Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 11:06 PM GMT

PDB ID	:	5FP2
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

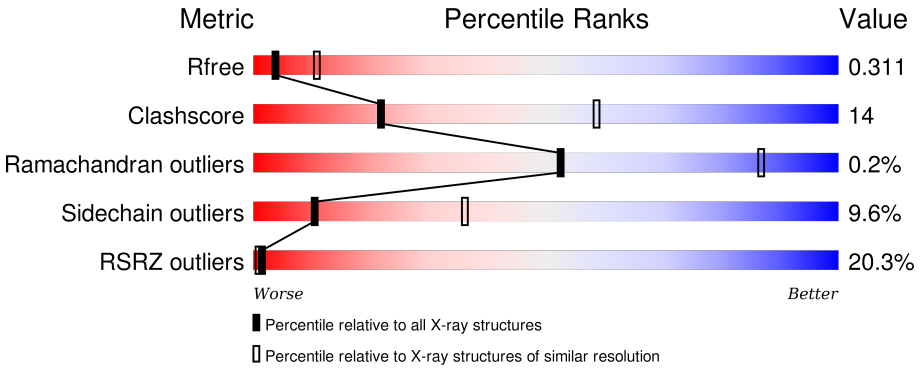
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 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}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	14% 50% 18% • 31%
1	B	725	15% 50% 21% • 26%
2	X	10	70% 30%
2	Z	10	90% 10%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OCT	B	801	-	-	-	X
3	OCT	B	802	-	-	-	X
4	SO4	B	1716	-	-	-	X

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
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			

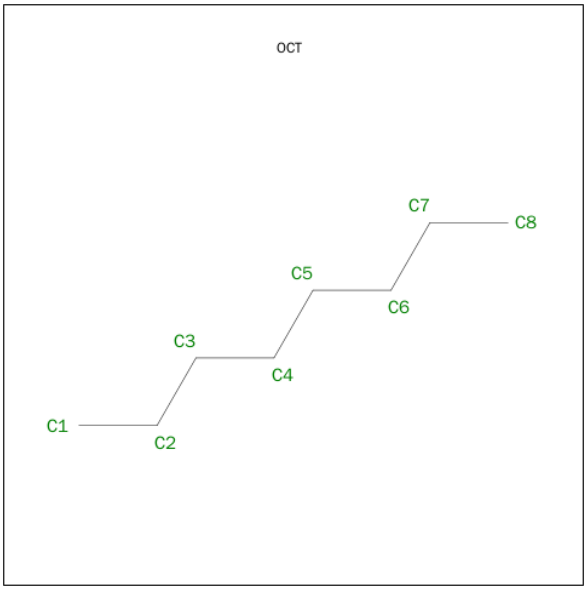
There are 22 discrepancies between the modelled and reference sequences:

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.

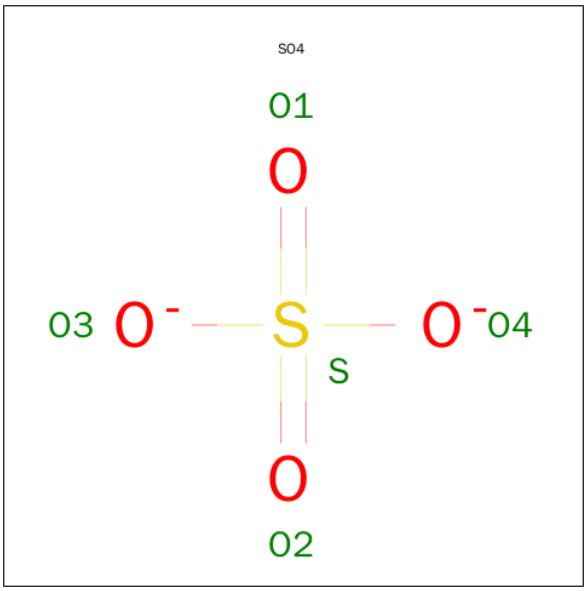
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	X	7	Total C N O 33 19 7 7	0	0	0
2	Z	10	Total C N O 46 26 10 10	0	0	0

