



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:02 PM UTC

PDB ID : 5FP2 / pdb\_00005fp2  
Title : Crystal structure of the siderophore receptor PirA from *Pseudomonas aeruginosa*  
Authors : Moynie, L.; Tortajada, A.; Naismith, J.H.  
Deposited on : 2015-11-27  
Resolution : 2.97 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

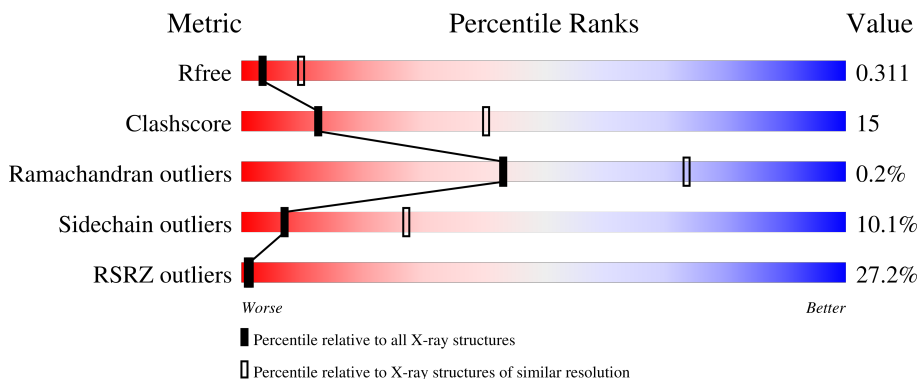
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.97 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	725	
1	B	725	
2	X	10	
2	Z	10	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8201 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 FERRIC ENTEROBACTIN RECEPTOR PIRA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	499	Total	C	N	O	S	0	0	0
			3908	2454	686	760	8			
1	B	538	Total	C	N	O	S	0	0	0
			4180	2611	740	818	11			

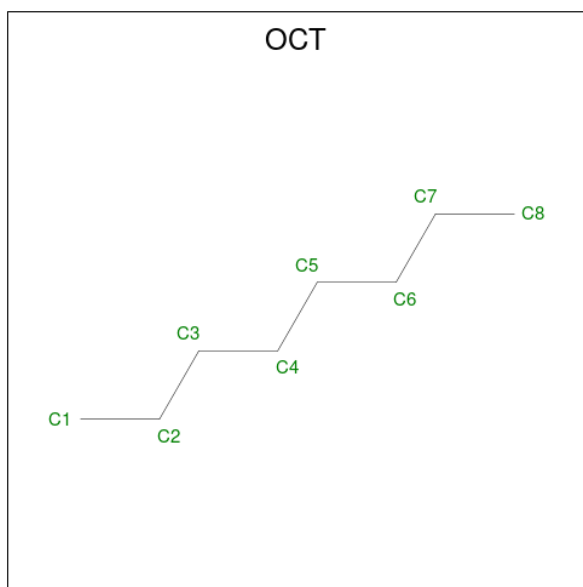
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q9I527
A	-1	ASP	-	expression tag	UNP Q9I527
A	0	ILE	-	expression tag	UNP Q9I527
A	715	LEU	-	expression tag	UNP Q9I527
A	716	SER	-	expression tag	UNP Q9I527
A	717	HIS	-	expression tag	UNP Q9I527
A	718	HIS	-	expression tag	UNP Q9I527
A	719	HIS	-	expression tag	UNP Q9I527
A	720	HIS	-	expression tag	UNP Q9I527
A	721	HIS	-	expression tag	UNP Q9I527
A	722	HIS	-	expression tag	UNP Q9I527
B	-2	MET	-	expression tag	UNP Q9I527
B	-1	ASP	-	expression tag	UNP Q9I527
B	0	ILE	-	expression tag	UNP Q9I527
B	715	LEU	-	expression tag	UNP Q9I527
B	716	SER	-	expression tag	UNP Q9I527
B	717	HIS	-	expression tag	UNP Q9I527
B	718	HIS	-	expression tag	UNP Q9I527
B	719	HIS	-	expression tag	UNP Q9I527
B	720	HIS	-	expression tag	UNP Q9I527
B	721	HIS	-	expression tag	UNP Q9I527
B	722	HIS	-	expression tag	UNP Q9I527

- Molecule 2 is a protein called FERRIC ENTEROBACTIN RECEPTOR PIRA.

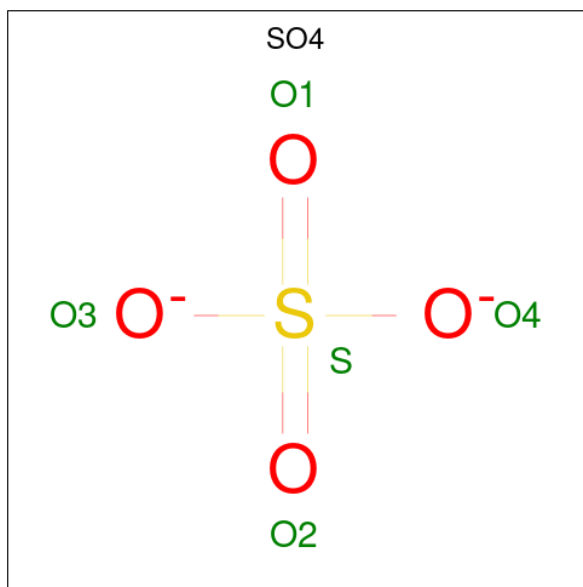
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
2	X	7	Total	C	N	O	0	0	0
			33	19	7	7			
2	Z	10	Total	C	N	O	0	0	0
			46	26	10	10			

- Molecule 3 is N-OCTANE (CCD ID: OCT) (formula: C<sub>8</sub>H<sub>18</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			8	8		
3	B	1	Total	C	0	0
			8	8		
3	B	1	Total	C	0	0
			8	8		

