Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:11 AM GMT

PDB ID	:	2W77
Title	:	STRUCTURES OF P. AERUGINOSA FPVA BOUND TO HETEROLOGOUS PYOVERDINES: FPVA-PVD(PFL18.1)-FE COMPLEX
Authors	:	Greenwald, J.; Nader, M.; Celia, H.; Gruffaz, C.; Meyer, J.-M.; Schalk, I.J.; Pattus, F.
Deposited on	:	2008-12-20
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:

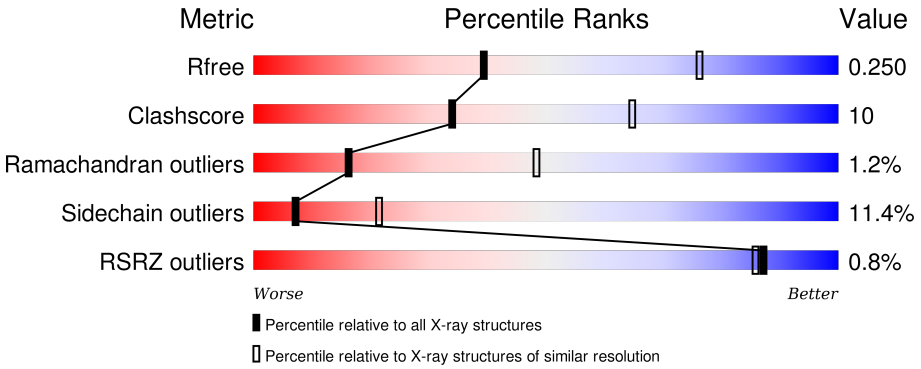
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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	% 72% 23% 5%
1	B	772	% 72% 22% . . .
2	C	10	60% 20% 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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12329 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.

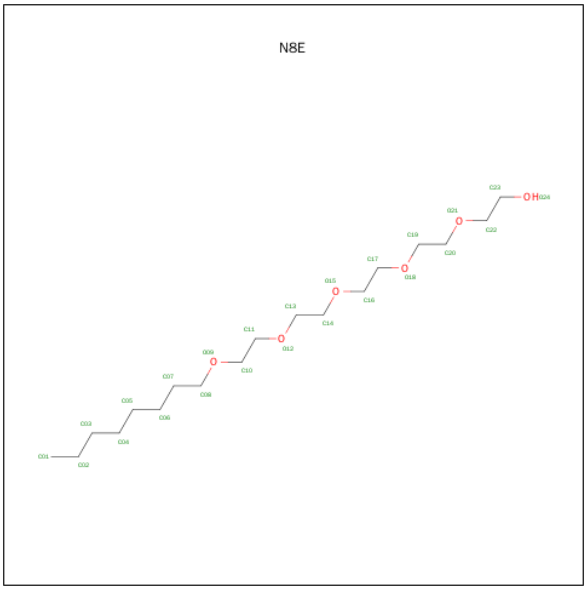
- Molecule 1 is a protein called FERRIPYOVERDINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	0	0	0
			6114	3845	1046	1211	12			
1	B	754	Total	C	N	O	S	0	0	0
			5994	3775	1027	1181	11			

- Molecule 2 is a protein called PYOVERDIN 18-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			72	40	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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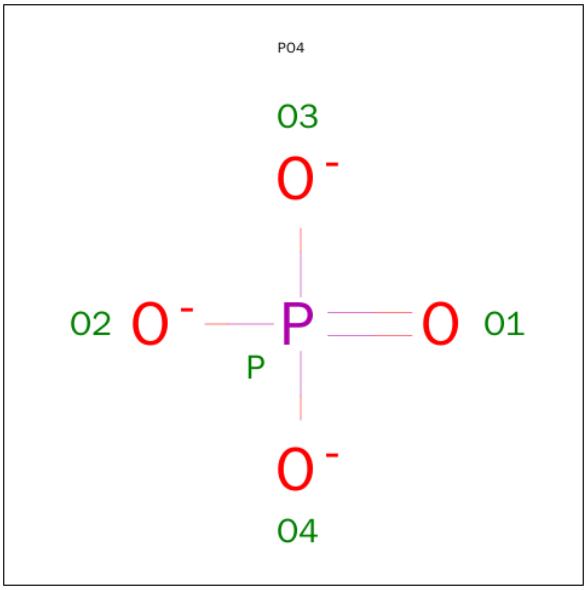
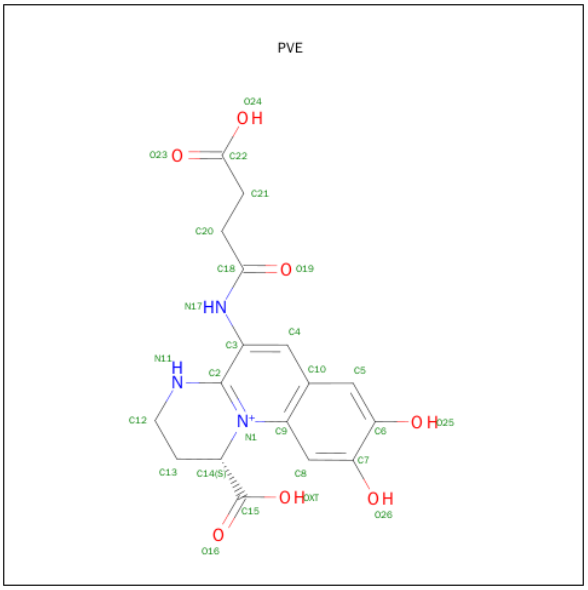
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 48 36 12	0	1

