311:ARG:HG3	1:2:311:ARG:HH11	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:456:HIS:HD2	1:2:463:TYR:CE1	1.86	0.92
1:1:37:LEU:HA	1:1:160:MET:HE1	1.53	0.90
1:1:324:MET:CE	1:1:364:LEU:HG	2.03	0.89
1:1:176:ARG:HH11	1:1:176:ARG:HG2	1.37	0.88
1:1:315:ASN:HB3	1:1:318:THR:HB	1.57	0.87
1:2:217:PHE:CD1	1:2:581:HIS:HD2	1.91	0.87
1:2:409:GLU:HG3	1:2:410:GLU:N	1.89	0.87
1:1:142:THR:HG21	1:1:161:HIS:CE1	2.11	0.85
1:1:409:GLU:HG3	1:1:410:GLU:N	1.91	0.84
1:1:241:ILE:HD12	1:1:358:LEU:HD21	1.59	0.83
1:1:346:ARG:NH2	1:1:350:LYS:HD3	1.96	0.81
1:2:39:THR:HG22	1:2:73:THR:CG2	2.10	0.79
1:1:228:LYS:H	1:1:228:LYS:CD	1.91	0.78
1:2:456:HIS:CD2	1:2:463:TYR:CE1	2.71	0.77
1:1:295:LEU:HD21	1:1:314:LEU:HD12	1.65	0.76
1:2:217:PHE:HD1	1:2:581:HIS:HD2	1.29	0.76
1:2:408:MET:HE2	1:2:408:MET:HA	1.68	0.75
1:2:517:TYR:CG	1:2:518:PRO:HD2	2.22	0.74
1:1:409:GLU:CG	1:1:410:GLU:H	2.01	0.72
1:2:409:GLU:CG	1:2:410:GLU:H	2.00	0.72
1:1:37:LEU:HA	1:1:160:MET:CE	2.19	0.72
1:2:241:ILE:HD12	1:2:358:LEU:HD21	1.70	0.72
1:2:217:PHE:CD1	1:2:581:HIS:CD2	2.76	0.72
1:1:553:ASN:C	1:1:553:ASN:HD22	1.93	0.72
1:1:559:ARG:HD3	1:1:573:PRO:HB2	1.71	0.71
1:2:559:ARG:HD3	1:2:573:PRO:HB2	1.73	0.70
1:2:39:THR:CG2	1:2:73:THR:HG23	2.14	0.70
1:2:217:PHE:HD1	1:2:581:HIS:CD2	2.08	0.70
1:2:553:ASN:C	1:2:553:ASN:HD22	1.95	0.70
1:1:499:ILE:HG13	1:1:500:ASP:H	1.55	0.69
1:2:295:LEU:HD21	1:2:314:LEU:HD12	1.73	0.69
1:2:567:TYR:HB3	1:2:569:PHE:CE2	2.28	0.69
1:1:62:LEU:HB3	1:1:70:LEU:HD12	1.74	0.69
1:1:19:THR:HB	1:1:48:VAL:HB	1.74	0.68
1:2:522:ASP:HB3	1:2:525:LEU:HD12	1.75	0.68
1:2:192:SER:HA	1:2:462:THR:HG22	1.76	0.67
1:1:217:PHE:CD1	1:1:581:HIS:HD2	2.13	0.67
1:1:598:ARG:NH1	3:1:649:SO4:O1	2.27	0.67
1:2:517:TYR:CD2	1:2:518:PRO:HD2	2.31	0.66
1:1:485:ASN:CA	1:1:506:MET:HE3	2.17	0.66
1:1:324:MET:HE3	1:1:364:LEU:HG	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:324:MET:HE1	1:1:364:LEU:HG	1.77	0.65
1:1:228:LYS:HD2	1:1:228:LYS:N	1.96	0.65
1:2:189:MET:HB2	1:2:463:TYR:HB3	1.78	0.65
1:2:192:SER:HA	1:2:462:THR:CG2	2.26	0.65
1:2:94:ILE:HD12	1:2:94:ILE:H	1.60	0.65
1:1:315:ASN:HB3	1:1:318:THR:CB	2.27	0.64
