Full wwPDB X-ray Structure Validation Report (i)

Dec 21, 2016 – 12:59 PM EST

PDB ID	:	2W6T
Title	:	Structures of P. aeruginosa FpvA bound to heterologous pyoverdines: FpvA-Pvd(DSM50106)-Fe complex
Authors	:	Greenwald, J.; Nader, M.; Celia, H.; Gruffaz, C.; Meyer, J.-M.; Schalk, I.J.; Pattus, F.
Deposited on	:	2008-12-19
Resolution	:	2.90 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:

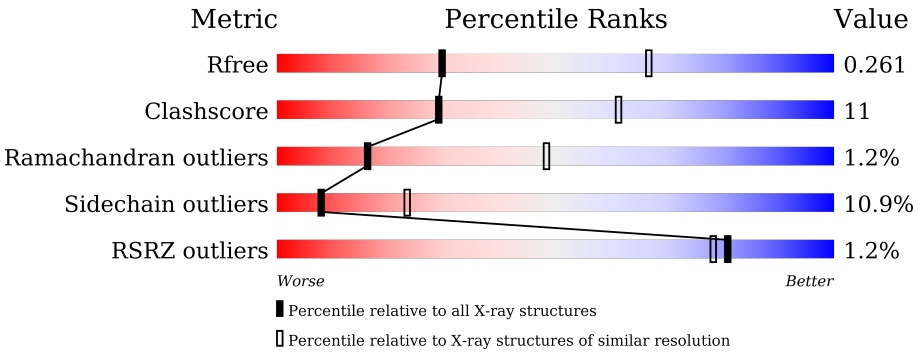
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	772	% 69% 25% 5%
1	B	772	% 70% 24%
2	C	10	80% 20%

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	N8E	A	1816	-	-	-	X
3	N8E	A	1817[A]	-	-	-	X
3	N8E	A	1817[B]	-	-	-	X
4	PO4	A	1822	-	-	-	X
4	PO4	A	1823	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12342 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.

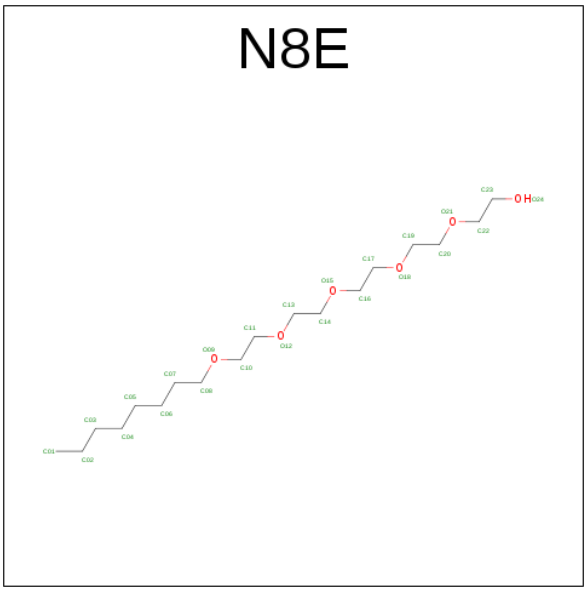
- Molecule 1 is a protein called FERRIPYOVERDINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	0	1	0
			6128	3856	1048	1212	12			
1	B	754	Total	C	N	O	S	0	0	0
			5994	3775	1027	1181	11			

- Molecule 2 is a protein called PYOVERDINE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			71	39	14	18			

- Molecule 3 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (three-letter code: N8E) (formula: $C_{18}H_{38}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	18	6		

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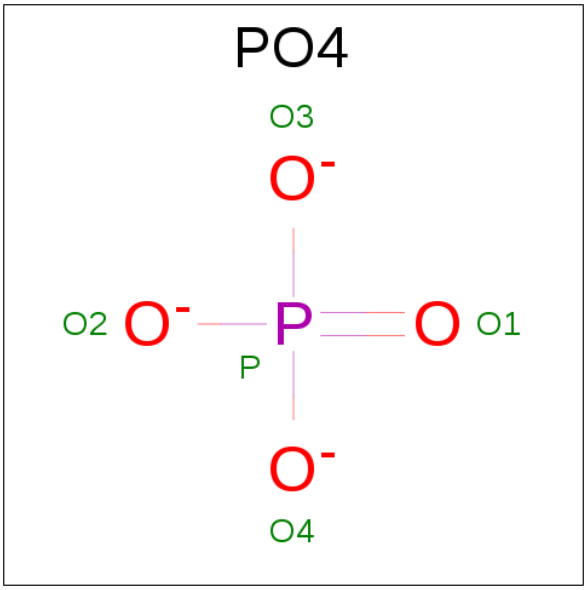
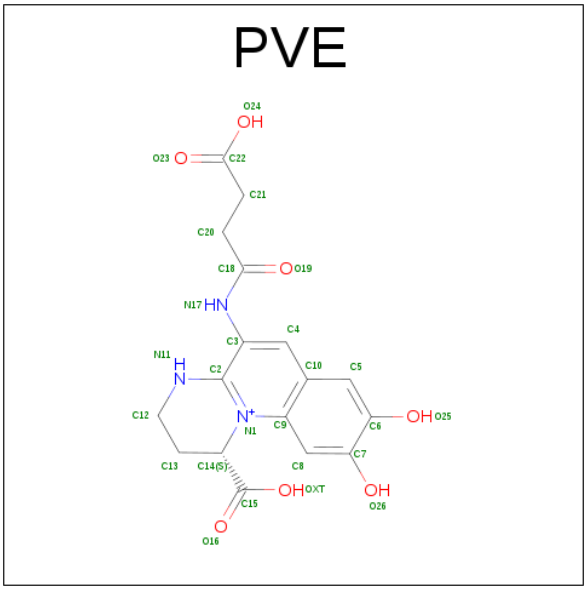
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 48 36 12	0	1

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is (1S)-1-CARBOXY-5-[(3-CARBOXYPROPANOYL)AMINO]-8,9-DIHYDROXY-1,2,3,4-TETRAHYDROPYRIMIDO[1,2-A]QUINOLIN-11-IUM (three-letter code: PVE) (formula: $C_{17}H_{18}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	5	0
			26	17	3	6		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