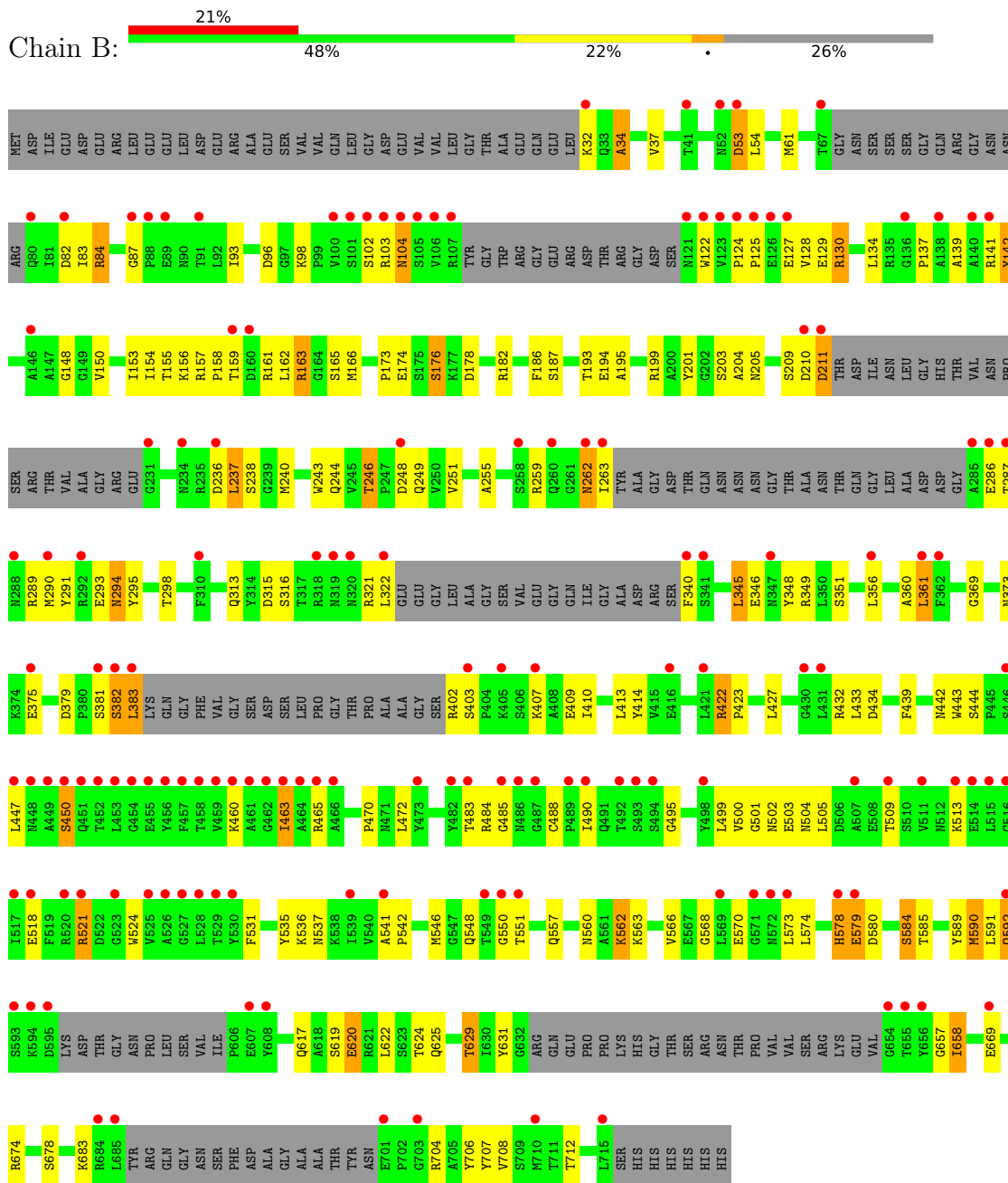
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



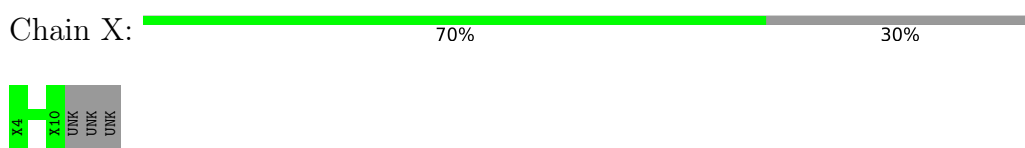
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		



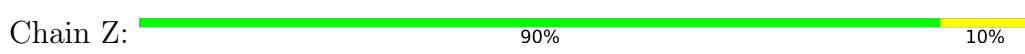
● Molecule 1: FERRIC ENTEROBACTIN RECEPTOR PIRA

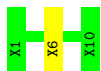


● Molecule 2: FERRIC ENTEROBACTIN RECEPTOR PIRA



● Molecule 2: FERRIC ENTEROBACTIN RECEPTOR PIRA





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.12Å 95.28Å 131.83Å 90.00° 127.52° 90.00°	Depositor
Resolution (Å)	52.49 – 2.97 52.49 – 2.97	Depositor EDS
% Data completeness (in resolution range)	98.8 (52.49-2.97) 98.8 (52.49-2.97)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.96Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.263 , 0.319 0.262 , 0.311	Depositor DCC
$R_{free}$ test set	1756 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.4	Xtrriage
Anisotropy	0.515	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 96.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8201	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: OCT, 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	0.54	0/3982	0.81	4/5394 (0.1%)
1	B	0.61	0/4257	0.88	9/5767 (0.2%)
All	All	0.58	0/8239	0.85	13/11161 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	34	ALA	CA-C-N	-8.82	110.64	119.90
1	B	34	ALA	C-N-CA	-8.82	110.64	119.90
1	A	34	ALA	CA-C-N	-6.37	112.40	120.23
1	A	34	ALA	C-N-CA	-6.37	112.40	120.23
1	B	87	GLY	CA-C-N	6.00	125.39	118.85
1	B	87	GLY	C-N-CA	6.00	125.39	118.85
1	B	128	VAL	CB-CA-C	-5.57	104.00	110.91
1	B	141	ARG	N-CA-C	5.34	118.89	112.38
1	B	246	THR	CA-C-N	-5.26	114.40	119.87
1	B	246	THR	C-N-CA	-5.26	114.40	119.87
1	B	153	ILE	N-CA-C	5.23	115.62	107.99
1	A	87	GLY	CA-C-N	5.14	124.45	118.85

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	GLY	C-N-CA	5.14	124.45	118.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	530	TYR	Sidechain
1	B	142	TYR	Sidechain

## 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	A	3908	0	3813	97	0
1	B	4180	0	4077	154	0
2	X	33	0	8	0	0
2	Z	46	0	9	1	0
3	A	8	0	18	0	0
3	B	16	0	36	0	0
4	B	10	0	0	0	0
All	All	8201	0	7961	246	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 15.