- Molecule 3 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



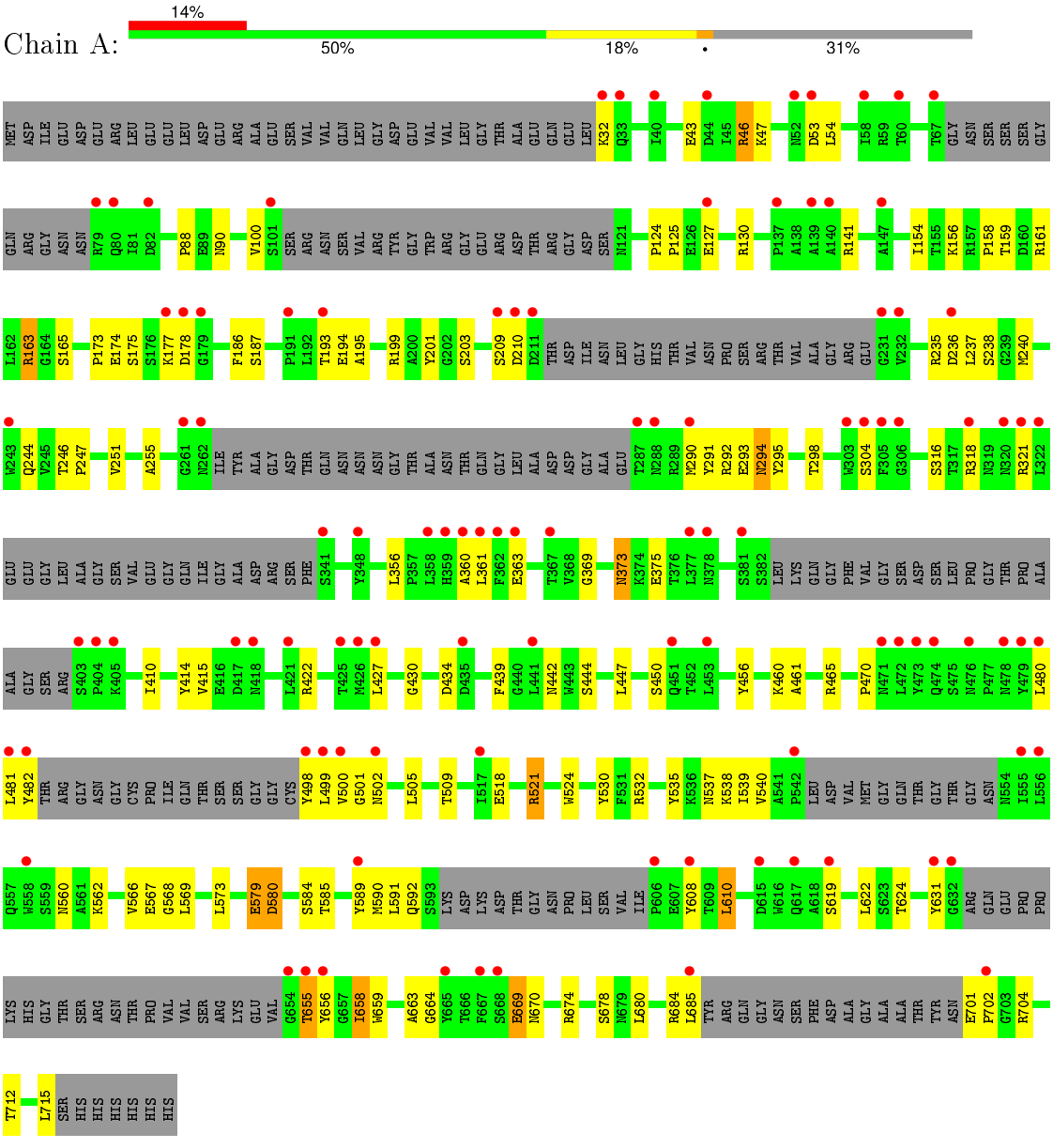
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