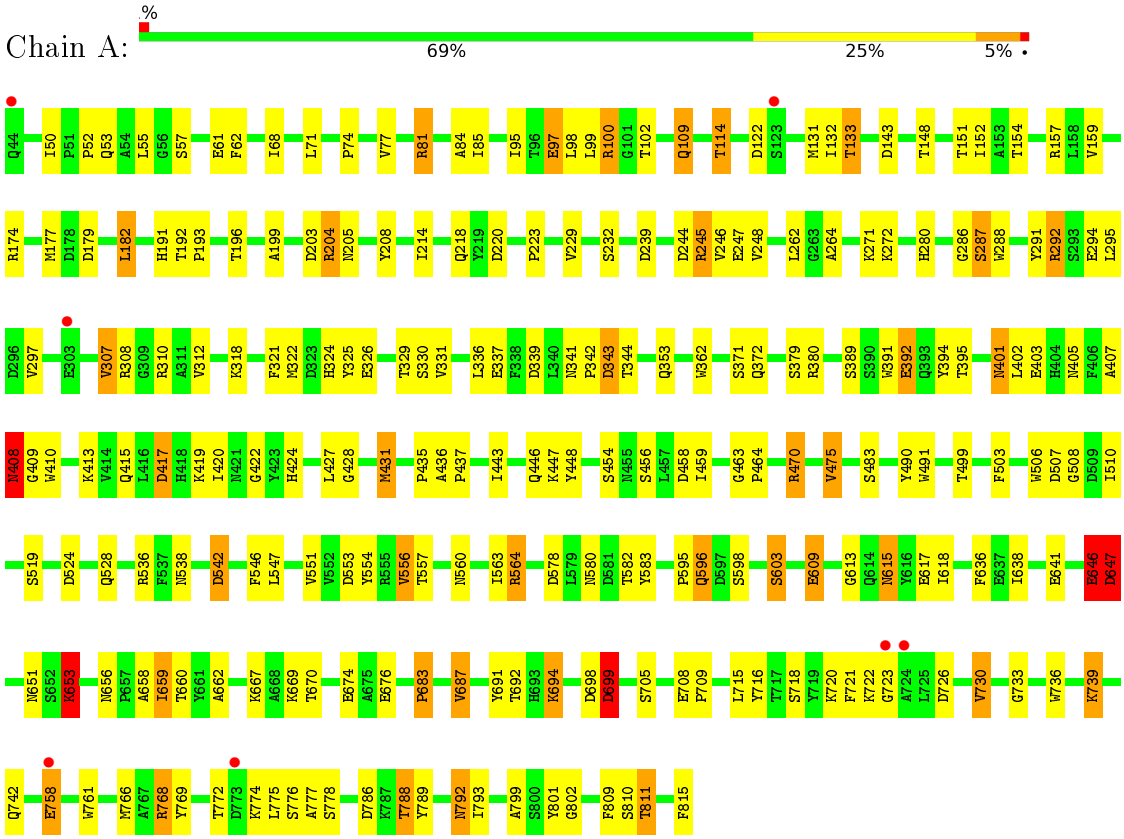
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Fe	0	0
			1	1		

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.

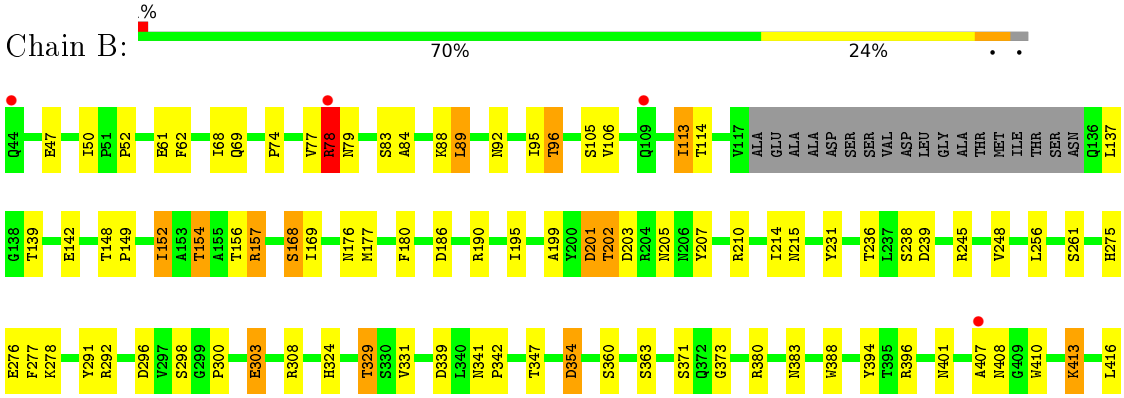
- Molecule 1: FERRIPYOVERDINE RECEPTOR

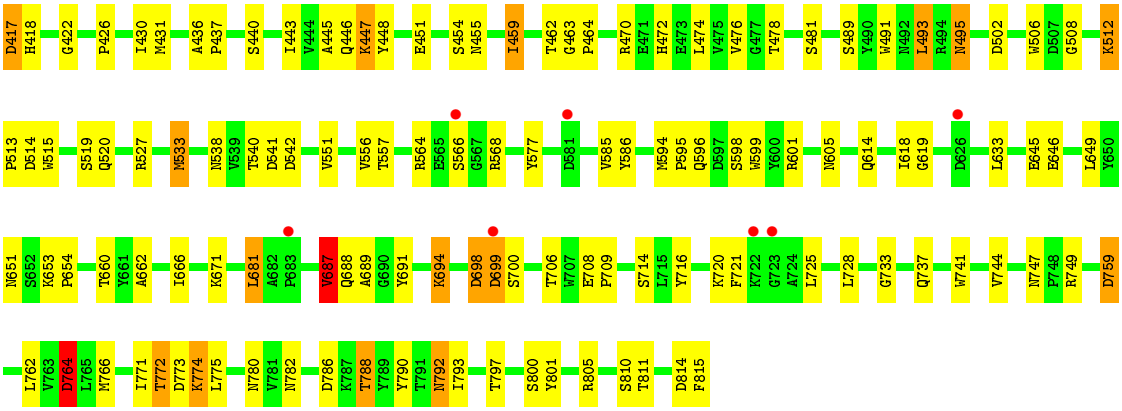
Chain A:



- Molecule 1: FERRIPYOVERDINE RECEPTOR

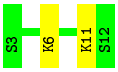
Chain B:





- Molecule 2: PYOVERDINE

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	194.56Å 129.13Å 141.82Å 90.00° 131.65° 90.00°	Depositor
Resolution (Å)	106.00 – 2.90 31.67 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (106.00-2.90) 93.5 (31.67-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.263 0.204 , 0.261	Depositor DCC
R_{free} test set	2785 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12342	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DSN, FHO, PO4, ORN, PVE, FE, N8E, FH7

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	0.97	2/6282 (0.0%)	1.00	13/8537 (0.2%)
1	B	0.89	1/6145 (0.0%)	0.94	10/8347 (0.1%)
2	C	0.81	0/25	0.87	0/25
All	All	0.93	3/12452 (0.0%)	0.97	23/16909 (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	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	GLU	CG-CD	9.91	1.66	1.51
1	A	758	GLU	CG-CD	5.63	1.60	1.51
1	B	599	TRP	CB-CG	-5.05	1.41	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	687	VAL	CB-CA-C	-7.05	98.00	111.40
1	B	687	VAL	CB-CA-C	-6.82	98.45	111.40
1	A	475	VAL	CB-CA-C	-6.31	99.42	111.40
1	B	514	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	81	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	647	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	190	ARG	NE-CZ-NH1	5.63	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	296	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	507	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	A	336	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	292	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	204	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	764	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	B	354	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	768	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	502	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	633	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	292	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	208	TYR	CA-CB-CG	5.15	123.19	113.40
1	B	89	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	204	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	786	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	354	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	407	ALA	Peptide
1	B	698	ASP	Peptide

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	6128	0	5797	143	0
1	B	5994	0	5675	135	0
2	C	71	0	62	3	0
3	A	72	0	114	6	0
4	A	30	0	0	2	0
4	B	20	0	0	3	0
5	C	26	0	14	0	0
6	C	1	0	0	0	0
All	All	12342	0	11662	274	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 11.