All (246) 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:A:295:TYR:OH	1:B:193:THR:HG21	1.48	1.11
1:A:193:THR:HG21	1:B:295:TYR:OH	1.57	1.02
1:B:246:THR:HG22	1:B:249:GLN:HB2	1.41	1.01
1:B:484:ARG:NH1	1:B:495:GLY:O	2.11	0.83
1:B:433:LEU:CD2	1:B:443:TRP:CD1	2.65	0.80
1:A:177:LYS:O	1:A:210:ASP:HB2	1.81	0.79
1:B:536:LYS:HE2	1:B:563:LYS:HE2	1.65	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:SER:O	1:B:383:LEU:HB3	1.84	0.76
1:B:537:ASN:HB3	1:B:560:ASN:ND2	2.00	0.76
1:B:104:ASN:ND2	1:B:472:LEU:HG	2.02	0.75
1:B:84:ARG:HG2	1:B:531:PHE:CD2	2.23	0.74
1:B:246:THR:HG22	1:B:249:GLN:CB	2.17	0.74
1:A:100:VAL:O	1:A:292:ARG:NH1	2.21	0.74
1:A:159:THR:HG23	1:A:161:ARG:O	1.88	0.74
1:A:470:PRO:HG3	1:A:539:ILE:HD11	1.69	0.73
1:B:102:SER:O	1:B:103:ARG:HG2	1.91	0.70
1:B:548:GLN:O	1:B:548:GLN:HG3	1.91	0.70
1:B:158:PRO:HD3	1:B:240:MET:CE	2.22	0.70
1:B:537:ASN:HB3	1:B:560:ASN:HD22	1.57	0.69
1:B:360:ALA:O	1:B:361:LEU:HB2	1.91	0.69
1:A:456:TYR:CE1	1:A:521:ARG:HD2	2.28	0.69
1:B:409:GLU:C	1:B:410:ILE:HD12	2.18	0.69
1:B:104:ASN:N	1:B:104:ASN:OD1	2.24	0.68
1:B:37:VAL:HG23	1:B:134:LEU:HD12	1.76	0.68
1:B:176:SER:O	1:B:178:ASP:O	2.11	0.68
1:B:433:LEU:CD2	1:B:443:TRP:NE1	2.57	0.68
1:B:246:THR:HG23	1:B:248:ASP:H	1.58	0.67
1:A:532:ARG:HG3	1:A:567:GLU:HG3	1.75	0.67
1:B:427:LEU:HD11	1:B:447:LEU:HD11	1.77	0.66
1:B:484:ARG:NH1	1:B:495:GLY:C	2.53	0.66
1:B:546:MET:HE1	1:B:557:GLN:OE1	1.95	0.66
1:A:470:PRO:HG3	1:A:539:ILE:CD1	2.26	0.66
1:B:373:ASN:HB3	1:B:410:ILE:HB	1.77	0.66
1:A:538:LYS:HG2	1:A:540:VAL:HG13	1.78	0.65
1:A:43:GLU:O	1:A:47:LYS:HG3	1.97	0.65
1:B:186:PHE:CD1	1:B:186:PHE:C	2.73	0.65
1:A:538:LYS:HG2	1:A:540:VAL:CG1	2.27	0.65
1:A:360:ALA:O	1:A:361:LEU:HB2	1.96	0.65
1:B:620:GLU:CD	1:B:620:GLU:H	2.05	0.64
1:B:159:THR:HG23	1:B:161:ARG:O	1.97	0.64
1:A:427:LEU:HD11	1:A:447:LEU:HD11	1.79	0.63
1:A:130:ARG:HH11	1:A:154:ILE:HD12	1.63	0.63
1:B:53:ASP:N	1:B:53:ASP:OD1	2.30	0.63
1:B:536:LYS:CE	1:B:563:LYS:HE2	2.29	0.63
1:A:158:PRO:HD3	1:A:240:MET:CE	2.29	0.63
1:A:291:TYR:CE2	1:A:293:GLU:HG3	2.34	0.62
1:B:102:SER:OG	1:B:345:LEU:HD11	1.99	0.62
1:B:61:MET:HE2	1:B:61:MET:HA	1.81	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:O	1:A:210:ASP:CB	2.47	0.62
1:B:433:LEU:HD23	1:B:443:TRP:CD1	2.35	0.62
1:B:574:LEU:HD12	1:B:584:SER:OG	2.00	0.62
1:B:704:ARG:HD3	1:B:706:TYR:OH	1.99	0.62
1:B:289:ARG:HH11	1:B:289:ARG:HG2	1.65	0.61
1:B:463:ILE:HD12	1:B:513:LYS:HG2	1.80	0.61
1:A:439:PHE:CE2	1:A:470:PRO:HD2	2.36	0.61
1:A:537:ASN:HB3	1:A:560:ASN:ND2	2.15	0.61
1:B:237:LEU:HD23	1:B:238:SER:N	2.16	0.60
1:A:701:GLU:HB2	1:A:702:PRO:HD2	1.82	0.60
1:B:382:SER:O	1:B:383:LEU:CB	2.49	0.60
1:B:625:GLN:OE1	1:B:674:ARG:NH1	2.35	0.60
1:A:61:MET:HA	1:A:61:MET:HE2	1.84	0.60
1:B:439:PHE:CE2	1:B:470:PRO:HD2	2.37	0.59
1:A:46:ARG:HG2	1:A:46:ARG:HH11	1.68	0.59
1:B:500:VAL:HG12	1:B:501:GLY:O	2.02	0.59
1:A:46:ARG:HG2	1:A:46:ARG:NH1	2.18	0.59
1:B:259:ARG:NH1	1:B:289:ARG:NH1	2.50	0.59
1:A:631:TYR:O	1:A:655:THR:HB	2.02	0.58
1:A:373:ASN:HB3	1:A:410:ILE:HB	1.86	0.58
1:B:321:ARG:HG3	1:B:322:LEU:N	2.19	0.57
1:A:237:LEU:HD23	1:A:238:SER:N	2.20	0.57
1:B:360:ALA:O	1:B:361:LEU:CB	2.52	0.57
1:A:500:VAL:HG12	1:A:501:GLY:O	2.03	0.57
1:A:127:GLU:OE1	1:A:187:SER:HB2	2.05	0.57
1:A:165:SER:O	1:A:186:PHE:HA	2.04	0.57
1:B:142:TYR:CD2	1:B:150:VAL:HG21	2.39	0.57
1:B:182:ARG:HH11	1:B:182:ARG:HG2	1.70	0.57
1:B:96:ASP:OD2	1:B:155:THR:OG1	2.18	0.56
1:B:542:PRO:HD3	1:B:557:GLN:O	2.04	0.56
1:A:53:ASP:OD1	1:A:53:ASP:N	2.38	0.56
1:B:657:GLY:O	1:B:658:ILE:HG13	2.05	0.56
1:B:210:ASP:OD1	1:B:210:ASP:O	2.23	0.56
1:A:201:TYR:CD1	1:A:201:TYR:C	2.84	0.55
1:B:573:LEU:HB3	1:B:585:THR:HG22	1.87	0.55
1:B:210:ASP:O	1:B:211:ASP:CB	2.54	0.55