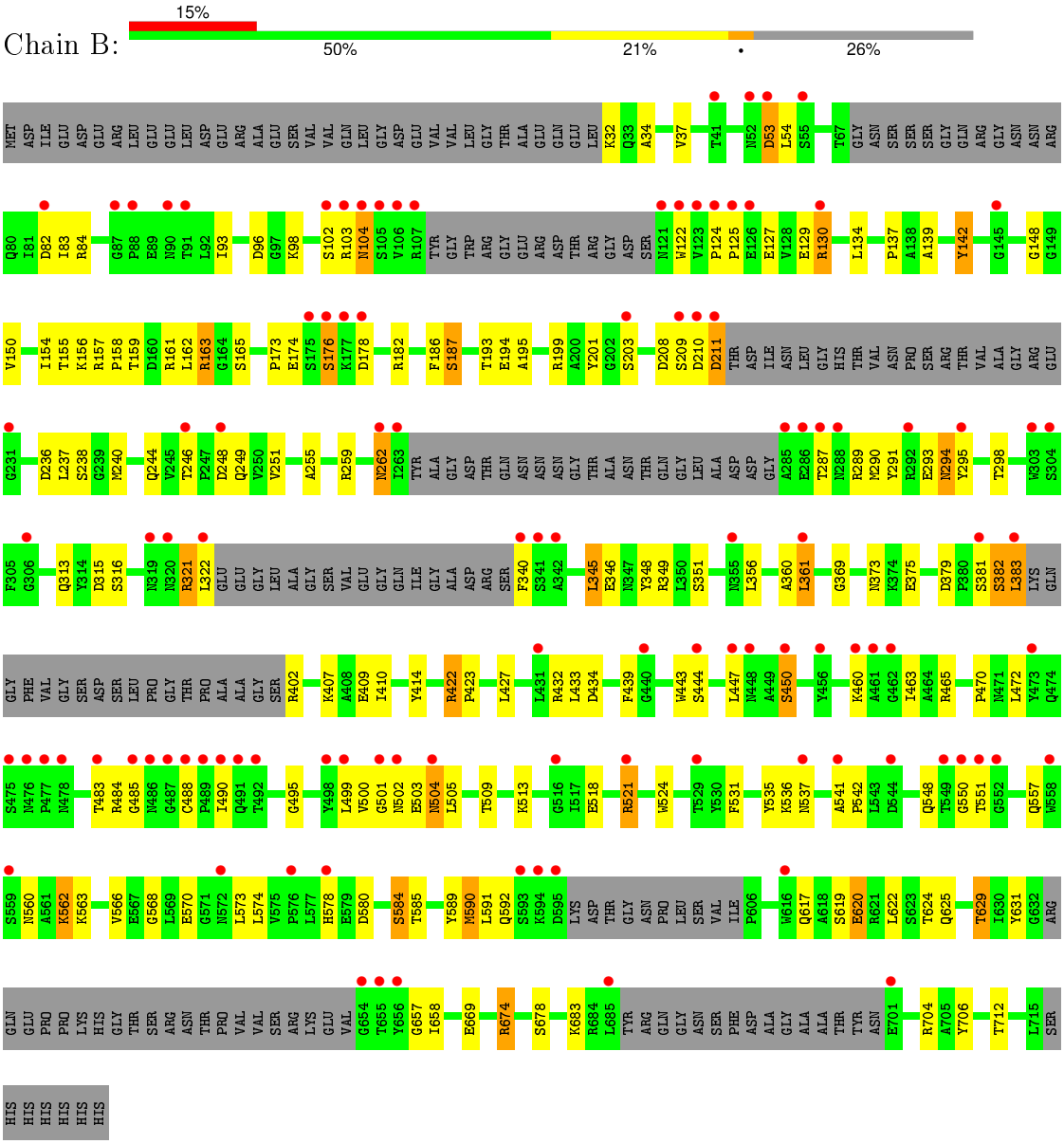
- Molecule 1: FERRIC ENTEROBACTIN RECEPTOR PIRA