All (274) 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:772:THR:HG21	1:B:291:TYR:OH	1.54	1.06
1:B:772:THR:HG22	1:B:774:LYS:H	1.24	1.01
1:A:362[B]:TRP:CD1	1:A:431:MET:HE1	1.97	0.99
1:A:694:LYS:HE3	1:A:708:GLU:OE1	1.65	0.96
1:A:772:THR:HG22	1:A:774:LYS:H	1.30	0.94
1:B:418:HIS:HD2	1:B:455:ASN:HD21	0.97	0.93
1:B:472:HIS:HD2	1:B:538:ASN:H	0.96	0.90
1:B:418:HIS:CD2	1:B:455:ASN:HD21	1.88	0.90
1:B:472:HIS:CD2	1:B:538:ASN:H	1.89	0.90
1:A:74:PRO:HG3	1:A:132:ILE:HG12	1.51	0.89
1:A:556:VAL:HG13	1:A:563:ILE:HB	1.56	0.88
1:A:362[B]:TRP:HH2	1:A:446:GLN:OE1	1.57	0.87
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.57	0.87
1:A:742:GLN:HG3	1:A:793:ILE:O	1.75	0.85
3:A:1817[B]:N8E:H031	1:B:805:ARG:HD2	1.56	0.85
1:A:408:ASN:HB3	1:A:410:TRP:CD1	2.14	0.82
1:A:109:GLN:OE1	1:A:114:THR:HG22	1.79	0.82
1:A:470:ARG:NH1	1:A:538:ASN:OD1	2.13	0.81
1:A:308:ARG:NH1	1:A:337:GLU:OE1	2.14	0.81
1:B:446:GLN:NE2	1:B:491:TRP:HB2	1.96	0.81
1:B:418:HIS:HD2	1:B:455:ASN:ND2	1.79	0.79
1:B:472:HIS:HD2	1:B:538:ASN:N	1.77	0.79
1:B:540:THR:HG22	1:B:541:ASP:H	1.47	0.79
1:B:446:GLN:NE2	1:B:491:TRP:CB	2.46	0.78
1:B:493:LEU:H	1:B:493:LEU:HD12	1.50	0.76
1:B:646:GLU:O	1:B:662:ALA:O	2.02	0.76
1:B:772:THR:HG22	1:B:774:LYS:N	1.99	0.76
1:B:512:LYS:HE3	4:B:1818:PO4:O3	1.86	0.76
1:A:772:THR:HG22	1:A:774:LYS:N	2.01	0.74
1:A:722:LYS:HG3	1:A:723:GLY:H	1.52	0.74
1:A:408:ASN:HB3	1:A:410:TRP:HD1	1.52	0.74
1:A:245:ARG:NH1	1:A:247:GLU:OE1	2.21	0.73
1:A:777:ALA:HB1	3:A:1817[B]:N8E:H191	1.70	0.73
1:A:53:GLN:OE1	1:A:57:SER:HB2	1.89	0.73
1:A:443:ILE:HG13	1:A:510:ILE:HD13	1.71	0.71
1:B:418:HIS:HE1	4:B:1821:PO4:O1	1.73	0.71
1:B:201:ASP:O	1:B:203:ASP:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:PHE:HB3	3:A:1817[B]:N8E:H201	1.71	0.71
1:B:50:ILE:HG12	1:B:61:GLU:HG2	1.71	0.70
1:A:239:ASP:OD2	1:A:292:ARG:NH2	2.23	0.70
1:B:347:THR:HB	1:B:401:ASN:HB2	1.73	0.70
1:A:778:SER:O	3:A:1817[B]:N8E:H192	1.92	0.70
1:B:195:ILE:HD11	1:B:248:VAL:HG11	1.72	0.69
1:A:443:ILE:HG13	1:A:510:ILE:CD1	2.22	0.69
1:A:214:ILE:HG12	1:A:264:ALA:HB3	1.75	0.69
1:B:666:ILE:HB	1:B:699:ASP:OD2	1.93	0.67
1:A:699:ASP:OD1	1:A:699:ASP:N	2.27	0.67
1:B:764:ASP:HB3	1:B:782:ASN:HA	1.76	0.67
1:A:239:ASP:CG	1:A:292:ARG:HH22	1.98	0.66
1:A:53:GLN:OE1	1:A:57:SER:CB	2.43	0.66
1:A:772:THR:HG21	1:B:291:TYR:HH	1.61	0.65
1:B:542:ASP:O	1:B:577:TYR:HA	1.97	0.65
1:B:156:THR:O	1:B:157:ARG:HB2	1.97	0.64
1:A:271:LYS:HD3	1:A:310:ARG:NH2	2.12	0.64
1:A:580:ASN:CB	1:A:582:THR:H	2.10	0.64
1:A:646:GLU:O	1:A:647:ASP:CB	2.45	0.64
1:B:694:LYS:HE3	1:B:708:GLU:OE1	1.98	0.64
1:A:667:LYS:O	1:A:699:ASP:OD1	2.17	0.63
1:A:109:GLN:OE1	1:A:114:THR:CG2	2.45	0.63
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.35	0.62
1:B:436:ALA:HB1	1:B:437:PRO:HD2	1.81	0.62
1:B:446:GLN:NE2	1:B:491:TRP:HB3	2.13	0.62
1:A:580:ASN:HB3	1:A:582:THR:H	1.65	0.62
1:B:324:HIS:CE1	1:B:383:ASN:HB3	2.35	0.62
1:A:656:ASN:HB3	1:A:659:ILE:HD12	1.82	0.61
1:B:772:THR:CG2	1:B:774:LYS:H	2.09	0.61
1:B:95:ILE:HG12	1:B:113:ILE:CD1	2.32	0.60
1:B:446:GLN:HE21	1:B:491:TRP:HB2	1.65	0.60
1:A:371:SER:OG	1:A:436:ALA:HA	2.02	0.60
1:B:388:TRP:CZ2	1:B:513:PRO:HD3	2.37	0.60
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.37	0.59
1:B:774:LYS:HB3	1:B:814:ASP:O	2.02	0.59
1:A:401:ASN:ND2	1:A:415:GLN:HG2	2.16	0.59
1:A:362[B]:TRP:CH2	1:A:446:GLN:OE1	2.48	0.59
1:A:410:TRP:CD2	1:A:463:GLY:HA3	2.37	0.59
1:A:721:PHE:O	1:A:726:ASP:HA	2.02	0.59
1:A:174:ARG:HB2	1:A:244:ASP:O	2.03	0.58
1:B:601:ARG:NH1	1:B:605:ASN:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLU:HG3	1:A:424:HIS:HB3	1.86	0.58
1:B:797:THR:HG22	1:B:797:THR:O	2.01	0.58
1:A:391:TRP:HB2	1:A:427:LEU:HD21	1.84	0.58
1:B:371:SER:OG	1:B:436:ALA:HA	2.03	0.58
1:A:97:GLU:O	1:A:100:ARG:HB2	2.04	0.58
1:B:95:ILE:HG12	1:B:113:ILE:HD13	1.85	0.58
1:B:394:TYR:OH	1:B:451:GLU:HG3	2.03	0.58
1:A:417:ASP:HB2	1:A:456:SER:HB2	1.85	0.58
1:A:362[B]:TRP:CG	1:A:431:MET:HE1	2.38	0.58
1:A:556:VAL:CG1	1:A:563:ILE:HB	2.32	0.58
1:A:447:LYS:HB3	1:A:490:TYR:HB2	1.86	0.57
1:A:199:ALA:HA	1:A:205:ASN:HD22	1.70	0.57
1:A:291:TYR:OH	1:B:772:THR:HG21	2.04	0.57
1:A:151:THR:O	1:A:152:ILE:HD13	2.05	0.56
1:A:446:GLN:OE1	1:A:448:TYR:OH	2.17	0.56
1:A:580:ASN:HB2	1:A:583:TYR:H	1.70	0.56
1:B:380:ARG:HA	1:B:801:TYR:CE2	2.41	0.55
1:B:92:ASN:O	1:B:96:THR:HB	2.06	0.55
1:A:772:THR:CG2	1:B:291:TYR:OH	2.43	0.55
3:A:1817[B]:N8E:H031	1:B:805:ARG:HH11	1.72	0.55
1:A:443:ILE:CG1	1:A:510:ILE:CD1	2.85	0.55
1:B:792:ASN:O	1:B:793:ILE:HG13	2.07	0.55
1:B:431:MET:SD	2:C:11:FH7:HB2C	2.45	0.55
1:A:554:TYR:CD2	1:A:595:PRO:HG2	2.42	0.55
1:A:280:HIS:NE2	4:A:1823:PO4:O4	2.39	0.54
1:A:739:LYS:HD2	1:A:739:LYS:H	1.73	0.54
1:A:775:LEU:HD23	1:A:776:SER:N	2.23	0.53
1:B:792:ASN:HB3	1:B:800:SER:HB2	1.90	0.53
1:A:454:SER:OG	1:A:483:SER:HB3	2.07	0.53
1:A:646:GLU:O	1:A:647:ASP:HB3	2.08	0.53
1:A:775:LEU:C	1:A:775:LEU:HD23	2.28	0.53
1:B:681:LEU:HD22	1:B:687:VAL:HG22	1.89	0.53
1:A:362[B]:TRP:HH2	1:A:446:GLN:CD	2.11	0.53
1:A:646:GLU:O	1:A:662:ALA:O	2.27	0.53
1:A:722:LYS:HG3	1:A:723:GLY:N	2.23	0.53
1:B:380:ARG:HD3	1:B:788:THR:HB	1.90	0.53
1:B:447:LYS:HE2	1:B:515:TRP:CD1	2.43	0.53
1:A:133:THR:HG21	1:A:159:VAL:HG21	1.90	0.53
1:A:362[B]:TRP:CH2	1:A:446:GLN:CD	2.81	0.53
1:A:674:GLU:HG3	1:A:692:THR:OG1	2.07	0.53
1:B:341:ASN:HB2	1:B:342:PRO:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:ASP:O	1:B:455:ASN:HA	2.09	0.53
1:A:262:LEU:HD21	1:A:613:GLY:HA3	1.91	0.52
1:A:491:TRP:CE2	1:A:519:SER:HB3	2.44	0.52
1:B:614:GLN:N	1:B:614:GLN:CD	2.63	0.52
1:B:689:ALA:HA	1:B:714:SER:O	2.09	0.52
1:B:275:HIS:O	1:B:300:PRO:HD3	2.09	0.52
1:A:542:ASP:HB3	1:A:578:ASP:HB2	1.92	0.51
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.46	0.51
1:A:775:LEU:HD21	1:A:811:THR:HG22	1.93	0.51
1:A:52:PRO:HG3	1:A:84:ALA:HB2	1.92	0.51
1:B:77:VAL:O	1:B:79:ASN:N	2.43	0.51
1:A:218:GLN:HG2	1:A:223:PRO:HA	1.92	0.51
1:A:769:TYR:OH	3:A:1817[B]:N8E:H041	2.11	0.51
1:B:156:THR:O	1:B:157:ARG:CB	2.58	0.51
1:A:419:LYS:HG2	1:A:420:ILE:N	2.24	0.51
1:A:341:ASN:HB2	1:A:342:PRO:CD	2.37	0.50
1:B:363:SER:HB2	1:B:431:MET:HE2	1.94	0.50
1:B:199:ALA:HA	1:B:205:ASN:ND2	2.25	0.50