1:1:94:ILE:H	1:1:94:ILE:HD12	1.62	0.64
1:1:176:ARG:HH11	1:1:176:ARG:CG	2.10	0.63
1:1:346:ARG:HH21	1:1:350:LYS:HD3	1.63	0.63
1:2:62:LEU:HD21	1:2:74:ILE:HG13	1.81	0.63
1:2:311:ARG:HH11	1:2:311:ARG:CG	2.09	0.62
1:2:3:GLY:HA2	1:2:154:THR:HG23	1.80	0.62
1:2:522:ASP:OD1	1:2:524:SER:HB3	2.00	0.62
1:1:324:MET:CE	1:1:364:LEU:CG	2.77	0.60
1:2:104:VAL:HB	1:2:112:MET:HB3	1.83	0.60
1:2:202:ALA:O	1:2:203:PRO:C	2.40	0.60
1:2:393:VAL:HA	1:2:509:TYR:CE2	2.36	0.60
1:2:517:TYR:CG	1:2:518:PRO:CD	2.84	0.60
1:2:346:ARG:NH2	1:2:350:LYS:HD3	2.16	0.60
1:1:79:ARG:HG2	1:1:80:ASN:N	2.17	0.60
1:2:619:ILE:O	1:2:625:GLY:HA3	2.01	0.60
1:2:3:GLY:CA	1:2:154:THR:HG23	2.31	0.59
1:1:61:ALA:HA	1:1:73:THR:HG22	1.84	0.59
1:1:315:ASN:CB	1:1:318:THR:HB	2.30	0.59
1:1:316:LYS:HG3	1:1:317:GLN:OE1	2.02	0.59
1:2:291:GLU:O	1:2:371:ARG:NH2	2.36	0.59
1:2:612:TYR:CE2	1:2:616:LEU:HD11	2.38	0.59
1:1:553:ASN:HD22	1:1:554:VAL:N	2.01	0.59
1:1:291:GLU:O	1:1:371:ARG:NH2	2.36	0.58
1:2:550:THR:H	1:2:553:ASN:ND2	2.01	0.58
1:1:14:ASN:OD1	1:1:84:ARG:HD2	2.04	0.58
1:2:22:LYS:HD2	1:2:42:SER:HB3	1.85	0.58
1:1:52:LYS:HG2	1:1:53:GLU:H	1.69	0.58
1:1:142:THR:HG21	1:1:161:HIS:NE2	2.19	0.58
1:2:36:ILE:O	1:2:160:MET:HE3	2.03	0.57
1:1:248:ASN:ND2	1:1:248:ASN:H	2.01	0.57
1:1:65:GLN:HE22	1:1:134:ARG:HH22	1.53	0.57
1:1:378:TYR:HD1	1:1:478:ILE:HD12	1.70	0.57
1:1:378:TYR:CD1	1:1:478:ILE:HD12	2.40	0.56
1:2:339:THR:HA	1:2:359:ILE:O	2.04	0.56
1:2:344:GLU:OE2	1:2:357:ARG:NH2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:455:HIS:ND1	1:1:464:CYS:HB2	2.21	0.56
1:2:148:GLY:HA2	1:2:160:MET:CE	2.36	0.56
1:1:190:ARG:HB2	1:1:191:PRO:HD2	1.88	0.55
1:1:619:ILE:O	1:1:625:GLY:HA3	2.06	0.55
1:1:244:LYS:HG3	1:1:245:TYR:N	2.21	0.55
1:1:313:ILE:HG23	1:1:323:GLU:HG3	1.88	0.55
1:1:347:SER:O	1:1:351:VAL:HG23	2.07	0.55
1:2:20:THR:HG22	1:2:47:ILE:HD12	1.88	0.55
1:1:140:PHE:O	1:1:142:THR:N	2.40	0.55
1:1:65:GLN:HE22	1:1:134:ARG:NH2	2.04	0.55
1:2:342:LYS:HB2	1:2:359:ILE:HG13	1.88	0.55
1:2:71:GLU:O	1:2:71:GLU:HG3	2.07	0.55
1:2:148:GLY:HA2	1:2:160:MET:HE1	1.88	0.55
1:1:455:HIS:ND1	1:1:464:CYS:CB	2.70	0.54
1:2:197:TYR:CE2	1:2:336:PRO:HG2	2.42	0.54