Chain A:



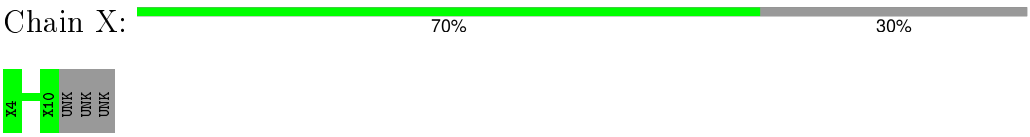
- Molecule 1: FERRIC ENTEROBACTIN RECEPTOR PIRA

Chain B:



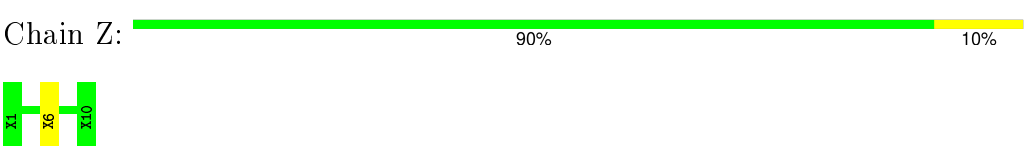
• Molecule 2: FERRIC ENTEROBACTIN RECEPTOR PIRA

Chain X:



• Molecule 2: FERRIC ENTEROBACTIN RECEPTOR PIRA

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.99 (at 2.96Å)	Xtriage
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 (5.00%)	DCC
Wilson B-factor (Å^2)	73.4	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 97.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 36860 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8201	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/3982	0.61	0/5394
1	B	0.48	0/4257	0.66	0/5767
All	All	0.45	0/8239	0.64	0/11161

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.

There are no bond angle outliers.