- 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
			Total	C	N	O		
5	C	1	26	17	3	6	5	0

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

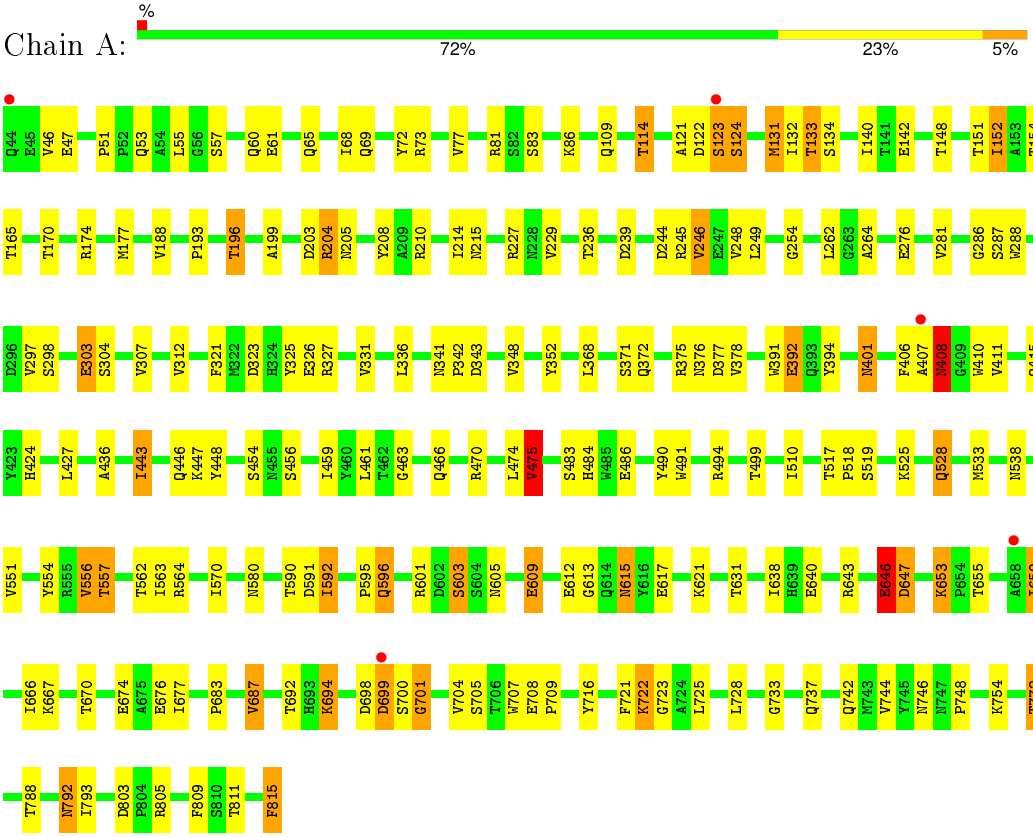
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
6	C	1	1	1	0	0

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.