1:A:481:LEU:O	1:A:498:TYR:HA	2.08	0.54
1:B:165:SER:O	1:B:186:PHE:HA	2.07	0.54
1:A:163:ARG:NH2	1:A:715:LEU:HD13	2.22	0.54
1:A:186:PHE:CD1	1:A:186:PHE:C	2.85	0.54
1:B:37:VAL:HG23	1:B:134:LEU:CD1	2.38	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:LEU:HD21	1:B:541:ALA:HB2	1.90	0.54
1:A:163:ARG:HH21	1:A:715:LEU:CD1	2.21	0.54
1:B:246:THR:HG23	1:B:248:ASP:N	2.24	0.53
1:B:174:GLU:OE1	1:B:704:ARG:HD2	2.08	0.53
1:B:484:ARG:NH1	1:B:495:GLY:CA	2.72	0.53
1:B:193:THR:HG22	1:B:195:ALA:H	1.73	0.53
1:B:706:TYR:N	1:B:706:TYR:CD1	2.77	0.53
1:B:137:PRO:C	1:B:139:ALA:H	2.17	0.52
1:A:251:VAL:HA	1:A:298:THR:O	2.09	0.52
1:A:521:ARG:O	1:A:524:TRP:HB2	2.10	0.52
1:A:656:TYR:HE2	1:A:658:ILE:CD1	2.23	0.52
1:A:369:GLY:HA3	1:A:414:TYR:CZ	2.45	0.52
1:A:562:LYS:HD3	1:A:562:LYS:N	2.24	0.52
1:B:182:ARG:HG2	1:B:182:ARG:NH1	2.26	0.51
1:A:659:TRP:O	1:A:680:LEU:HB2	2.10	0.51
1:A:174:GLU:OE1	1:A:704:ARG:HD2	2.09	0.51
1:A:502:ASN:HB3	1:A:505:LEU:HG	1.93	0.51
1:B:201:TYR:CD1	1:B:201:TYR:C	2.89	0.51
1:B:313:GLN:HB3	1:B:349:ARG:HB3	1.93	0.51
1:B:484:ARG:CZ	1:B:495:GLY:HA3	2.40	0.51
1:B:521:ARG:O	1:B:524:TRP:HB2	2.11	0.50
1:B:251:VAL:HA	1:B:298:THR:O	2.12	0.50
1:A:127:GLU:OE1	1:A:187:SER:CB	2.60	0.50
1:A:193:THR:HG23	1:B:293:GLU:CD	2.36	0.50
1:A:535:TYR:HE1	1:A:566:VAL:HG23	1.76	0.50
1:A:46:ARG:HH11	1:A:46:ARG:CG	2.24	0.50
1:B:433:LEU:HD22	1:B:443:TRP:NE1	2.26	0.50
1:B:104:ASN:HD21	1:B:472:LEU:HG	1.75	0.49
1:B:502:ASN:HB3	1:B:505:LEU:HG	1.94	0.49
1:A:573:LEU:HB3	1:A:585:THR:HG22	1.92	0.49
1:B:127:GLU:OE1	1:B:187:SER:HB2	2.12	0.49
1:B:246:THR:HG23	1:B:249:GLN:N	2.27	0.49
1:A:193:THR:HG22	1:A:195:ALA:H	1.77	0.49
1:B:360:ALA:C	1:B:361:LEU:HD12	2.37	0.49
1:A:663:ALA:O	1:A:674:ARG:HG3	2.12	0.49
1:B:433:LEU:HD21	1:B:443:TRP:NE1	2.27	0.48
1:B:54:LEU:HD21	1:B:125:PRO:HA	1.95	0.48
1:A:481:LEU:HB2	1:A:499:LEU:HD12	1.95	0.48
1:B:104:ASN:HD22	1:B:472:LEU:HG	1.78	0.48
1:B:210:ASP:O	1:B:211:ASP:HB2	2.13	0.48
1:B:503:GLU:HG3	1:B:504:ASN:OD1	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:HG2	1:B:423:PRO:HD2	1.94	0.48
1:A:175:SER:OG	1:A:177:LYS:HB3	2.13	0.48
1:B:450:SER:HB2	1:B:460:LYS:HG3	1.95	0.48
1:B:550:GLY:C	1:B:551:THR:HG23	2.39	0.48
1:A:124:PRO:HG3	1:A:203:SER:HB3	1.95	0.48
1:A:684:ARG:O	1:A:685:LEU:C	2.57	0.47
1:A:255:ALA:HA	1:A:294:ASN:O	2.14	0.47
1:B:535:TYR:HE2	1:B:566:VAL:HG23	1.78	0.47
1:B:483:THR:HG22	1:B:484:ARG:N	2.29	0.47
1:B:237:LEU:HD23	1:B:238:SER:H	1.79	0.47
1:B:287:THR:O	1:B:321:ARG:HA	2.14	0.47
1:B:369:GLY:HA3	1:B:414:TYR:CZ	2.50	0.47
1:A:236:ASP:C	1:A:236:ASP:OD1	2.59	0.47
1:B:102:SER:OG	1:B:345:LEU:CD1	2.62	0.47
1:A:664:GLY:HA3	1:A:674:ARG:HH11	1.79	0.46
1:B:34:ALA:HB3	1:B:37:VAL:CG1	2.45	0.46
1:B:82:ASP:OD1	1:B:82:ASP:C	2.57	0.46
1:A:193:THR:HG22	1:A:194:GLU:N	2.30	0.46
1:B:157:ARG:O	1:B:158:PRO:C	2.55	0.46
1:B:124:PRO:HG3	1:B:203:SER:HB3	1.98	0.46
1:B:255:ALA:HA	1:B:294:ASN:O	2.15	0.46
1:A:178:ASP:HA	1:A:210:ASP:HB3	1.98	0.46
1:A:193:THR:HG21	1:B:295:TYR:CZ	2.46	0.46
1:B:590:MET:HB2	1:B:592:GLN:OE1	2.16	0.46
1:A:482:TYR:HB3	1:A:498:TYR:HD1	1.81	0.46
1:B:289:ARG:HG2	1:B:289:ARG:NH1	2.28	0.45
1:B:360:ALA:C	1:B:361:LEU:CD1	2.89	0.45
1:B:409:GLU:O	1:B:410:ILE:HD12	2.15	0.45
1:A:173:PRO:CB	1:A:178:ASP:HB3	2.47	0.45
1:B:84:ARG:HD2	1:B:570:GLU:OE2	2.16	0.45
1:B:414:TYR:HB3	1:B:432:ARG:HG3	1.98	0.45
1:A:88:PRO:C	1:A:90:ASN:H	2.24	0.45
1:B:162:LEU:HG	1:B:163:ARG:N	2.30	0.45
1:B:130:ARG:HG2	1:B:154:ILE:HB	1.99	0.45
1:A:130:ARG:NH1	1:A:154:ILE:HD12	2.31	0.45
1:B:379:ASP:OD1	1:B:381:SER:N	2.50	0.45
1:B:536:LYS:HG2	1:B:563:LYS:HG2	1.99	0.45
1:B:360:ALA:HB1	1:B:361:LEU:HD12	1.98	0.45
1:B:484:ARG:HH11	1:B:485:GLY:H	1.64	0.45
1:A:499:LEU:HD12	1:A:499:LEU:O	2.16	0.44