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

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	91	0
1	B	4180	0	4077	141	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	226	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 (226) 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
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:246:THR:HG22	1:B:249:GLN:CB	2.17	0.74
1:B:84:ARG:HG2	1:B:531:PHE:CD2	2.23	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:360:ALA:O	1:B:361:LEU:HB2	1.91	0.71
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:A:456:TYR:CE1	1:A:521:ARG:HD2	2.28	0.69
1:B:104:ASN:N	1:B:104:ASN:OD1	2.24	0.68
1:B:433:LEU:CD2	1:B:443:TRP:NE1	2.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:LEU:HD11	1:B:447:LEU:HD11	1.77	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: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:409:GLU:C	1:B:410:ILE:HD12	2.18	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:OD1	1:B:53:ASP:N	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:433:LEU:HD23	1:B:443:TRP:CD1	2.35	0.62
1:A:177:LYS:O	1:A:210:ASP:CB	2.47	0.62
1:B:484:ARG:NH1	1:B:495:GLY:C	2.53	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:HG2	1:B:289:ARG:HH11	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:B:186:PHE:C	1:B:186:PHE:CD1	2.73	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:B:620:GLU:H	1:B:620:GLU:CD	2.05	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:96:ASP:OD2	1:B:155:THR:OG1	2.18	0.57
1:B:321:ARG:HG3	1:B:322:LEU:N	2.19	0.57
1:B:360:ALA:O	1:B:361:LEU:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:HD23	1:A:238:SER:N	2.20	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:542:PRO:HD3	1:B:557:GLN:O	2.04	0.56
1:A:53:ASP:N	1:A:53:ASP:OD1	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: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:B:165:SER:O	1:B:186:PHE:HA	2.07	0.54
1:A:481:LEU:O	1:A:498:TYR:HA	2.08	0.54
1:B:37:VAL:HG23	1:B:134:LEU:CD1	2.38	0.54
1:B:499:LEU:HD21	1:B:541:ALA:HB2	1.90	0.54
1:A:163:ARG:NH2	1:A:715:LEU:HD13	2.22	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:CD1	1:B:706:TYR:N	2.77	0.53
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:562:LYS:HD3	1:A:562:LYS:N	2.24	0.52
1:A:369:GLY:HA3	1:A:414:TYR:CZ	2.45	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: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:A:201:TYR:CD1	1:A:201:TYR:C	2.84	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:535:TYR:HE1	1:A:566:VAL:HG23	1.76	0.50
1:A:46:ARG:CG	1:A:46:ARG:HH11	2.24	0.50
1:B:433:LEU:HD22	1:B:443:TRP:NE1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:186:PHE:CD1	1:A:186:PHE:C	2.85	0.49
1:A:193:THR:HG22	1:A:195:ALA:H	1.77	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: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:A:481:LEU:HB2	1:A:499:LEU:HD12	1.95	0.48
1:B:503:GLU:HG3	1:B:504:ASN:OD1	2.14	0.48
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:A:124:PRO:HG3	1:A:203:SER:HB3	1.95	0.48
1:B:137:PRO:C	1:B:139:ALA:H	2.17	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:B:102:SER:OG	1:B:345:LEU:CD1	2.62	0.47
1:B:34:ALA:HB3	1:B:37:VAL:CG1	2.45	0.46
1:A:664:GLY:HA3	1:A:674:ARG:HH11	1.79	0.46
1:A:193:THR:HG22	1:A:194:GLU:N	2.30	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:201:TYR:C	1:B:201:TYR:CD1	2.89	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:409:GLU:O	1:B:410:ILE:HD12	2.15	0.45
1:B:289:ARG:HG2	1:B:289:ARG:NH1	2.28	0.45
1:A:193:THR:HG23	1:B:293:GLU:CD	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:TYR:HB3	1:B:432:ARG:HG3	1.98	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:B:536:LYS:HG2	1:B:563:LYS:HG2	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:484:ARG:HH11	1:B:485:GLY:H	1.64	0.45
1:B:360:ALA:HB1	1:B:361:LEU:HD12	1.98	0.45
1:B:173:PRO:CB	1:B:178:ASP:HB3	2.46	0.44
1:A:499:LEU:O	1:A:499:LEU:HD12	2.16	0.44
1:B:236:ASP:OD1	1:B:236:ASP:O	2.35	0.44
1:B:360:ALA:C	1:B:361:LEU:HD12	2.37	0.44
1:B:289:ARG:HH12	1:B:291:TYR:HB2	1.82	0.44
1:B:173:PRO:HB3	1:B:178:ASP:HB3	2.00	0.44
1:A:47:LYS:O	1:A:674:ARG:NE	2.51	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:A:54:LEU:HD21	1:A:125:PRO:HA	1.99	0.44
1:B:262:ASN:O	1:B:262:ASN:ND2	2.49	0.43
1:A:580:ASP:N	1:A:580:ASP:OD1	2.50	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:B:82:ASP:C	1:B:82:ASP:OD1	2.57	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:608:TYR:CE2	1:A:610:LEU:HD12	2.52	0.43
1:B:156:LYS:O	1:B:199:ARG:HD3	2.18	0.43
1:B:550:GLY:C	1:B:551:THR:HG23	2.39	0.43
1:B:484:ARG:NH1	1:B:495:GLY:HA3	2.33	0.43
1:A:684:ARG:O	1:A:685:LEU:C	2.57	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:568:GLY:CA	1:A:589:TYR:O	2.67	0.43
1:B:348:TYR:CD1	1:B:348:TYR:N	2.86	0.42
1:A:460:LYS:HG3	1:A:461:ALA:N	2.33	0.42
1:A:579:GLU:HA	1:A:579:GLU:OE1	2.18	0.42
1:A:664:GLY:HA3	1:A:674:ARG:NH1	2.33	0.42
1:B:704:ARG:HD3	1:B:706:TYR:CZ	2.54	0.42
1:B:127:GLU:O	1:B:156:LYS:HG3	2.19	0.42
1:B:83:ILE:CG2	1:B:148:GLY:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:SER:OG	1:A:622:LEU:N	2.47	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
1:A:46:ARG:CG	1:A:46:ARG:NH1	2.83	0.42
1:B:134:LEU:HD21	2:Z:6:UNK:CB	2.50	0.42
1:A:656:TYR:CE2	1:A:701:GLU:OE2	2.73	0.42
1:B:433:LEU:HD21	1:B:443:TRP:HE1	1.83	0.42
1:B:137:PRO:O	1:B:139:ALA:N	2.52	0.42
1:A:236:ASP:C	1:A:236:ASP:OD1	2.59	0.42
1:B:157:ARG:O	1:B:158:PRO:C	2.55	0.41
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:619:SER:OG	1:B:622:LEU:N	2.43	0.41
1:B:678:SER:O	1:B:704:ARG:HA	2.20	0.41
1:A:537:ASN:HB3	1:A:560:ASN:HD22	1.81	0.41
1:A:415:VAL:O	1:A:430:GLY:HA2	2.21	0.41
1:B:360:ALA:C	1:B:361:LEU:CD1	2.89	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:A:295:TYR:HH	1:B:193:THR:HG21	1.71	0.40
1:B:542:PRO:CD	1:B:557:GLN:O	2.67	0.40
1:A:88:PRO:C	1:A:90:ASN:H	2.24	0.40
1:B:629:THR:CG2	1:B:631:TYR:CE2	3.04	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:A:678:SER:O	1:A:704:ARG:HA	2.21	0.40
1:A:193:THR:HG21	1:B:295:TYR:HH	1.77	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:HG12	1:A:100:VAL:O	2.20	0.40
1:A:318:ARG:HG3	1:A:318:ARG:HH11	1.86	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%)	52 87
1	B	518/725 (71%)	493 (95%)	24 (5%)	1 (0%)	52 87
All	All	993/1450 (68%)	948 (96%)	43 (4%)	2 (0%)	52 87