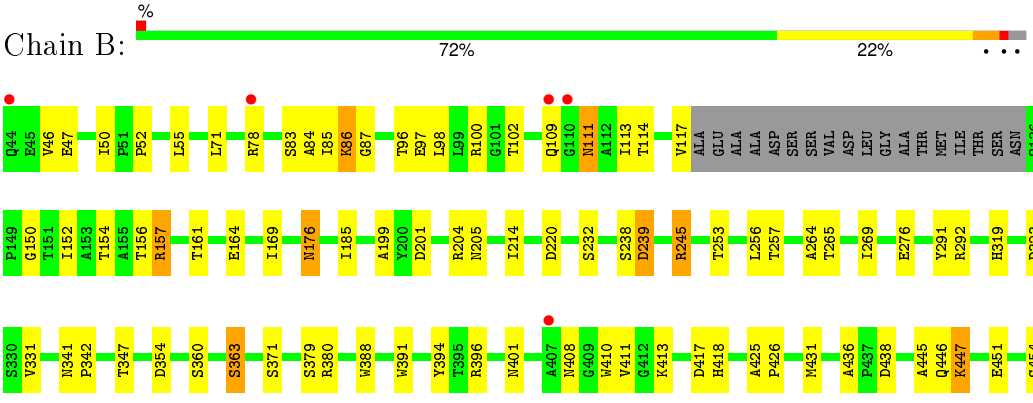
- Molecule 1: FERRIPYOVERDINE RECEPTOR

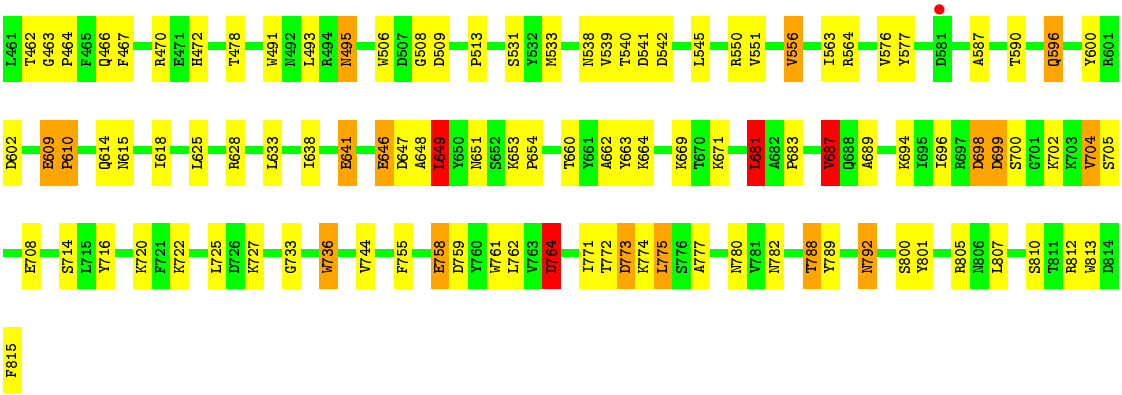
Chain A:



- Molecule 1: FERRIPYOVERDINE RECEPTOR

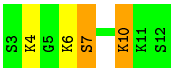
Chain B:





- Molecule 2: PYOVERDIN 18-1

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	194.77Å 130.02Å 141.33Å 90.00° 130.92° 90.00°	Depositor
Resolution (Å)	25.57 – 2.90 24.86 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (25.57-2.90) 96.9 (24.86-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.253 0.202 , 0.250	Depositor DCC
R_{free} test set	2892 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.6	EDS
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 57117 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12329	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: DSN, FHO, PO4, N8E, PVE, FE, 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	0.93	1/6266 (0.0%)	0.98	11/8514 (0.1%)
1	B	0.85	4/6145 (0.1%)	0.91	10/8347 (0.1%)
2	C	0.82	0/34	0.95	0/36
All	All	0.89	5/12445 (0.0%)	0.95	21/16897 (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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	758	GLU	CG-CD	6.28	1.61	1.51
1	A	61	GLU	CG-CD	6.17	1.61	1.51
1	B	326	GLU	CG-CD	5.66	1.60	1.51
1	B	736	TRP	CB-CG	5.37	1.59	1.50
1	B	758	GLU	CB-CG	5.27	1.62	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	687	VAL	CB-CA-C	-7.60	96.95	111.40
1	B	681	LEU	CA-CB-CG	6.44	130.12	115.30
1	B	150	GLY	N-CA-C	-6.33	97.28	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	683	PRO	C-N-CA	-6.14	109.41	122.30
1	B	764	ASP	CB-CG-OD1	-6.04	112.86	118.30
1	B	649	LEU	CB-CG-CD1	5.91	121.05	111.00
1	A	474	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	336	LEU	CA-CB-CG	5.87	128.81	115.30
1	A	803	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	475	VAL	CB-CA-C	-5.78	100.43	111.40
1	A	647	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	687	VAL	CB-CA-C	-5.70	100.57	111.40
1	B	239	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	B	220	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	208	TYR	CA-CB-CG	5.31	123.50	113.40
1	A	292	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	377	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	354	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	A	210	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	633	LEU	CA-CB-CG	5.07	126.96	115.30
1	B	323	ASP	CB-CG-OD1	-5.03	113.77	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	408	ASN	Peptide
1	B	698	ASP	Peptide