1:B:173:PRO:CB	1:B:178:ASP:HB3	2.46	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ASP:OD1	1:B:236:ASP:O	2.35	0.44
1:A:233:ARG:HH21	1:A:262:ASN:C	2.25	0.44
1:B:289:ARG:HH12	1:B:291:TYR:HB2	1.82	0.44
1:B:158:PRO:CD	1:B:240:MET:HE3	2.47	0.44
1:B:236:ASP:OD1	1:B:236:ASP:C	2.61	0.44
1:B:173:PRO:HB3	1:B:178:ASP:HB3	2.00	0.44
1:B:137:PRO:C	1:B:139:ALA:N	2.75	0.44
1:A:47:LYS:O	1:A:674:ARG:NE	2.51	0.44
1:A:54:LEU:HD21	1:A:125:PRO:HA	1.99	0.44
1:A:127:GLU:O	1:A:156:LYS:HG3	2.18	0.44
1:B:127:GLU:OE1	1:B:187:SER:CB	2.65	0.44
1:B:488:CYS:HB3	1:B:490:ILE:O	2.18	0.44
1:B:243:TRP:C	1:B:243:TRP:CD1	2.95	0.43
1:A:580:ASP:OD1	1:A:580:ASP:N	2.50	0.43
1:A:707:TYR:CD1	1:A:707:TYR:C	2.95	0.43
1:B:262:ASN:O	1:B:262:ASN:ND2	2.49	0.43
1:B:568:GLY:CA	1:B:589:TYR:O	2.66	0.43
1:B:432:ARG:NE	1:B:434:ASP:OD2	2.36	0.43
1:A:608:TYR:CE2	1:A:610:LEU:HD12	2.52	0.43
1:B:61:MET:HE2	1:B:61:MET:CA	2.49	0.43
1:B:158:PRO:CD	1:B:240:MET:CE	2.94	0.43
1:B:321:ARG:O	1:B:340:PHE:HA	2.18	0.43
1:A:166:MET:HE2	1:A:166:MET:HB3	1.86	0.43
1:B:156:LYS:O	1:B:199:ARG:HD3	2.18	0.43
1:B:484:ARG:NH1	1:B:495:GLY:HA3	2.33	0.43
1:A:568:GLY:CA	1:A:589:TYR:O	2.67	0.43
1:B:83:ILE:HG21	1:B:148:GLY:O	2.19	0.43
1:B:315:ASP:O	1:B:346:GLU:HA	2.19	0.43
1:A:460:LYS:HG3	1:A:461:ALA:N	2.33	0.42
1:B:348:TYR:CD1	1:B:348:TYR:N	2.86	0.42
1:A:579:GLU:OE1	1:A:579:GLU:HA	2.18	0.42
1:A:664:GLY:HA3	1:A:674:ARG:NH1	2.33	0.42
1:B:707:TYR:C	1:B:707:TYR:CD1	2.97	0.42
1:A:61:MET:HE2	1:A:61:MET:CA	2.49	0.42
1:A:619:SER:OG	1:A:622:LEU:N	2.47	0.42
1:B:83:ILE:CG2	1:B:148:GLY:O	2.68	0.42
1:B:127:GLU:O	1:B:156:LYS:HG3	2.19	0.42
1:B:704:ARG:HD3	1:B:706:TYR:CZ	2.54	0.42
1:A:293:GLU:CD	1:B:193:THR:HG23	2.44	0.42
1:B:433:LEU:HD21	1:B:443:TRP:CD1	2.51	0.42
1:B:562:LYS:HG2	1:B:563:LYS:N	2.32	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:NH1	1:A:46:ARG:CG	2.83	0.42
1:A:656:TYR:CE2	1:A:701:GLU:OE2	2.73	0.42
1:B:134:LEU:HD21	2:Z:6:UNK:CB	2.50	0.42
1:B:137:PRO:O	1:B:139:ALA:N	2.52	0.42
1:B:433:LEU:HD21	1:B:443:TRP:HE1	1.83	0.42
1:B:589:TYR:CD1	1:B:589:TYR:C	2.97	0.42
1:A:670:ASN:O	1:A:712:THR:HA	2.19	0.41
1:A:173:PRO:HB3	1:A:178:ASP:HB3	2.02	0.41
1:A:246:THR:HG22	1:A:247:PRO:N	2.35	0.41
1:A:156:LYS:O	1:A:199:ARG:HD3	2.20	0.41
1:A:656:TYR:CE2	1:A:658:ILE:CD1	3.02	0.41
1:A:680:LEU:HA	1:A:680:LEU:HD23	1.88	0.41
1:B:166:MET:HE2	1:B:166:MET:HB3	1.85	0.41
1:B:619:SER:OG	1:B:622:LEU:N	2.43	0.41
1:B:620:GLU:CD	1:B:620:GLU:N	2.77	0.41
1:B:678:SER:O	1:B:704:ARG:HA	2.20	0.41
1:B:578:HIS:O	1:B:579:GLU:C	2.63	0.41
1:A:415:VAL:O	1:A:430:GLY:HA2	2.21	0.41
1:A:537:ASN:HB3	1:A:560:ASN:HD22	1.81	0.41
1:A:679:ASN:O	1:A:680:LEU:C	2.64	0.41
1:B:93:ILE:HD13	1:B:122:TRP:CZ3	2.55	0.41
1:B:536:LYS:HE2	1:B:563:LYS:CE	2.43	0.41
1:B:542:PRO:CD	1:B:557:GLN:O	2.67	0.40
1:B:629:THR:CG2	1:B:631:TYR:CE2	3.04	0.40
1:A:678:SER:O	1:A:704:ARG:HA	2.21	0.40
1:B:84:ARG:HG2	1:B:531:PHE:CE2	2.55	0.40
1:B:159:THR:HG21	1:B:163:ARG:HD2	2.02	0.40
1:B:204:ALA:C	1:B:205:ASN:OD1	2.65	0.40
1:A:669:GLU:H	1:A:669:GLU:HG3	1.65	0.40
1:B:580:ASP:HB3	1:B:617:GLN:O	2.21	0.40
1:A:100:VAL:O	1:A:100:VAL:HG12	2.20	0.40
1:A:157:ARG:O	1:A:158:PRO:C	2.62	0.40
1:A:318:ARG:HG3	1:A:318:ARG:HH11	1.86	0.40
1:B:379:ASP:OD1	1:B:379:ASP:C	2.64	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	475/725 (66%)	455 (96%)	19 (4%)	1 (0%)	43	73
1	B	518/725 (71%)	493 (95%)	24 (5%)	1 (0%)	43	73
All	All	993/1450 (68%)	948 (96%)	43 (4%)	2 (0%)	43	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ARG
1	B	361	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	424/604 (70%)	389 (92%)	35 (8%)	10	35
1	B	454/604 (75%)	400 (88%)	54 (12%)	5	20
All	All	878/1208 (73%)	789 (90%)	89 (10%)	7	27