1:1:310:LYS:HE3	1:1:364:LEU:HD13	1.88	0.54
1:2:30:VAL:HB	1:2:34:VAL:HG23	1.89	0.54
1:2:87:ARG:N	1:2:88:PRO:HD2	2.23	0.54
1:1:217:PHE:CD1	1:1:581:HIS:CD2	2.95	0.54
1:2:47:ILE:HG12	1:2:56:ILE:HD11	1.89	0.53
1:1:580:ILE:HG23	1:1:600:LEU:HD22	1.89	0.53
1:1:527:ALA:HA	1:1:537:MET:HE1	1.90	0.53
1:2:311:ARG:HG3	1:2:311:ARG:NH1	2.10	0.53
1:2:190:ARG:HB2	1:2:191:PRO:HD2	1.91	0.53
1:2:271:LEU:HD11	1:2:389:THR:HG22	1.91	0.53
1:2:517:TYR:CD1	1:2:518:PRO:HD2	2.44	0.53
1:1:324:MET:HE1	1:1:364:LEU:CD2	2.39	0.52
1:1:458:TYR:HB2	1:1:463:TYR:HE2	1.75	0.52
1:2:188:TRP:CE2	1:2:464:CYS:HB2	2.45	0.52
1:1:393:VAL:HA	1:1:509:TYR:CE2	2.45	0.52
1:2:408:MET:HA	1:2:408:MET:CE	2.37	0.51
1:1:142:THR:HG21	1:1:161:HIS:HE1	1.72	0.51
1:1:87:ARG:N	1:1:88:PRO:HD2	2.25	0.51
1:1:179:PHE:O	1:1:180:THR:C	2.49	0.51
1:2:412:LEU:HD21	1:2:551:TRP:CZ2	2.46	0.51
1:1:38:PRO:HD3	1:1:160:MET:HE1	1.92	0.50
1:1:493:LEU:HD23	1:1:499:ILE:CG2	2.41	0.50
1:2:626:ARG:C	1:2:628:LEU:H	2.15	0.50
1:1:499:ILE:HG13	1:1:500:ASP:N	2.25	0.50
1:2:20:THR:HG22	1:2:47:ILE:CD1	2.42	0.50
1:1:147:ALA:HA	1:1:161:HIS:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:569:PHE:HE2	1:2:570:LEU:HD23	1.77	0.50
1:2:553:ASN:HD22	1:2:554:VAL:N	2.09	0.50
1:1:150:VAL:HG11	1:1:157:VAL:HG13	1.93	0.50
1:2:228:LYS:NZ	1:2:459:LYS:HE2	2.25	0.50
1:2:567:TYR:C	1:2:569:PHE:H	2.15	0.50
1:2:195:VAL:HG23	1:2:197:TYR:HD1	1.77	0.49
1:1:262:ASP:HA	1:1:438:LYS:HE3	1.93	0.49
1:1:52:LYS:HG2	1:1:53:GLU:N	2.27	0.49
1:2:20:THR:C	1:2:22:LYS:H	2.16	0.49
1:2:61:ALA:HA	1:2:73:THR:HG22	1.95	0.49
1:2:527:ALA:HA	1:2:537:MET:HE1	1.93	0.49
1:1:514:ILE:HG23	1:1:514:ILE:O	2.12	0.49
1:2:567:TYR:HD2	1:2:569:PHE:CE2	2.31	0.49
1:2:71:GLU:HG2	1:2:162:VAL:HB	1.94	0.48
1:2:181:GLN:O	1:2:181:GLN:HG2	2.11	0.48
1:2:577:MET:HB3	1:2:581:HIS:CE1	2.47	0.48
1:1:489:ARG:NH1	1:1:506:MET:HE2	2.29	0.48
1:2:27:MET:HG3	1:2:36:ILE:O	2.14	0.48
1:2:615:PHE:CZ	1:2:619:ILE:HD11	2.48	0.48
1:2:626:ARG:O	1:2:628:LEU:N	2.37	0.48
1:2:350:LYS:HE2	3:2:648:SO4:O3	2.13	0.48
1:2:455:HIS:CB	1:2:463:TYR:O	2.61	0.48
1:1:640:TRP:HA	1:1:643:SER:OG	2.14	0.48
1:1:71:GLU:OE2	1:1:71:GLU:HA	2.13	0.47