1:B:540:THR:HG22	1:B:541:ASP:N	2.23	0.50
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.47	0.50
1:B:52:PRO:HD3	1:B:84:ALA:HB2	1.93	0.50
1:A:50:ILE:HD12	1:A:85:ILE:HD11	1.94	0.49
1:A:389:SER:HB2	1:A:428:GLY:H	1.77	0.49
1:A:772:THR:CG2	1:A:774:LYS:H	2.13	0.49
1:B:445:ALA:O	1:B:446:GLN:HG3	2.13	0.49
1:B:448:TYR:CZ	2:C:6:FHO:HD2C	2.48	0.49
1:B:69:GLN:HG2	1:B:276:GLU:HA	1.93	0.49
1:A:132:ILE:HD11	1:A:464:PRO:HD3	1.94	0.49
1:A:380:ARG:HA	1:A:801:TYR:CD2	2.48	0.49
1:B:586:TYR:CE1	1:B:619:GLY:HA3	2.48	0.49
1:A:152:ILE:HG22	1:A:154:THR:H	1.77	0.49
1:A:286:GLY:O	1:A:287:SER:C	2.51	0.49
1:B:329:THR:HA	1:B:354:ASP:O	2.13	0.49
1:B:308:ARG:NH2	1:B:339:ASP:OD2	2.46	0.49
1:B:445:ALA:O	1:B:446:GLN:CG	2.61	0.48
1:B:152:ILE:HD12	1:B:169:ILE:HG12	1.94	0.48
1:A:715:LEU:C	1:A:715:LEU:HD23	2.34	0.48
1:A:182:LEU:HD21	1:A:191:HIS:CD2	2.48	0.48
1:B:698:ASP:HB3	1:B:700:SER:H	1.78	0.48
1:B:771:ILE:HG13	1:B:771:ILE:H	1.50	0.48
1:A:344:THR:HA	1:A:403:GLU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:C	1:A:98:LEU:HD23	2.34	0.47
1:A:410:TRP:CE2	1:A:463:GLY:HA3	2.49	0.47
1:A:653:LYS:O	1:A:653:LYS:HG3	2.13	0.47
1:B:694:LYS:HD2	1:B:694:LYS:C	2.34	0.47
1:A:536:ARG:HD2	1:A:546:PHE:CZ	2.50	0.47
1:A:53:GLN:OE1	1:A:57:SER:HB3	2.14	0.47
1:B:646:GLU:HG3	1:B:651:ASN:HD22	1.78	0.47
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.49	0.47
1:B:470:ARG:NH1	1:B:540:THR:O	2.45	0.47
1:B:436:ALA:HB1	1:B:437:PRO:CD	2.44	0.47
1:B:201:ASP:O	1:B:202:THR:C	2.53	0.47
1:B:231:TYR:CZ	2:C:6:FHO:HG1C	2.50	0.47
1:B:721:PHE:HB2	1:B:725:LEU:O	2.15	0.47
1:A:177:MET:HA	1:A:182:LEU:HD12	1.97	0.47
1:A:736:TRP:HB2	1:A:761:TRP:CE3	2.50	0.47
1:B:142:GLU:HG3	4:B:1820:PO4:O1	2.15	0.47
1:B:493:LEU:N	1:B:493:LEU:HD12	2.25	0.47
1:A:321:PHE:CE2	1:A:322:MET:HG3	2.50	0.46
1:B:426:PRO:HB3	1:B:447:LYS:HG3	1.97	0.46
1:B:594:MET:SD	1:B:595:PRO:HD2	2.55	0.46
1:B:653:LYS:HA	1:B:654:PRO:HD2	1.68	0.46
1:A:99:LEU:O	1:A:102:THR:HG23	2.16	0.46
1:B:410:TRP:CD2	1:B:463:GLY:HA3	2.51	0.46
1:A:436:ALA:HB1	1:A:437:PRO:CD	2.45	0.46
1:B:154:THR:O	1:B:256:LEU:HD12	2.15	0.46
1:A:638:ILE:O	1:A:669:LYS:HA	2.15	0.46
1:A:694:LYS:O	1:A:694:LYS:HD2	2.15	0.46
1:B:410:TRP:CG	1:B:463:GLY:HA3	2.51	0.46
1:B:721:PHE:CE2	1:B:728:LEU:HD23	2.51	0.46
1:B:506:TRP:CZ2	1:B:508:GLY:HA2	2.51	0.46
1:A:615:ASN:HD21	1:A:617:GLU:HB2	1.81	0.46
1:B:772:THR:HG22	1:B:775:LEU:H	1.80	0.45
1:A:596:GLN:NE2	1:A:609:GLU:O	2.49	0.45
1:B:459:ILE:HG12	1:B:478:THR:HG22	1.98	0.45
1:A:402:LEU:O	1:A:413:LYS:HA	2.17	0.45
1:A:560:ASN:HB3	1:A:598:SER:OG	2.17	0.45
1:A:691:TYR:CD2	1:A:691:TYR:C	2.90	0.45
1:B:476:VAL:HG12	1:B:533:MET:HG3	1.98	0.45
1:B:489:SER:O	1:B:519:SER:N	2.48	0.45
1:B:790:TYR:CG	1:B:793:ILE:HD11	2.52	0.44
1:A:174:ARG:CZ	1:A:177:MET:HE3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASP:HB2	1:A:405:ASN:HB2	1.99	0.44
1:B:277:PHE:HA	1:B:298:SER:O	2.17	0.44
1:B:772:THR:CG2	1:B:773:ASP:N	2.81	0.44
1:B:489:SER:HB2	1:B:520:GLN:HB3	1.99	0.44
1:A:196:THR:HG21	1:A:709:PRO:HD3	1.98	0.44
1:B:186:ASP:OD1	1:B:207:TYR:OH	2.27	0.44
1:A:179:ASP:OD1	1:A:768:ARG:NH1	2.37	0.44
1:B:239:ASP:OD2	1:B:292:ARG:NH2	2.51	0.44
1:B:792:ASN:HD22	1:B:800:SER:CB	2.31	0.44
1:B:462:THR:HA	1:B:474:LEU:O	2.18	0.43
1:A:580:ASN:HB2	1:A:582:THR:H	1.82	0.43
1:A:687:VAL:HG23	1:A:687:VAL:O	2.18	0.43
1:B:201:ASP:C	1:B:203:ASP:H	2.20	0.43
1:B:762:LEU:HD23	1:B:762:LEU:HA	1.85	0.43
1:B:77:VAL:O	1:B:78:ARG:C	2.57	0.43
1:A:736:TRP:HB2	1:A:761:TRP:CD2	2.53	0.43
1:B:215:ASN:HB3	1:B:261:SER:HB3	2.00	0.43
1:A:392:GLU:CG	1:A:424:HIS:HB3	2.47	0.43
1:A:636:PHE:C	1:A:636:PHE:CD1	2.91	0.43
1:A:656:ASN:OD1	1:A:658:ALA:HB3	2.18	0.43
1:B:446:GLN:HE21	1:B:491:TRP:CB	2.27	0.43
1:A:307:VAL:HA	1:A:337:GLU:O	2.18	0.43
1:A:431:MET:HB2	1:A:431:MET:HE2	1.83	0.43
1:B:430:ILE:HG13	1:B:443:ILE:CD1	2.49	0.43
1:A:792:ASN:O	1:A:799:ALA:HA	2.18	0.43
1:B:168:SER:CB	1:B:210:ARG:HH22	2.31	0.43
1:B:527:ARG:C	1:B:527:ARG:HD2	2.38	0.43
1:A:789:TYR:CZ	1:A:802:GLY:HA3	2.54	0.43
1:B:418:HIS:CD2	1:B:455:ASN:ND2	2.66	0.43
1:A:553:ASP:OD1	1:A:564:ARG:NH2	2.52	0.42
1:A:638:ILE:HB	1:A:670:THR:HB	2.00	0.42
1:B:464:PRO:HA	1:B:472:HIS:O	2.19	0.42
1:B:694:LYS:NZ	1:B:709:PRO:O	2.51	0.42
1:B:47:GLU:OE1	1:B:88:LYS:HB2	2.19	0.42
1:B:691:TYR:C	1:B:691:TYR:CD1	2.93	0.42
1:A:380:ARG:HD3	1:A:788:THR:HB	2.01	0.42
1:A:506:TRP:CZ2	1:A:508:GLY:HA2	2.55	0.42
1:B:394:TYR:CZ	1:B:422:GLY:HA3	2.55	0.42
1:B:737:GLN:O	1:B:759:ASP:HA	2.19	0.42
1:A:380:ARG:HA	1:A:801:TYR:CE2	2.55	0.42
1:A:435:PRO:HD3	1:A:503:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:THR:HB	1:B:741:TRP:CE2	2.55	0.42
1:B:180:PHE:HA	1:B:780:ASN:HD21	1.85	0.42
1:A:435:PRO:HD3	1:A:503:PHE:CE1	2.55	0.41
1:B:341:ASN:HB2	1:B:342:PRO:HD2	2.02	0.41
1:B:137:LEU:HD21	1:B:413:LYS:NZ	2.34	0.41
1:B:430:ILE:CG1	1:B:443:ILE:CD1	2.98	0.41
1:B:646:GLU:HG3	1:B:651:ASN:ND2	2.36	0.41
1:B:373:GLY:HA3	1:B:749:ARG:HG3	2.01	0.41
1:B:792:ASN:HD22	1:B:800:SER:HB2	1.85	0.41
1:A:192:THR:HA	1:A:193:PRO:HD2	1.92	0.41
1:B:148:THR:OG1	1:B:149:PRO:HD2	2.20	0.41
1:A:407:ALA:O	1:A:409:GLY:N	2.52	0.41
1:A:436:ALA:HB1	1:A:437:PRO:HD2	2.02	0.41
1:A:395:THR:HA	1:A:420:ILE:O	2.21	0.41
1:B:74:PRO:HG3	1:B:303:GLU:CG	2.50	0.41
1:A:330:SER:O	1:A:353:GLN:HA	2.21	0.41
1:B:410:TRP:HH2	1:B:474:LEU:HD23	1.86	0.41
1:A:308:ARG:NH2	1:A:339:ASP:OD1	2.54	0.41
1:A:547:LEU:HD23	1:A:547:LEU:HA	1.89	0.41
1:A:718:SER:HA	1:A:730:VAL:O	2.21	0.41
1:B:169:ILE:HD12	1:B:248:VAL:O	2.21	0.41
1:B:62:PHE:CZ	1:B:95:ILE:HB	2.56	0.41
1:B:207:TYR:HB2	1:B:214:ILE:HB	2.04	0.40
1:B:88:LYS:O	1:B:89:LEU:HD23	2.20	0.40
1:A:294:GLU:OE2	4:A:1823:PO4:O4	2.38	0.40
1:A:203:ASP:OD1	1:A:325:TYR:OH	2.33	0.40
1:A:674:GLU:HA	1:A:691:TYR:O	2.22	0.40
1:A:62:PHE:CZ	1:A:95:ILE:HB	2.56	0.40
1:B:645:GLU:HG3	1:B:646:GLU:H	1.86	0.40
1:A:229:VAL:HA	1:A:232:SER:HB3	2.03	0.40
1:A:55:LEU:HD23	1:A:77:VAL:HG12	2.03	0.40
1:B:506:TRP:CE2	1:B:508:GLY:HA2	2.56	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	771/772 (100%)	718 (93%)	40 (5%)	13 (2%)	11 38
1	B	750/772 (97%)	707 (94%)	38 (5%)	5 (1%)	26 63
2	C	4/10 (40%)	4 (100%)	0	0	100 100
All	All	1525/1554 (98%)	1429 (94%)	78 (5%)	18 (1%)	16 48