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	46	ARG
1	A	47	LYS
1	A	209	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	235	ARG
1	A	244	GLN
1	A	290	MET
1	A	294	ASN
1	A	304	SER
1	A	316	SER
1	A	356	LEU
1	A	363	GLU
1	A	373	ASN
1	A	375	GLU
1	A	422	ARG
1	A	442	ASN
1	A	444	SER
1	A	450	SER
1	A	460	LYS
1	A	480	LEU
1	A	509	THR
1	A	518	GLU
1	A	569	LEU
1	A	579	GLU
1	A	580	ASP
1	A	584	SER
1	A	590	MET
1	A	591	LEU
1	A	592	GLN
1	A	610	LEU
1	A	624	THR
1	A	655	THR
1	A	658	ILE
1	A	669	GLU
1	A	715	LEU
1	B	32	LYS
1	B	53	ASP
1	B	84	ARG
1	B	98	LYS
1	B	104	ASN
1	B	129	GLU
1	B	130	ARG
1	B	163	ARG
1	B	176	SER
1	B	194	GLU
1	B	209	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	211	ASP
1	B	237	LEU
1	B	244	GLN
1	B	262	ASN
1	B	263	ILE
1	B	286	GLU
1	B	290	MET
1	B	294	ASN
1	B	316	SER
1	B	345	LEU
1	B	351	SER
1	B	356	LEU
1	B	375	GLU
1	B	382	SER
1	B	383	LEU
1	B	402	ARG
1	B	403	SER
1	B	407	LYS
1	B	413	LEU
1	B	422	ARG
1	B	442	ASN
1	B	444	SER
1	B	450	SER
1	B	463	ILE
1	B	465	ARG
1	B	509	THR
1	B	518	GLU
1	B	521	ARG
1	B	562	LYS
1	B	578	HIS
1	B	579	GLU
1	B	584	SER
1	B	590	MET
1	B	591	LEU
1	B	592	GLN
1	B	620	GLU
1	B	624	THR
1	B	629	THR
1	B	658	ILE
1	B	669	GLU
1	B	683	LYS
1	B	708	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	712	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	244	GLN
1	A	249	GLN
1	A	260	GLN
1	A	313	GLN
1	B	249	GLN