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%)	387 (91%)	37 (9%)	13 41
1	B	454/604 (75%)	407 (90%)	47 (10%)	9 31
All	All	878/1208 (73%)	794 (90%)	84 (10%)	10 36

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	46	ARG
1	A	163	ARG
1	A	209	SER

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Mol	Chain	Res	Type
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	321	ARG
1	A	356	LEU
1	A	363	GLU
1	A	373	ASN
1	A	375	GLU
1	A	422	ARG
1	A	434	ASP
1	A	442	ASN
1	A	444	SER
1	A	450	SER
1	A	465	ARG
1	A	480	LEU
1	A	509	THR
1	A	518	GLU
1	A	521	ARG
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	B	32	LYS
1	B	53	ASP
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	187	SER

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Mol	Chain	Res	Type
1	B	194	GLU
1	B	208	ASP
1	B	209	SER
1	B	211	ASP
1	B	244	GLN
1	B	262	ASN
1	B	290	MET
1	B	294	ASN
1	B	316	SER
1	B	321	ARG
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	407	LYS
1	B	422	ARG
1	B	444	SER
1	B	450	SER
1	B	465	ARG
1	B	504	ASN
1	B	509	THR
1	B	518	GLU
1	B	521	ARG
1	B	562	LYS
1	B	578	HIS
1	B	584	SER
1	B	590	MET
1	B	591	LEU
1	B	620	GLU
1	B	624	THR
1	B	629	THR
1	B	669	GLU
1	B	674	ARG
1	B	683	LYS
1	B	712	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	A	249	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	OCT	A	801	-	7,7,7	0.24	0	6,6,6	0.41	0
4	SO4	B	1716	-	4,4,4	0.17	0	6,6,6	0.17	0
4	SO4	B	1717	-	4,4,4	0.31	0	6,6,6	0.11	0
3	OCT	B	801	-	7,7,7	0.24	0	6,6,6	0.40	0
3	OCT	B	802	-	7,7,7	0.22	0	6,6,6	0.46	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	0/0/0/0
4	SO4	B	1716	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1717	-	-	0/0/0/0	0/0/0/0
3	OCT	B	801	-	-	0/5/5/5	0/0/0/0
3	OCT	B	802	-	-	0/5/5/5	0/0/0/0