1:2:192:SER:CA	1:2:462:THR:HG22	2.44	0.47
1:2:455:HIS:HB3	1:2:464:CYS:CA	2.29	0.47
1:1:577:MET:SD	1:1:607:ASN:ND2	2.87	0.47
1:2:324:MET:O	1:2:327:LEU:HB2	2.14	0.47
1:1:189:MET:O	1:1:190:ARG:HB3	2.14	0.47
1:1:517:TYR:CG	1:1:518:PRO:HD2	2.50	0.47
1:1:324:MET:HE1	1:1:364:LEU:CG	2.41	0.47
1:1:493:LEU:HD23	1:1:499:ILE:HG22	1.96	0.47
1:2:125:LEU:HD11	1:2:170:PHE:CG	2.49	0.47
1:2:557:LEU:C	1:2:559:ARG:H	2.16	0.47
1:1:34:VAL:HG13	1:1:74:ILE:CG2	2.45	0.47
1:1:225:VAL:HG13	1:1:230:ASP:CB	2.44	0.47
1:2:244:LYS:HG3	1:2:245:TYR:N	2.28	0.47
1:2:567:TYR:O	1:2:569:PHE:N	2.48	0.47
1:1:324:MET:CE	1:1:364:LEU:CD2	2.93	0.47
1:2:262:ASP:HA	1:2:438:LYS:HE3	1.97	0.47
1:1:14:ASN:O	1:1:28:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:553:ASN:C	1:1:553:ASN:ND2	2.65	0.47
1:1:36:ILE:HG22	1:1:74:ILE:HG12	1.96	0.46
1:1:62:LEU:HD11	1:1:74:ILE:HD11	1.97	0.46
1:2:315:ASN:HB3	1:2:318:THR:HB	1.96	0.46
1:2:557:LEU:HD23	1:2:557:LEU:HA	1.47	0.46
1:2:210:PRO:HB3	1:2:214:HIS:CG	2.50	0.46
1:2:242:PHE:C	1:2:244:LYS:H	2.18	0.46
1:2:286:GLY:O	1:2:319:ARG:NH2	2.48	0.46
1:2:404:ILE:N	1:2:405:PRO:HD2	2.30	0.46
1:1:344:GLU:OE2	1:1:357:ARG:NH2	2.48	0.46
1:1:605:TRP:HA	1:1:612:TYR:HB2	1.98	0.46
1:1:248:ASN:N	1:1:248:ASN:HD22	2.13	0.46
1:1:29:GLY:HA3	1:1:83:PHE:CD1	2.51	0.46
1:1:186:ILE:HD11	1:1:245:TYR:CD1	2.51	0.46
1:1:522:ASP:HB3	1:1:525:LEU:HD12	1.96	0.46
1:2:384:ASN:N	1:2:385:PRO:HD3	2.31	0.46
1:1:185:GLU:HB3	1:1:245:TYR:HB2	1.96	0.46
1:1:24:GLU:OE1	1:1:106:THR:HB	2.16	0.46
1:1:577:MET:HB3	1:1:581:HIS:CE1	2.51	0.46
1:1:550:THR:H	1:1:553:ASN:ND2	2.14	0.45
1:2:92:THR:HG22	1:2:176:ARG:NH1	2.30	0.45
1:2:371:ARG:O	1:2:375:GLY:CA	2.64	0.45
1:1:52:LYS:CG	1:1:53:GLU:H	2.30	0.45
1:1:303:TYR:OH	1:1:327:LEU:HB3	2.15	0.45
1:1:190:ARG:CB	1:1:191:PRO:HD2	2.45	0.45
1:2:503:HIS:O	1:2:518:PRO:HD3	2.16	0.45
1:2:38:PRO:HD3	1:2:160:MET:HE1	1.97	0.45
1:2:315:ASN:CB	1:2:318:THR:HB	2.46	0.45
1:1:71:GLU:HG3	1:1:71:GLU:O	2.17	0.45
1:1:399:LEU:HD21	1:1:643:SER:HB3	1.98	0.45
1:2:567:TYR:C	1:2:569:PHE:N	2.69	0.45
1:2:62:LEU:HD21	1:2:74:ILE:CD1	2.47	0.45
1:1:79:ARG:HG2	1:1:80:ASN:H	1.79	0.45