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	6114	0	5788	128	0
1	B	5994	0	5675	115	0
2	C	72	0	65	2	0
3	A	72	0	114	8	0
4	A	30	0	0	0	0
4	B	20	0	0	2	0
5	C	26	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1	0	0	0	0
All	All	12329	0	11656	243	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 10.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:772:THR:HG22	1:B:774:LYS:H	1.07	1.16
1:A:722:LYS:HE2	1:A:723:GLY:H	1.21	1.01
1:A:742:GLN:HG3	1:A:793:ILE:O	1.63	0.97
1:B:446:GLN:HE21	1:B:491:TRP:HB2	1.27	0.97
1:A:772:THR:HG22	1:A:774:LYS:H	1.29	0.96
1:B:772:THR:HG22	1:B:774:LYS:N	1.87	0.89
1:B:694:LYS:HE3	1:B:708:GLU:OE1	1.74	0.87
1:A:60:GLN:NE2	1:A:134:SER:HA	1.90	0.85
1:B:744:VAL:HG22	1:B:755:PHE:HE1	1.40	0.83
1:A:556:VAL:HG13	1:A:563:ILE:HB	1.60	0.83
1:B:744:VAL:CG2	1:B:755:PHE:HE1	1.92	0.82
1:A:772:THR:HG21	1:B:291:TYR:OH	1.79	0.81
1:A:53:GLN:OE1	1:A:57:SER:HB2	1.81	0.81
1:B:698:ASP:HB3	1:B:700:SER:H	1.43	0.81
1:B:446:GLN:HE21	1:B:491:TRP:CB	1.94	0.80
1:B:472:HIS:HD2	1:B:538:ASN:H	1.25	0.80
1:A:470:ARG:NH1	1:A:538:ASN:OD1	2.15	0.79
1:B:646:GLU:O	1:B:662:ALA:O	2.00	0.79
1:B:764:ASP:HB3	1:B:782:ASN:HA	1.65	0.79
1:A:777:ALA:HB1	3:A:1817[B]:N8E:H192	1.63	0.78
1:A:73:ARG:HG3	1:A:131:MET:CE	2.13	0.78
1:B:744:VAL:HG22	1:B:755:PHE:CE1	2.18	0.77
1:A:805:ARG:HD2	3:A:1817[A]:N8E:H031	1.66	0.77
1:A:722:LYS:HE2	1:A:723:GLY:N	2.00	0.76
1:A:151:THR:O	1:A:152:ILE:HD13	1.85	0.76
1:B:744:VAL:CG2	1:B:755:PHE:CE1	2.69	0.76
1:B:772:THR:CG2	1:B:774:LYS:H	1.96	0.73
1:B:446:GLN:NE2	1:B:491:TRP:HB2	2.01	0.73
1:B:446:GLN:NE2	1:B:491:TRP:CB	2.51	0.73
1:A:239:ASP:OD2	1:A:292:ARG:NH2	2.20	0.72
1:B:681:LEU:HD13	1:B:687:VAL:HG22	1.69	0.72
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:HG3	1:A:131:MET:HE1	1.71	0.71
1:B:341:ASN:HB2	1:B:342:PRO:CD	2.21	0.70
1:A:410:TRP:CD2	1:A:463:GLY:HA3	2.27	0.70
1:A:694:LYS:HE3	1:A:708:GLU:OE1	1.92	0.69
1:A:443:ILE:N	1:A:443:ILE:HD13	2.08	0.68
1:A:371:SER:OG	1:A:436:ALA:HA	1.94	0.67
1:B:111:ASN:N	1:B:111:ASN:HD22	1.91	0.67
1:A:408:ASN:HB3	1:A:410:TRP:H	1.60	0.67
1:A:410:TRP:CE2	1:A:463:GLY:HA3	2.30	0.66
1:A:73:ARG:CG	1:A:131:MET:HE3	2.26	0.66
1:B:540:THR:HG22	1:B:541:ASP:N	2.11	0.66
1:B:472:HIS:CD2	1:B:538:ASN:H	2.11	0.66
1:A:707:TRP:CH2	1:A:793:ILE:HG13	2.31	0.65
1:B:542:ASP:O	1:B:577:TYR:HA	1.95	0.65
1:B:204:ARG:HD3	1:B:391:TRP:CH2	2.31	0.65
1:A:53:GLN:OE1	1:A:57:SER:CB	2.44	0.65
1:B:614:GLN:OE1	1:B:641:GLU:OE2	2.15	0.64
1:B:587:ALA:HB2	1:B:618:ILE:HG13	1.80	0.62
1:A:73:ARG:HG3	1:A:131:MET:HE3	1.81	0.61
1:B:97:GLU:OE2	1:B:100:ARG:HD2	2.00	0.61
1:A:72:TYR:C	1:A:131:MET:HE2	2.21	0.61
1:B:111:ASN:H	1:B:111:ASN:HD22	1.47	0.60
1:A:109:GLN:OE1	1:A:114:THR:HG22	2.01	0.60
1:B:744:VAL:HG21	1:B:755:PHE:CE1	2.36	0.60
1:A:406:PHE:C	1:A:408:ASN:H	2.05	0.60