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 (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^{th} 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	A	499/725 (68%)	1.29	103 (20%)	1	1	101, 126, 164, 197	0
1	B	538/725 (74%)	1.44	108 (20%)	1	1	103, 124, 159, 191	0
2	X	0/10	-	-			-	-
2	Z	0/10	-	-			-	-
All	All	1037/1470 (70%)	1.37	211 (20%)	1	1	101, 125, 161, 197	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	ALA	10.4
1	B	263	ILE	9.1
1	B	210	ASP	7.8
1	A	361	LEU	7.5
1	A	287	THR	7.3
1	A	288	ASN	6.8
1	B	102	SER	6.8
1	A	480	LEU	6.7
1	A	362	PHE	6.6
1	B	655	THR	6.5
1	B	104	ASN	6.3
1	A	498	TYR	6.0
1	B	549	THR	5.9
1	B	105	SER	5.8
1	B	211	ASP	5.8
1	B	106	VAL	5.5
1	B	322	LEU	5.4
1	A	404	PRO	5.3
1	B	103	ARG	5.2
1	A	403	SER	5.2
1	B	340	PHE	5.1
1	B	107	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	287	THR	5.0
1	A	655	THR	4.9
1	A	305	PHE	4.8
1	A	211	ASP	4.8
1	B	288	ASN	4.7
1	A	231	GLY	4.5
1	B	685	LEU	4.5
1	B	498	TYR	4.5
1	A	322	LEU	4.4
1	B	320	ASN	4.4
1	A	262	ASN	4.3
1	B	552	GLY	4.3
1	A	654	GLY	4.3
1	B	485	GLY	4.3
1	A	80	GLN	4.3
1	A	209	SER	4.2
1	A	341	SER	4.1
1	A	210	ASP	4.1
1	A	558	TRP	4.1
1	B	502	ASN	4.1
1	A	473	TYR	4.1
1	B	478	ASN	4.1
1	A	479	TYR	4.0
1	A	320	ASN	4.0
1	B	286	GLU	4.0
1	A	482	TYR	3.9
1	A	304	SER	3.9
1	B	473	TYR	3.8
1	A	405	LYS	3.8
1	A	500	VAL	3.8
1	B	559	SER	3.7
1	B	486	ASN	3.7
1	B	550	GLY	3.7
1	A	360	ALA	3.7
1	A	177	LYS	3.6
1	B	122	TRP	3.6
1	B	504	ASN	3.6
1	B	319	ASN	3.6
1	B	490	ILE	3.6
1	A	476	ASN	3.6
1	B	654	GLY	3.4
1	A	381	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	359	HIS	3.4
1	B	125	PRO	3.4
1	B	701	GLU	3.4
1	A	702	PRO	3.3
1	B	381	SER	3.3
1	A	137	PRO	3.3
1	B	231	GLY	3.3
1	B	477	PRO	3.3
1	A	418	ASN	3.3
1	A	542	PRO	3.3
1	B	121	ASN	3.3
1	A	656	TYR	3.2
1	A	321	ARG	3.2
1	B	176	SER	3.2
1	A	127	GLU	3.2
1	A	67	THR	3.2
1	A	147	ALA	3.2
1	A	318	ARG	3.2
1	A	471	ASN	3.1
1	A	425	THR	3.1
1	B	475	SER	3.1
1	B	541	ALA	3.1
1	A	179	GLY	3.1
1	B	341	SER	3.1
1	A	427	LEU	3.0
1	A	358	LEU	3.0
1	B	488	CYS	3.0
1	B	656	TYR	3.0
1	A	631	TYR	3.0
1	B	262	ASN	3.0
1	A	178	ASP	3.0
1	A	451	GLN	2.9
1	B	53	ASP	2.9
1	B	87	GLY	2.9
1	B	448	ASN	2.9
1	B	594	LYS	2.9
1	B	440	GLY	2.9
1	B	521	ARG	2.9
1	A	261	GLY	2.9
1	B	203	SER	2.8
1	B	177	LYS	2.8