1:1:455:HIS:ND1	1:1:464:CYS:HB3	2.33	0.44
1:2:550:THR:H	1:2:553:ASN:HD21	1.64	0.44
1:2:191:PRO:HG2	1:2:194:GLU:CD	2.37	0.44
1:1:315:ASN:O	1:1:318:THR:N	2.50	0.44
1:1:557:LEU:HA	1:1:557:LEU:HD23	1.69	0.44
1:2:62:LEU:HD21	1:2:74:ILE:CG1	2.47	0.44
1:2:48:VAL:HA	1:2:53:GLU:HA	2.00	0.44
1:1:248:ASN:ND2	1:1:248:ASN:N	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:189:MET:HE2	1:2:461:LYS:HB3	2.00	0.44
1:2:263:HIS:CE1	1:2:501:LEU:HB3	2.52	0.44
1:1:592:ASN:O	1:1:593:THR:C	2.54	0.44
1:2:456:HIS:CD2	1:2:463:TYR:HE1	2.34	0.44
1:2:183:GLN:O	1:2:245:TYR:O	2.34	0.43
1:1:407:LEU:HD23	1:1:407:LEU:HA	1.73	0.43
1:2:62:LEU:CD2	1:2:74:ILE:HG13	2.47	0.43
1:2:457:LEU:HD23	1:2:462:THR:HB	2.00	0.43
1:2:567:TYR:HB3	1:2:569:PHE:CZ	2.53	0.43
1:1:321:THR:O	1:1:322:LYS:C	2.57	0.43
1:2:634:SER:O	1:2:635:THR:C	2.55	0.43
1:1:138:TYR:OH	1:1:161:HIS:ND1	2.43	0.43
1:2:336:PRO:HA	1:2:455:HIS:O	2.19	0.43
1:1:192:SER:HA	1:1:462:THR:HG23	2.00	0.43
1:1:69:ASN:OD1	1:1:70:LEU:N	2.52	0.43
1:1:456:HIS:O	1:1:462:THR:HA	2.19	0.43
1:2:512:ASP:OD2	1:2:556:PHE:O	2.36	0.43
1:2:189:MET:CB	1:2:463:TYR:HB3	2.45	0.42
1:1:79:ARG:HG2	1:1:80:ASN:OD1	2.20	0.42
1:1:412:LEU:HD21	1:1:551:TRP:CZ2	2.54	0.42
1:1:594:GLN:HA	1:1:628:LEU:HD22	2.02	0.42
1:1:634:SER:O	1:1:635:THR:C	2.57	0.42
1:2:561:PHE:O	1:2:562:ARG:HD3	2.19	0.42
1:1:315:ASN:O	1:1:317:GLN:N	2.53	0.42
1:2:127:LEU:O	1:2:128:GLY:C	2.57	0.42
1:2:493:LEU:HD23	1:2:499:ILE:HG22	2.00	0.42
1:1:60:LYS:O	1:1:73:THR:HA	2.19	0.42
1:1:320:ASP:OD2	1:1:320:ASP:C	2.58	0.42
1:2:598:ARG:NH2	3:2:649:SO4:O2	2.52	0.42
1:1:469:MET:HG2	1:1:480:ASN:OD1	2.19	0.42
1:2:202:ALA:O	1:2:204:SER:N	2.53	0.42
1:1:367:SER:O	1:1:371:ARG:HG3	2.20	0.42
1:1:150:VAL:CG1	1:1:157:VAL:HG13	2.49	0.42
1:1:362:SER:HB2	1:1:450:TYR:OH	2.20	0.42
1:1:408:MET:HA	1:1:408:MET:CE	2.50	0.42
1:1:321:THR:O	1:1:324:MET:N	2.53	0.42
1:2:605:TRP:CD1	1:2:636:LEU:HD13	2.55	0.42
1:1:27:MET:HG3	1:1:36:ILE:O	2.20	0.41
1:2:322:LYS:O	1:2:323:GLU:C	2.58	0.41
1:1:408:MET:HE3	1:1:507:ILE:HG13	2.01	0.41
1:2:624:ILE:O	1:2:628:LEU:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:186:ILE:HG21	1:1:463:TYR:HB2	2.01	0.41