1:B:681:LEU:HD13	1:B:687:VAL:CG2	2.30	0.60
1:A:239:ASP:CG	1:A:292:ARG:HH22	2.05	0.60
1:B:161:THR:OG1	1:B:164:GLU:HG3	2.01	0.60
1:A:443:ILE:HG12	1:A:510:ILE:CD1	2.32	0.60
1:B:540:THR:HG22	1:B:541:ASP:H	1.67	0.60
1:A:443:ILE:CG1	1:A:510:ILE:HD12	2.31	0.59
2:C:10:LYS:O	2:C:10:LYS:HG3	2.03	0.59
1:B:71:LEU:HD12	1:B:114:THR:HG22	1.85	0.58
1:A:443:ILE:HG12	1:A:510:ILE:HD12	1.85	0.58
1:A:188:VAL:HG11	1:A:246:VAL:CG1	2.32	0.58
1:A:615:ASN:HD21	1:A:617:GLU:HB2	1.68	0.58
1:A:188:VAL:HG11	1:A:246:VAL:HG13	1.86	0.58
1:A:325:TYR:OH	1:A:327:ARG:NH1	2.36	0.58
1:B:418:HIS:CD2	1:B:455:ASN:HD21	2.21	0.57
1:B:156:THR:O	1:B:157:ARG:HB2	2.04	0.57
1:A:262:LEU:HD23	1:A:592:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.86	0.57
1:A:199:ALA:HA	1:A:205:ASN:HD22	1.68	0.57
1:B:111:ASN:N	1:B:111:ASN:ND2	2.53	0.56
1:B:470:ARG:HH12	1:B:540:THR:CA	2.17	0.56
1:A:157:ARG:HB3	1:A:475:VAL:HG11	1.87	0.56
1:B:276:GLU:N	1:B:276:GLU:OE1	2.38	0.56
1:A:570:ILE:HG23	1:A:591:ASP:HB3	1.87	0.56
1:B:418:HIS:HD2	1:B:455:ASN:HD21	1.54	0.55
1:B:52:PRO:HD3	1:B:84:ALA:HB2	1.88	0.55
1:B:470:ARG:NH2	1:B:541:ASP:OD1	2.39	0.55
1:A:262:LEU:HD11	1:A:613:GLY:HA3	1.87	0.55
1:B:156:THR:O	1:B:157:ARG:CB	2.55	0.55
1:A:368:LEU:O	1:A:376:ASN:HB2	2.06	0.55
1:A:709:PRO:HG3	1:A:737:GLN:NE2	2.22	0.55
1:A:51:PRO:O	1:A:53:GLN:HG2	2.08	0.54
1:B:698:ASP:HB3	1:B:700:SER:N	2.18	0.54
1:A:470:ARG:HD3	1:A:538:ASN:O	2.08	0.53
1:A:55:LEU:HB3	1:A:77:VAL:HB	1.89	0.53
1:B:694:LYS:HD2	1:B:694:LYS:C	2.29	0.53
1:A:254:GLY:CA	1:A:592:ILE:HG13	2.38	0.53
1:B:459:ILE:O	1:B:459:ILE:HG13	2.06	0.53
1:B:55:LEU:HD22	1:B:102:THR:HG21	1.91	0.53
1:B:736:TRP:HB2	1:B:761:TRP:CE3	2.44	0.53
1:A:391:TRP:HB2	1:A:427:LEU:HD21	1.89	0.53
1:B:446:GLN:NE2	1:B:491:TRP:HB3	2.22	0.53
1:A:447:LYS:HB3	1:A:490:TYR:HB2	1.90	0.52
1:A:291:TYR:OH	1:B:772:THR:HG21	2.09	0.52
1:A:109:GLN:OE1	1:A:114:THR:CG2	2.57	0.52
1:B:596:GLN:HG2	1:B:600:TYR:HB2	1.92	0.52
1:A:254:GLY:HA2	1:A:592:ILE:HG13	1.90	0.52
1:B:792:ASN:HB3	1:B:800:SER:HB2	1.91	0.52
1:B:775:LEU:HD12	1:B:813:TRP:HB2	1.90	0.52
1:A:525:LYS:HB2	1:A:557:THR:HG22	1.92	0.52
1:A:406:PHE:C	1:A:408:ASN:N	2.63	0.52
1:B:176:ASN:C	1:B:176:ASN:HD22	2.13	0.52
1:A:214:ILE:HG12	1:A:264:ALA:HB3	1.92	0.52
1:B:772:THR:CG2	1:B:773:ASP:N	2.72	0.51
1:A:204:ARG:NH1	1:A:229:VAL:HG12	2.26	0.51
1:B:199:ALA:HA	1:B:205:ASN:HD22	1.76	0.51
1:A:288:TRP:CZ2	1:A:321:PHE:HB3	2.44	0.51
1:A:174:ARG:CZ	1:A:177:MET:CE	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ILE:HD12	1:B:85:ILE:HD11	1.93	0.51
1:A:653:LYS:O	1:A:653:LYS:HG3	2.11	0.51
1:A:262:LEU:CD2	1:A:592:ILE:HG22	2.41	0.51
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.46	0.51
1:A:60:GLN:HE22	1:A:134:SER:HA	1.74	0.51
1:B:506:TRP:CE2	1:B:508:GLY:HA2	2.45	0.51
1:B:689:ALA:HA	1:B:714:SER:O	2.10	0.51