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	408	ASN
1	A	646	GLU
1	A	653	LYS
1	A	699	ASP
1	B	202	THR
1	B	408	ASN
1	A	182	LEU
1	A	324	HIS
1	A	651	ASN
1	B	78	ARG
1	B	495	ASN
1	A	287	SER
1	A	603	SER
1	A	647	ASP
1	A	220	ASP
1	B	786	ASP
1	A	683	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	A	651/650 (100%)	579 (89%)	72 (11%)	8 22
1	B	637/650 (98%)	569 (89%)	68 (11%)	8 24
2	C	3/3 (100%)	3 (100%)	0	100 100
All	All	1291/1303 (99%)	1151 (89%)	140 (11%)	8 24

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ILE
1	A	71	LEU
1	A	81	ARG
1	A	97	GLU
1	A	100	ARG
1	A	109	GLN
1	A	114	THR
1	A	131	MET
1	A	133	THR
1	A	143	ASP
1	A	148	THR
1	A	157	ARG
1	A	204	ARG
1	A	245	ARG
1	A	246	VAL
1	A	248	VAL
1	A	272	LYS
1	A	288	TRP
1	A	295	LEU
1	A	297	VAL
1	A	307	VAL
1	A	312	VAL
1	A	318	LYS
1	A	326	GLU
1	A	329	THR
1	A	331	VAL
1	A	343	ASP
1	A	372	GLN
1	A	379	SER
1	A	392	GLU
1	A	401	ASN
1	A	408	ASN
1	A	417	ASP
1	A	431	MET