1	B	491	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	489	PRO	2.8
1	B	248	ASP	2.8
1	A	668	SER	2.8
1	A	615	ASP	2.8
1	A	367	THR	2.8
1	B	551	THR	2.8
1	A	139	ALA	2.8
1	B	460	LYS	2.7
1	A	232	VAL	2.7
1	A	589	TYR	2.7
1	B	383	LEU	2.7
1	A	421	LEU	2.7
1	B	529	THR	2.7
1	A	606	PRO	2.7
1	B	178	ASP	2.7
1	B	55	SER	2.6
1	B	90	ASN	2.6
1	A	303	TRP	2.6
1	A	617	GLN	2.6
1	B	595	ASP	2.6
1	A	478	ASN	2.6
1	A	472	LEU	2.6
1	A	101	SER	2.6
1	B	123	VAL	2.6
1	B	544	ASP	2.6
1	A	193	THR	2.6
1	B	246	THR	2.5
1	A	435	ASP	2.5
1	B	292	ARG	2.5
1	B	476	ASN	2.5
1	B	487	GLY	2.5
1	B	126	GLU	2.5
1	B	41	THR	2.5
1	A	441	LEU	2.5
1	A	608	TYR	2.4
1	B	175	SER	2.4
1	A	32	LYS	2.4
1	A	502	ASN	2.4
1	B	306	GLY	2.4
1	B	483	THR	2.4
1	B	209	SER	2.4
1	A	58	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	91	THR	2.4
1	B	444	SER	2.4
1	B	501	GLY	2.4
1	A	667	PHE	2.4
1	B	82	ASP	2.4
1	B	355	ASN	2.4
1	A	363	GLU	2.4
1	B	516	GLY	2.4
1	A	243	TRP	2.4
1	A	556	LEU	2.4
1	B	499	LEU	2.4
1	B	130	ARG	2.3
1	B	537	ASN	2.3
1	A	378	ASN	2.3
1	A	44	ASP	2.3
1	B	361	LEU	2.3
1	B	578	HIS	2.3
1	B	342	ALA	2.3
1	B	450	SER	2.3
1	A	481	LEU	2.3
1	B	447	LEU	2.3
1	A	290	MET	2.2
1	A	426	MET	2.2
1	A	52	ASN	2.2
1	B	572	ASN	2.2
1	B	593	SER	2.2
1	A	40	ILE	2.2
1	B	456	TYR	2.2
1	A	60	THR	2.2
1	A	191	PRO	2.2
1	A	665	TYR	2.2
1	A	453	LEU	2.2
1	A	79	ARG	2.2
1	A	685	LEU	2.2
1	B	88	PRO	2.2
1	A	499	LEU	2.2
1	B	52	ASN	2.2
1	B	304	SER	2.2
1	A	377	LEU	2.1
1	A	33	GLN	2.1
1	A	619	SER	2.1
1	A	555	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	53	ASP	2.1
1	A	82	ASP	2.1
1	A	236	ASP	2.1
1	B	558	TRP	2.1
1	B	431	LEU	2.1
1	B	461	ALA	2.1
1	B	303	TRP	2.1
1	B	295	TYR	2.1
1	B	492	THR	2.1
1	A	417	ASP	2.1
1	B	124	PRO	2.1
1	B	576	PRO	2.1
1	A	306	GLY	2.1
1	B	616	TRP	2.1
1	A	632	GLY	2.1
1	B	145	GLY	2.1
1	B	462	GLY	2.1
1	A	517	ILE	2.0
1	A	348	TYR	2.0
1	A	140	ALA	2.0
1	A	474	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	OCT	B	802	8/8	0.61	0.69	9.82	160,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	OCT	B	801	8/8	0.78	0.59	8.58	160,160,160,160	0
4	SO4	B	1716	5/5	0.76	0.39	2.10	160,160,160,160	0
3	OCT	A	801	8/8	0.77	0.46	-	160,160,160,160	0
4	SO4	B	1717	5/5	0.79	0.23	-	160,160,160,160	0

6.5 Other polymers (i)

There are no such residues in this entry.