1:A:174:ARG:HB2	1:A:244:ASP:O	2.11	0.50
1:A:596:GLN:NE2	1:A:609:GLU:O	2.44	0.50
2:C:6:FHO:O	2:C:7:SER:HB2	2.10	0.50
1:A:446:GLN:OE1	1:A:448:TYR:OH	2.17	0.50
1:B:152:ILE:HD12	1:B:169:ILE:HG12	1.94	0.50
1:B:506:TRP:CZ2	1:B:508:GLY:HA2	2.46	0.50
1:A:239:ASP:CG	1:A:292:ARG:NH2	2.64	0.50
1:B:426:PRO:HB3	1:B:447:LYS:HG3	1.93	0.49
1:A:809:PHE:HD2	3:A:1817[B]:N8E:H201	1.77	0.49
1:A:73:ARG:HG2	1:A:131:MET:HE3	1.93	0.49
1:A:203:ASP:OD1	1:A:325:TYR:OH	2.23	0.49
1:A:725:LEU:HD22	3:A:1817[B]:N8E:H062	1.93	0.49
3:A:1817[B]:N8E:H031	1:B:805:ARG:HD2	1.95	0.49
1:A:158:LEU:HD21	1:A:475:VAL:HG22	1.95	0.48
1:A:165:THR:O	1:A:621:LYS:NZ	2.45	0.48
1:A:638:ILE:HB	1:A:670:THR:HB	1.95	0.48
1:B:410:TRP:CD1	1:B:464:PRO:HD2	2.48	0.48
1:A:646:GLU:O	1:A:662:ALA:O	2.32	0.48
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.49	0.48
1:B:762:LEU:HD21	1:B:789:TYR:CE1	2.49	0.48
1:A:484:HIS:CE1	1:A:486:GLU:OE2	2.66	0.48
1:A:123:SER:O	1:A:124:SER:HB3	2.14	0.48
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.49	0.47
1:B:363:SER:OG	1:B:431:MET:CE	2.62	0.47
1:B:86:LYS:HG3	1:B:87:GLY:N	2.30	0.47
1:B:602:ASP:HA	1:B:663:TYR:O	2.14	0.47
1:A:631:THR:HG22	1:A:677:ILE:HG13	1.96	0.47
1:A:666:ILE:HD12	1:A:698:ASP:HB2	1.97	0.47
1:B:371:SER:OG	1:B:436:ALA:HA	2.15	0.47
1:A:805:ARG:HH11	3:A:1817[A]:N8E:H031	1.78	0.47
1:A:196:THR:HG21	1:A:709:PRO:CD	2.45	0.47
1:A:605:ASN:HA	1:A:659:ILE:HG12	1.96	0.47
1:B:696:ILE:HG23	1:B:704:VAL:HG12	1.97	0.47
1:B:380:ARG:HD3	1:B:788:THR:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ILE:HD13	1:B:264:ALA:HB3	1.97	0.46
1:A:694:LYS:HE3	1:A:708:GLU:CD	2.34	0.46
1:A:491:TRP:CE2	1:A:519:SER:HB3	2.51	0.46
1:A:417:ASP:HB2	1:A:456:SER:HB2	1.96	0.46
1:B:540:THR:CG2	1:B:541:ASP:N	2.77	0.46
1:B:98:LEU:HD23	1:B:98:LEU:C	2.34	0.46
1:A:443:ILE:CD1	1:A:443:ILE:N	2.78	0.46
1:B:647:ASP:HB2	1:B:664:LYS:HG2	1.97	0.46
1:B:556:VAL:HG13	1:B:563:ILE:HB	1.98	0.46
1:B:638:ILE:O	1:B:669:LYS:HA	2.16	0.46
1:A:454:SER:OG	1:A:483:SER:HB3	2.16	0.46
1:B:467:PHE:HB3	1:B:472:HIS:HE1	1.80	0.45
1:B:470:ARG:HH12	1:B:540:THR:N	2.14	0.45
1:B:418:HIS:HE1	4:B:1819:PO4:O1	1.98	0.45
1:A:700:SER:OG	1:A:701:GLY:N	2.48	0.45
1:A:72:TYR:C	1:A:131:MET:CE	2.84	0.45
1:B:625:LEU:O	1:B:628:ARG:HD3	2.17	0.45
1:A:170:THR:HG21	1:A:193:PRO:HD2	1.98	0.45
1:B:467:PHE:HB3	1:B:472:HIS:CE1	2.51	0.45
1:A:655:THR:O	1:A:655:THR:HG22	2.17	0.45
1:A:443:ILE:CG1	1:A:510:ILE:CD1	2.91	0.45
1:A:746:ASN:OD1	1:A:748:PRO:HD2	2.16	0.45
1:A:392:GLU:HG3	1:A:424:HIS:HB3	1.98	0.45
1:B:394:TYR:OH	1:B:451:GLU:HG3	2.16	0.45
1:A:640:GLU:CD	1:A:643:ARG:HB2	2.37	0.45
1:B:540:THR:CG2	1:B:541:ASP:H	2.29	0.44
1:B:388:TRP:CZ2	1:B:513:PRO:HD3	2.52	0.44
1:A:281:VAL:HG23	1:A:815:PHE:CZ	2.52	0.44
1:A:694:LYS:CE	1:A:708:GLU:OE1	2.62	0.44
1:B:425:ALA:O	1:B:447:LYS:HA	2.18	0.44