### 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](#)

5 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	$\# Z  > 2$
4	SO4	B	1716	-	4,4,4	0.35	0	6,6,6	0.25	0
3	OCT	A	801	-	7,7,7	0.23	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OCT	B	801	-	7,7,7	0.23	0	6,6,6	0.41	0
4	SO4	B	1717	-	4,4,4	0.42	0	6,6,6	0.14	0
3	OCT	B	802	-	7,7,7	0.21	0	6,6,6	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OCT	A	801	-	-	0/5/5/5	-
3	OCT	B	801	-	-	1/5/5/5	-
3	OCT	B	802	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	OCT	C4-C5-C6-C7
3	B	802	OCT	C4-C5-C6-C7

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	499/725 (68%)	1.51	133 (26%) <b>1</b> <b>1</b>	101, 126, 164, 197	0
1	B	538/725 (74%)	1.59	149 (27%) <b>1</b> <b>1</b>	103, 124, 159, 191	0
2	X	0/10	-	-	-	-
2	Z	0/10	-	-	-	-
All	All	1037/1470 (70%)	1.55	282 (27%) <b>1</b> <b>1</b>	101, 125, 161, 197	0

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	ARG	6.1
1	A	715	LEU	5.9
1	B	322	LEU	5.8
1	B	102	SER	5.8
1	B	452	THR	5.4
1	B	449	ALA	5.4
1	B	715	LEU	5.4
1	A	34	ALA	5.3
1	B	340	PHE	5.2
1	B	655	THR	5.1
1	A	80	GLN	5.0
1	B	122	TRP	5.0
1	A	288	ASN	4.8
1	B	447	LEU	4.8
1	B	210	ASP	4.8
1	B	526	ALA	4.7
1	A	361	LEU	4.6
1	B	701	GLU	4.6
1	B	105	SER	4.6
1	B	107	ARG	4.5
1	B	448	ASN	4.5
1	A	454	GLY	4.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	123	VAL	4.5
1	A	211	ASP	4.4
1	A	231	GLY	4.4
1	B	541	ALA	4.3
1	A	67	THR	4.3
1	A	685	LEU	4.3
1	A	423	PRO	4.3
1	B	656	TYR	4.2
1	B	460	LYS	4.2
1	B	453	LEU	4.1
1	B	525	VAL	4.1
1	A	232	VAL	4.1
1	A	101	SER	4.1
1	A	32	LYS	4.1
1	B	106	VAL	4.1
1	B	450	SER	4.0
1	A	319	ASN	4.0
1	A	127	GLU	4.0
1	B	446	SER	4.0
1	B	260	GLN	4.0
1	B	125	PRO	4.0
1	A	140	ALA	3.9
1	B	341	SER	3.9
1	B	160	ASP	3.9
1	B	461	ALA	3.8
1	B	594	LYS	3.8
1	A	234	ASN	3.8
1	B	231	GLY	3.8
1	B	459	VAL	3.8
1	B	375	GLU	3.7
1	B	263	ILE	3.7
1	B	451	GLN	3.7
1	A	52	ASN	3.7
1	B	685	LEU	3.7
1	A	455	GLU	3.7
1	B	53	ASP	3.7
1	B	290	MET	3.7
1	B	457	PHE	3.7
1	A	382	SER	3.7
1	B	489	PRO	3.7
1	A	482	TYR	3.7
1	A	287	THR	3.6

*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	322	LEU	3.6
1	B	138	ALA	3.6
1	A	305	PHE	3.6
1	B	126	GLU	3.6
1	A	615	ASP	3.6
1	B	517	ILE	3.6
1	A	404	PRO	3.6
1	A	606	PRO	3.6
1	B	516	GLY	3.5
1	A	498	TYR	3.5
1	A	318	ARG	3.5
1	B	121	ASN	3.5
1	A	33	GLN	3.5
1	B	140	ALA	3.5
1	B	464	ALA	3.5
1	B	490	ILE	3.5
1	B	462	GLY	3.5
1	B	487	GLY	3.5
1	B	515	LEU	3.5
1	B	319	ASN	3.5
1	A	122	TRP	3.4
1	B	287	THR	3.4
1	B	486	ASN	3.4
1	A	453	LEU	3.4
1	B	511	VAL	3.4
1	B	127	GLU	3.4
1	A	260	GLN	3.4
1	A	626	LEU	3.3
1	B	383	LEU	3.3
1	A	378	ASN	3.3
1	B	104	ASN	3.3
1	B	124	PRO	3.3
1	A	261	GLY	3.2
1	B	407	LYS	3.2
1	B	463	ILE	3.2
1	B	518	GLU	3.2
1	B	87	GLY	3.2
1	B	551	THR	3.2
1	A	302	THR	3.1
1	A	555	ILE	3.1
1	A	342	ALA	3.1
1	B	361	LEU	3.1