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Mol	Chain	Res	Type
1	A	458	ASP
1	A	459	ILE
1	A	470	ARG
1	A	475	VAL
1	A	499	THR
1	A	524	ASP
1	A	528	GLN
1	A	542	ASP
1	A	551	VAL
1	A	556	VAL
1	A	557	THR
1	A	564	ARG
1	A	596	GLN
1	A	603	SER
1	A	609	GLU
1	A	615	ASN
1	A	618	ILE
1	A	641	GLU
1	A	646	GLU
1	A	653	LYS
1	A	659	ILE
1	A	660	THR
1	A	676	GLU
1	A	683	PRO
1	A	694	LYS
1	A	698	ASP
1	A	699	ASP
1	A	705	SER
1	A	720	LYS
1	A	730	VAL
1	A	739	LYS
1	A	758	GLU
1	A	766	MET
1	A	788	THR
1	A	792	ASN
1	A	810	SER
1	A	811	THR
1	A	815	PHE
1	B	68	ILE
1	B	78	ARG
1	B	83	SER
1	B	96	THR

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Mol	Chain	Res	Type
1	B	105	SER
1	B	106	VAL
1	B	113	ILE
1	B	114	THR
1	B	139	THR
1	B	152	ILE
1	B	154	THR
1	B	157	ARG
1	B	168	SER
1	B	176	ASN
1	B	177	MET
1	B	201	ASP
1	B	236	THR
1	B	238	SER
1	B	245	ARG
1	B	278	LYS
1	B	303	GLU
1	B	329	THR
1	B	331	VAL
1	B	360	SER
1	B	396	ARG
1	B	413	LYS
1	B	416	LEU
1	B	417	ASP
1	B	440	SER
1	B	447	LYS
1	B	454	SER
1	B	459	ILE
1	B	481	SER
1	B	493	LEU
1	B	495	ASN
1	B	512	LYS
1	B	533	MET
1	B	551	VAL
1	B	556	VAL
1	B	557	THR
1	B	564	ARG
1	B	566	SER
1	B	568	ARG
1	B	585	VAL
1	B	596	GLN
1	B	598	SER

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Mol	Chain	Res	Type
1	B	618	ILE
1	B	649	LEU
1	B	660	THR
1	B	671	LYS
1	B	681	LEU
1	B	687	VAL
1	B	688	GLN
1	B	694	LYS
1	B	699	ASP
1	B	720	LYS
1	B	744	VAL
1	B	747	ASN
1	B	759	ASP
1	B	764	ASP
1	B	766	MET
1	B	772	THR
1	B	774	LYS
1	B	788	THR
1	B	792	ASN
1	B	810	SER
1	B	811	THR
1	B	815	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	79	ASN
1	A	183	ASN
1	A	205	ASN
1	A	218	GLN
1	A	372	GLN
1	A	401	ASN
1	A	408	ASN
1	A	439	ASN
1	A	455	ASN
1	A	505	ASN
1	A	520	GLN
1	A	596	GLN
1	A	615	ASN
1	A	710	GLN
1	A	806	ASN