1:A:196:THR:HG21	1:A:709:PRO:HD3	1.99	0.44
1:B:380:ARG:HA	1:B:801:TYR:CE2	2.52	0.44
1:B:157:ARG:HD3	1:B:256:LEU:HD13	1.99	0.44
1:A:262:LEU:HD23	1:A:592:ILE:CG2	2.47	0.44
1:A:554:TYR:CD2	1:A:595:PRO:HG2	2.53	0.44
1:B:117:VAL:HG12	1:B:117:VAL:O	2.18	0.44
3:A:1817[A]:N8E:H062	1:B:725:LEU:HD23	2.00	0.44
1:B:470:ARG:NH1	1:B:539:VAL:C	2.71	0.44
1:A:46:VAL:CG1	1:A:47:GLU:N	2.80	0.43
1:A:667:LYS:HB2	1:A:699:ASP:OD2	2.19	0.43
1:B:590:THR:O	1:B:614:GLN:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:O	1:A:264:ALA:HA	2.19	0.43
1:A:596:GLN:HB2	1:A:596:GLN:HE21	1.55	0.43
1:A:140:ILE:HG23	1:A:244:ASP:OD1	2.17	0.43
1:A:158:LEU:CD2	1:A:475:VAL:HG22	2.49	0.43
1:B:410:TRP:CD2	1:B:463:GLY:HA3	2.54	0.43
1:A:533:MET:O	1:A:548:GLY:HA3	2.19	0.43
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.54	0.42
1:A:443:ILE:HG13	1:A:510:ILE:HD12	2.00	0.42
1:B:780:ASN:O	1:B:807:LEU:HA	2.19	0.42
1:B:648:ALA:HA	1:B:651:ASN:HB2	2.00	0.42
1:B:812:ARG:NH2	4:B:1818:PO4:O4	2.35	0.42
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.55	0.42
1:A:674:GLU:HG3	1:A:692:THR:OG1	2.20	0.42
1:B:245:ARG:NH1	1:B:269:ILE:HG13	2.33	0.42
1:B:239:ASP:OD2	1:B:292:ARG:NH2	2.52	0.42
1:B:438:ASP:OD1	1:B:438:ASP:N	2.53	0.42
1:A:281:VAL:HG22	1:A:295:LEU:HD13	2.00	0.42
1:A:772:THR:HG22	1:A:774:LYS:N	2.13	0.41
1:A:615:ASN:ND2	1:A:617:GLU:HB2	2.35	0.41
1:A:517:THR:O	1:A:518:PRO:C	2.57	0.41
1:A:408:ASN:CB	1:A:410:TRP:HB2	2.50	0.41
1:A:528:GLN:HG2	1:A:554:TYR:HD1	1.86	0.41
1:A:244:ASP:O	1:A:245:ARG:HB3	2.20	0.41
1:B:413:LYS:HE2	1:B:460:TYR:OH	2.20	0.41
1:B:609:GLU:HG3	1:B:610:PRO:HD2	2.03	0.41
3:A:1817[A]:N8E:H201	1:B:777:ALA:HB1	2.02	0.41
1:B:347:THR:HB	1:B:401:ASN:HB2	2.02	0.41
1:A:721:PHE:CD2	1:A:728:LEU:HD23	2.56	0.41
1:B:646:GLU:O	1:B:647:ASP:HB3	2.21	0.41
1:A:590:THR:OG1	1:A:615:ASN:HB3	2.21	0.41
1:A:199:ALA:O	1:A:792:ASN:HB2	2.21	0.41
1:B:46:VAL:HG12	1:B:47:GLU:N	2.35	0.41
1:A:69:GLN:NE2	1:A:133:THR:HG23	2.36	0.41
1:A:406:PHE:O	1:A:408:ASN:N	2.54	0.41
1:B:649:LEU:HD12	1:B:649:LEU:O	2.22	0.40
1:A:401:ASN:ND2	1:A:415:GLN:HG2	2.36	0.40
1:A:286:GLY:O	1:A:287:SER:C	2.59	0.40
1:B:253:THR:O	1:B:257:THR:HB	2.22	0.40
1:B:363:SER:OG	1:B:431:MET:HE2	2.21	0.40
1:A:331:VAL:HA	1:A:352:TYR:O	2.21	0.40
1:B:445:ALA:O	1:B:446:GLN:CG	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ALA:HA	1:B:205:ASN:ND2	2.37	0.40
1:A:174:ARG:CZ	1:A:177:MET:HE2	2.52	0.40
1:B:531:SER:O	1:B:550:ARG:HA	2.21	0.40
1:A:646:GLU:O	1:A:663:TYR:HA	2.21	0.40
1:B:653:LYS:HA	1:B:654:PRO:HD2	1.81	0.40
1:B:185:ILE:N	1:B:238:SER:O	2.49	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	770/772 (100%)	716 (93%)	42 (6%)	12 (2%)	12 40
1	B	750/772 (97%)	702 (94%)	43 (6%)	5 (1%)	26 63
2	C	5/10 (50%)	4 (80%)	0	1 (20%)	0 0
All	All	1525/1554 (98%)	1422 (93%)	85 (6%)	18 (1%)	16 48