*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	457	PHE	3.1
1	A	289	ARG	3.0
1	B	458	THR	3.0
1	A	53	ASP	3.0
1	B	262	ASN	3.0
1	A	439	PHE	3.0
1	B	654	GLY	3.0
1	A	320	ASN	3.0
1	B	288	ASN	3.0
1	B	593	SER	3.0
1	B	527	GLY	2.9
1	B	482	TYR	2.9
1	A	290	MET	2.9
1	B	32	LYS	2.9
1	A	418	ASN	2.9
1	A	714	PHE	2.9
1	A	542	PRO	2.9
1	A	362	PHE	2.8
1	A	452	THR	2.8
1	A	480	LEU	2.8
1	A	121	ASN	2.8
1	A	441	LEU	2.8
1	B	211	ASP	2.8
1	B	101	SER	2.8
1	B	571	GLY	2.8
1	B	669	GLU	2.8
1	A	456	TYR	2.8
1	B	285	ALA	2.8
1	B	529	THR	2.8
1	B	595	ASP	2.8
1	A	593	SER	2.8
1	B	455	GLU	2.7
1	A	433	LEU	2.7
1	B	320	ASN	2.7
1	A	655	THR	2.7
1	B	80	GLN	2.7
1	B	421	LEU	2.7
1	A	359	HIS	2.7
1	A	445	PRO	2.7
1	B	318	ARG	2.7
1	A	473	TYR	2.6
1	A	246	THR	2.6

*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	317	THR	2.6
1	B	507	ALA	2.6
1	B	578	HIS	2.6
1	A	292	ARG	2.6
1	B	454	GLY	2.6
1	A	467	PHE	2.6
1	A	343	SER	2.6
1	B	258	SER	2.6
1	A	206	LYS	2.6
1	B	473	TYR	2.6
1	A	499	LEU	2.6
1	A	168	VAL	2.6
1	B	465	ARG	2.5
1	A	100	VAL	2.5
1	A	426	MET	2.5
1	B	89	GLU	2.5
1	B	483	THR	2.5
1	B	236	ASP	2.5
1	A	87	GLY	2.5
1	B	286	GLU	2.5
1	B	362	PHE	2.5
1	B	521	ARG	2.5
1	A	500	VAL	2.5
1	B	456	TYR	2.5
1	A	358	LEU	2.5
1	B	485	GLY	2.5
1	B	494	SER	2.5
1	B	100	VAL	2.5
1	A	592	GLN	2.5
1	B	141	ARG	2.5
1	B	67	THR	2.5
1	A	654	GLY	2.4
1	B	684	ARG	2.4
1	A	478	ASN	2.4
1	B	248	ASP	2.4
1	A	403	SER	2.4
1	A	562	LYS	2.4
1	B	579	GLU	2.4
1	B	492	THR	2.4
1	B	514	GLU	2.4
1	A	138	ALA	2.4
1	B	592	GLN	2.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	549	THR	2.4
1	A	427	LEU	2.4
1	A	591	LEU	2.4
1	B	234	ASN	2.4
1	A	440	GLY	2.4
1	A	160	ASP	2.4
1	B	607	GLU	2.4
1	A	381	SER	2.4
1	A	376	THR	2.4
1	A	589	TYR	2.4
1	B	530	TYR	2.4
1	A	405	LYS	2.3
1	A	254	GLU	2.3
1	A	624	THR	2.3
1	B	382	SER	2.3
1	A	177	LYS	2.3
1	A	310	PHE	2.3
1	B	539	ILE	2.3
1	A	520	ARG	2.3
1	A	608	TYR	2.3
1	B	292	ARG	2.3
1	A	459	VAL	2.3
1	B	136	GLY	2.3
1	A	354	LEU	2.3
1	A	580	ASP	2.3
1	B	573	LEU	2.3
1	B	513	LYS	2.3
1	A	584	SER	2.3
1	B	159	THR	2.3
1	B	88	PRO	2.3
1	B	310	PHE	2.2
1	B	572	ASN	2.2
1	A	44	ASP	2.2
1	B	430	GLY	2.2
1	A	447	LEU	2.2
1	A	556	LEU	2.2
1	A	463	ILE	2.2
1	A	625	GLN	2.2
1	A	157	ARG	2.2
1	A	303	TRP	2.2
1	B	493	SER	2.2
1	A	344	LYS	2.2

*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	360	ALA	2.2
1	A	443	TRP	2.2
1	A	407	LYS	2.2
1	A	656	TYR	2.2
1	A	421	LEU	2.2
1	A	431	LEU	2.2
1	A	668	SER	2.2
1	B	381	SER	2.2
1	B	431	LEU	2.2
1	B	466	ALA	2.2
1	A	46	ARG	2.1
1	B	520	ARG	2.1
1	A	313	GLN	2.1
1	A	554	ASN	2.1
1	A	578	HIS	2.1
1	A	438	ASP	2.1
1	B	523	GLY	2.1
1	A	146	ALA	2.1
1	B	146	ALA	2.1
1	A	247	PRO	2.1
1	B	41	THR	2.1
1	B	528	LEU	2.1
1	A	466	ALA	2.1
1	A	705	ALA	2.1
1	A	460	LYS	2.1
1	B	347	ASN	2.1
1	B	405	LYS	2.1
1	B	356	LEU	2.1
1	A	159	THR	2.1
1	B	509	THR	2.1
1	A	701	GLU	2.1
1	B	608	TYR	2.1
1	B	403	SER	2.1
1	A	37	VAL	2.1
1	B	550	GLY	2.1
1	A	182	ARG	2.1
1	B	91	THR	2.1
1	B	569	LEU	2.0
1	A	79	ARG	2.0
1	A	253	PHE	2.0
1	A	465	ARG	2.0
1	B	703	GLY	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	82	ASP	2.0
1	A	129	GLU	2.0
1	A	437	SER	2.0
1	B	52	ASN	2.0
1	A	139	ALA	2.0
1	B	416	GLU	2.0
1	B	710	MET	2.0
1	B	498	TYR	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
4	SO4	B	1716	5/5	0.72	0.28	160,160,160,160	0
4	SO4	B	1717	5/5	0.74	0.18	160,160,160,160	0
3	OCT	A	801	8/8	0.83	0.42	160,160,160,160	0
3	OCT	B	801	8/8	0.86	0.36	160,160,160,160	0
3	OCT	B	802	8/8	0.87	0.42	160,160,160,160	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.