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Mol	Chain	Res	Type
1	B	109	GLN
1	B	176	ASN
1	B	205	ASN
1	B	418	HIS
1	B	455	ASN
1	B	466	GLN
1	B	472	HIS
1	B	780	ASN
1	B	792	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ORN	C	10	2	5,7,8	0.44	0	5,7,9	1.13	1 (20%)
2	FH7	C	11	2,6	7,10,11	2.76	1 (14%)	6,11,13	1.98	2 (33%)
2	DSN	C	3	2,5	3,5,6	0.68	0	3,5,7	1.13	0
2	FHO	C	6	2,6	7,10,11	2.51	1 (14%)	6,11,13	1.92	2 (33%)
2	DSN	C	8	2	3,5,6	0.61	0	3,5,7	1.17	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
2	ORN	C	10	2	-	0/4/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FH7	C	11	2,6	-	0/6/10/12	0/0/0/0
2	DSN	C	3	2,5	-	0/2/4/6	0/0/0/0
2	FHO	C	6	2,6	-	0/6/10/12	0/0/0/0
2	DSN	C	8	2	-	0/2/4/6	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	FH7	OZ-NE	-7.23	1.23	1.43
2	C	6	FHO	OZ-NE	-6.38	1.26	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	11	FH7	O-C-CA	-2.72	118.43	125.72
2	C	6	FHO	O-C-CA	-2.11	120.06	125.72
2	C	10	ORN	O-C-CA	-2.10	120.08	125.72
2	C	11	FH7	CG-CD-NE	2.53	116.06	111.09
2	C	6	FHO	CG-CD-NE	3.13	117.25	111.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	11	FH7	1	0
2	C	6	FHO	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	N8E	A	1816	-	23,23,23	0.60	0	22,22,22	0.44	0
3	N8E	A	1817[A]	-	23,23,23	0.77	0	22,22,22	0.83	0
3	N8E	A	1817[B]	-	23,23,23	0.80	0	22,22,22	0.77	1 (4%)
4	PO4	A	1818	-	4,4,4	0.21	0	6,6,6	0.31	0
4	PO4	A	1819	-	4,4,4	0.66	0	6,6,6	0.35	0
4	PO4	A	1820	-	4,4,4	0.70	0	6,6,6	0.28	0
4	PO4	A	1821	-	4,4,4	0.71	0	6,6,6	0.24	0
4	PO4	A	1822	-	4,4,4	0.62	0	6,6,6	0.24	0
4	PO4	A	1823	-	4,4,4	0.62	0	6,6,6	0.25	0
4	PO4	B	1818	-	4,4,4	0.54	0	6,6,6	0.30	0
4	PO4	B	1819	-	4,4,4	0.54	0	6,6,6	0.26	0
4	PO4	B	1820	-	4,4,4	0.62	0	6,6,6	0.23	0
4	PO4	B	1821	-	4,4,4	0.69	0	6,6,6	0.25	0
5	PVE	C	1	2,6	23,28,29	2.64	5 (21%)	22,40,42	1.38	5 (22%)

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	N8E	A	1816	-	-	0/21/21/21	0/0/0/0
3	N8E	A	1817[A]	-	-	0/21/21/21	0/0/0/0
3	N8E	A	1817[B]	-	-	0/21/21/21	0/0/0/0
4	PO4	A	1818	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1819	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1820	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1821	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1822	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1823	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1818	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1819	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1820	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1821	-	-	0/0/0/0	0/0/0/0
5	PVE	C	1	2,6	-	0/7/21/23	0/2/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	PVE	C20-C18	-9.82	1.32	1.51
5	C	1	PVE	C9-N1	-2.26	1.37	1.40
5	C	1	PVE	C4-C3	2.25	1.42	1.37
5	C	1	PVE	C5-C6	4.61	1.41	1.37
5	C	1	PVE	C8-C7	4.68	1.42	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1	PVE	C21-C20-C18	-3.00	105.36	112.93
5	C	1	PVE	C8-C7-C6	-2.12	118.68	119.91
5	C	1	PVE	O19-C18-N17	2.02	127.31	123.77
5	C	1	PVE	O26-C7-C8	2.05	125.91	120.67
3	A	1817[B]	N8E	O18-C19-C20	2.32	120.71	110.40
5	C	1	PVE	C5-C6-C7	2.40	121.30	119.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1817[B]	N8E	6	0
4	A	1823	PO4	2	0
4	B	1818	PO4	1	0
4	B	1820	PO4	1	0
4	B	1821	PO4	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

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	772/772 (100%)	-0.50	7 (0%) 85 84	3, 17, 27, 37	0
1	B	754/772 (97%)	-0.34	11 (1%) 76 74	3, 15, 24, 62	0
2	C	5/10 (50%)	-0.74	0 100 100	6, 7, 9, 10	0
All	All	1531/1554 (98%)	-0.42	18 (1%) 81 78	3, 16, 26, 62	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	ALA	4.4
1	A	123	SER	4.1
1	B	581	ASP	3.3
1	B	566	SER	3.2
1	A	44	GLN	3.1
1	B	109	GLN	3.0
1	B	44	GLN	2.9
1	B	723	GLY	2.7
1	B	683	PRO	2.5
1	B	722	LYS	2.5
1	B	626	ASP	2.4
1	A	724	ALA	2.4
1	A	303	GLU	2.4
1	B	699	ASP	2.3
1	B	78	ARG	2.2
1	A	773	ASP	2.1
1	A	723	GLY	2.1
1	A	758	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	FHO	C	6	11/12	0.99	0.12	-	4,6,7,8	0
2	ORN	C	10	8/9	0.97	0.14	-	7,8,8,9	0
2	FH7	C	11	11/12	0.97	0.14	-	4,7,8,8	0
2	DSN	C	8	6/7	0.93	0.16	-	9,10,10,11	0
2	DSN	C	3	6/7	0.94	0.16	-	5,7,7,8	0

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	N8E	A	1816	24/24	0.85	0.39	6.86	40,57,59,60	0
4	PO4	A	1822	5/5	0.95	0.18	4.30	55,56,57,58	0
3	N8E	A	1817[A]	24/24	0.86	0.28	3.35	2,4,10,12	24
3	N8E	A	1817[B]	24/24	0.86	0.28	2.39	2,2,8,11	24
4	PO4	A	1823	5/5	0.96	0.20	2.39	46,46,48,49	0
4	PO4	B	1818	5/5	0.97	0.29	1.40	37,38,39,39	0
5	PVE	C	1	26/27	0.95	0.15	0.36	2,5,35,39	5
4	PO4	A	1820	5/5	0.97	0.12	-0.37	25,26,28,29	0
4	PO4	B	1820	5/5	0.96	0.11	-0.79	40,40,42,42	0
4	PO4	B	1819	5/5	0.98	0.08	-2.42	19,20,22,22	0
4	PO4	A	1819	5/5	0.98	0.09	-3.18	16,17,18,22	0
4	PO4	A	1818	5/5	0.99	0.12	-4.38	10,11,15,16	0
4	PO4	A	1821	5/5	0.96	0.42	-	54,54,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	PO4	B	1821	5/5	0.97	0.17	-	41,43,43,44	0
6	FE	C	2	1/1	1.00	0.12	-	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.