1:1:517:TYR:CD2	1:1:518:PRO:HD2	2.55	0.41
1:1:176:ARG:HG2	1:1:176:ARG:NH1	2.17	0.41
1:2:242:PHE:C	1:2:244:LYS:N	2.73	0.41
1:2:469:MET:HG2	1:2:480:ASN:OD1	2.20	0.41
1:2:553:ASN:C	1:2:553:ASN:ND2	2.67	0.41
1:2:626:ARG:C	1:2:628:LEU:N	2.74	0.41
1:1:541:ASP:O	1:1:542:LYS:C	2.57	0.41
1:2:27:MET:SD	1:2:37:LEU:HD21	2.60	0.41
1:2:140:PHE:O	1:2:142:THR:N	2.53	0.41
1:2:271:LEU:CD1	1:2:389:THR:HG22	2.50	0.41
1:2:322:LYS:HA	1:2:325:GLN:HB3	2.01	0.41
1:1:178:TYR:HD1	1:1:178:TYR:H	1.68	0.41
1:2:285:TYR:OH	1:2:320:ASP:O	2.26	0.41
1:1:153:CYS:SG	1:1:156:LYS:HD2	2.61	0.41
1:1:570:LEU:HA	1:1:570:LEU:HD23	1.79	0.40
1:2:229:ASN:O	1:2:230:ASP:C	2.59	0.40
1:1:280:LEU:HD22	1:1:325:GLN:NE2	2.35	0.40
1:1:605:TRP:CD1	1:1:636:LEU:HD13	2.56	0.40
1:2:71:GLU:HB2	1:2:132:THR:HG21	2.04	0.40
1:2:230:ASP:HA	1:2:231:PRO:HD2	1.68	0.40
1:2:324:MET:HB2	1:2:324:MET:HE2	1.94	0.40
1:2:570:LEU:HD22	1:2:644:PHE:CE1	2.56	0.40
1:1:191:PRO:HG2	1:1:194:GLU:CD	2.41	0.40
1:2:347:SER:O	1:2:351:VAL:HG23	2.21	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	1	642/644 (100%)	574 (89%)	56 (9%)	12 (2%)	8 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	2	642/644 (100%)	569 (89%)	63 (10%)	10 (2%)	9 34
All	All	1284/1288 (100%)	1143 (89%)	119 (9%)	22 (2%)	9 34

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	128	GLY
1	1	178	TYR
1	1	316	LYS
1	2	134	ARG
1	2	322	LYS
1	1	141	PRO
1	1	297	THR
1	1	568	PRO
1	2	32	ASP
1	2	43	PRO
1	2	128	GLY
1	1	32	ASP
1	1	42	SER
1	1	247	GLY
1	2	141	PRO
1	2	154	THR
1	1	94	ILE
1	1	322	LYS
1	2	191	PRO
1	2	123	GLY
1	2	230	ASP
1	1	590	PRO

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	1	546/546 (100%)	531 (97%)	15 (3%)	44 70
1	2	546/546 (100%)	532 (97%)	14 (3%)	46 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1092/1092 (100%)	1063 (97%)	29 (3%)	44 70

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	37	LEU
1	1	65	GLN
1	1	105	ASN
1	1	126	ASN
1	1	176	ARG
1	1	246	VAL
1	1	324	MET
1	1	397	PRO
1	1	401	TRP
1	1	421	ASP
1	1	461	LYS
1	1	464	CYS
1	1	545	THR
1	1	553	ASN
1	1	569	PHE
1	2	13	ARG
1	2	45	GLU
1	2	105	ASN
1	2	138	TYR
1	2	154	THR
1	2	187	GLN
1	2	311	ARG
1	2	334	ASN
1	2	401	TRP
1	2	455	HIS
1	2	462	THR
1	2	466	LYS
1	2	545	THR
1	2	553	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	31	HIS
1	1	65	GLN
1	1	93	GLN

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Mol	Chain	Res	Type
1	1	105	ASN
1	1	122	GLN
1	1	126	ASN
1	1	146	GLN
1	1	274	ASN
1	1	315	ASN
1	1	325	GLN
1	1	553	ASN
1	1	581	HIS
1	1	607	ASN
1	2	33	ASN
1	2	93	GLN
1	2	105	ASN
1	2	122	GLN
1	2	131	GLN
1	2	146	GLN
1	2	168	HIS
1	2	183	GLN
1	2	187	GLN
1	2	267	GLN
1	2	315	ASN
1	2	456	HIS
1	2	553	ASN
1	2	581	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
3	SO4	2	647	-	4,4,4	0.18	0	6,6,6	0.28	0
3	SO4	1	648	-	4,4,4	0.19	0	6,6,6	0.26	0
3	SO4	2	649	-	4,4,4	0.20	0	6,6,6	0.23	0
3	SO4	2	648	-	4,4,4	0.27	0	6,6,6	0.29	0
3	SO4	1	646	-	4,4,4	0.14	0	6,6,6	0.24	0
3	SO4	1	649	-	4,4,4	0.19	0	6,6,6	0.27	0
3	SO4	2	646	-	4,4,4	0.10	0	6,6,6	0.17	0
3	SO4	1	647	-	4,4,4	0.19	0	6,6,6	0.32	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2	649	SO4	1	0
3	2	648	SO4	1	0
3	1	649	SO4	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	1	644/644 (100%)	-0.44	2 (0%)	94	93	11, 37, 61, 102	0
1	2	644/644 (100%)	-0.40	7 (1%)	80	79	13, 37, 61, 110	0
All	All	1288/1288 (100%)	-0.42	9 (0%)	87	87	11, 37, 61, 110	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	182	SER	5.4
1	2	183	GLN	4.5
1	2	184	GLY	3.9
1	1	183	GLN	2.6
1	2	181	GLN	2.3
1	2	204	SER	2.2
1	2	129	GLY	2.2
1	2	65	GLN	2.1
1	1	184	GLY	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 monosaccharides 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, 95th 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^2)	Q<0.9
3	SO4	1	648	5/5	0.73	0.41	109,112,114,116	0
3	SO4	2	647	5/5	0.83	0.38	101,104,106,108	0
3	SO4	2	646	5/5	0.87	0.30	118,120,122,124	0
3	SO4	2	648	5/5	0.88	0.26	77,78,88,89	0
3	SO4	1	646	5/5	0.90	0.23	104,104,106,106	0
3	SO4	1	647	5/5	0.92	0.28	84,85,88,89	0
3	SO4	1	649	5/5	0.95	0.32	87,88,92,92	0
3	SO4	2	649	5/5	0.95	0.33	88,95,96,97	0
2	ZN	1	645	1/1	0.98	0.06	25,25,25,25	0
2	ZN	2	645	1/1	0.98	0.05	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.