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
1	A	124	SER
1	A	603	SER
1	A	646	GLU
1	A	122	ASP
1	A	407	ALA
1	A	647	ASP
1	A	699	ASP
1	B	363	SER
1	B	408	ASN
1	B	699	ASP

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Mol	Chain	Res	Type
1	A	227	ARG
2	C	7	SER
1	A	303	GLU
1	A	562	THR
1	B	495	ASN
1	A	701	GLY
1	B	610	PRO

5.3.2 Protein sidechains

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	650/650 (100%)	571 (88%)	79 (12%)	6 18
1	B	637/650 (98%)	571 (90%)	66 (10%)	9 26
2	C	4/4 (100%)	2 (50%)	2 (50%)	0 0
All	All	1291/1304 (99%)	1144 (89%)	147 (11%)	7 21

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	68	ILE
1	A	81	ARG
1	A	83	SER
1	A	86	LYS
1	A	114	THR
1	A	123	SER
1	A	131	MET
1	A	132	ILE
1	A	133	THR
1	A	142	GLU
1	A	148	THR
1	A	152	ILE
1	A	154	THR
1	A	157	ARG

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Mol	Chain	Res	Type
1	A	196	THR
1	A	204	ARG
1	A	215	ASN
1	A	236	THR
1	A	246	VAL
1	A	248	VAL
1	A	276	GLU
1	A	297	VAL
1	A	298	SER
1	A	303	GLU
1	A	304	SER
1	A	307	VAL
1	A	312	VAL
1	A	323	ASP
1	A	326	GLU
1	A	343	ASP
1	A	348	VAL
1	A	372	GLN
1	A	375	ARG
1	A	378	VAL
1	A	392	GLU
1	A	401	ASN
1	A	408	ASN
1	A	411	VAL
1	A	416	LEU
1	A	417	ASP
1	A	443	ILE
1	A	459	ILE
1	A	461	LEU
1	A	466	GLN
1	A	475	VAL
1	A	494	ARG
1	A	499	THR
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	580	ASN
1	A	592	ILE
1	A	596	GLN

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Mol	Chain	Res	Type
1	A	601	ARG
1	A	603	SER
1	A	609	GLU
1	A	612	GLU
1	A	615	ASN
1	A	646	GLU
1	A	653	LYS
1	A	659	ILE
1	A	660	THR
1	A	676	GLU
1	A	687	VAL
1	A	694	LYS
1	A	704	VAL
1	A	705	SER
1	A	722	LYS
1	A	744	VAL
1	A	754	LYS
1	A	772	THR
1	A	788	THR
1	A	792	ASN
1	A	811	THR
1	A	815	PHE
1	B	78	ARG
1	B	83	SER
1	B	86	LYS
1	B	96	THR
1	B	109	GLN
1	B	111	ASN
1	B	113	ILE
1	B	148	THR
1	B	154	THR
1	B	157	ARG
1	B	176	ASN
1	B	201	ASP
1	B	232	SER
1	B	245	ARG
1	B	265	THR
1	B	319	HIS
1	B	329	THR
1	B	331	VAL
1	B	360	SER
1	B	379	SER

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Mol	Chain	Res	Type
1	B	396	ARG
1	B	411	VAL
1	B	417	ASP
1	B	447	LYS
1	B	454	SER
1	B	459	ILE
1	B	462	THR
1	B	466	GLN
1	B	478	THR
1	B	493	LEU
1	B	495	ASN
1	B	509	ASP
1	B	533	MET
1	B	545	LEU
1	B	551	VAL
1	B	556	VAL
1	B	564	ARG
1	B	576	VAL
1	B	596	GLN
1	B	609	GLU
1	B	615	ASN
1	B	641	GLU
1	B	646	GLU
1	B	649	LEU
1	B	660	THR
1	B	671	LYS
1	B	681	LEU
1	B	683	PRO
1	B	687	VAL
1	B	699	ASP
1	B	702	LYS
1	B	704	VAL
1	B	705	SER
1	B	720	LYS
1	B	722	LYS
1	B	727	LYS
1	B	758	GLU
1	B	759	ASP
1	B	764	ASP
1	B	771	ILE
1	B	773	ASP
1	B	775	LEU

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Mol	Chain	Res	Type
1	B	788	THR
1	B	792	ASN
1	B	810	SER
1	B	815	PHE
2	C	4	LYS
2	C	10	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	136	GLN
1	A	205	ASN
1	A	218	GLN
1	A	401	ASN
1	A	408	ASN
1	A	439	ASN
1	A	455	ASN
1	A	505	ASN
1	A	580	ASN
1	A	596	GLN
1	A	615	ASN
1	A	737	GLN
1	B	109	GLN
1	B	111	ASN
1	B	176	ASN
1	B	183	ASN
1	B	205	ASN
1	B	418	HIS
1	B	472	HIS
1	B	596	GLN
1	B	615	ASN
1	B	688	GLN
1	B	710	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	FH7	C	11	2,6	7,10,11	0.53	0	6,11,13	1.56	2 (33%)
2	DSN	C	3	2,5	4,5,6	0.96	0	2,5,7	1.54	1 (50%)
2	FHO	C	6	2,6	7,10,11	0.64	0	6,11,13	1.68	2 (33%)
2	DSN	C	8	2	4,5,6	0.63	0	2,5,7	1.22	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	FH7	C	11	2,6	-	0/5/10/12	0/0/0/0
2	DSN	C	3	2,5	-	0/2/4/6	0/0/0/0
2	FHO	C	6	2,6	-	0/5/10/12	0/0/0/0
2	DSN	C	8	2	-	0/2/4/6	0/0/0/0

There are no bond length outliers.

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	-2.13	119.95	125.49
2	C	6	FHO	O-C-CA	-2.12	119.96	125.49
2	C	3	DSN	O-C-CA	-2.11	119.98	125.49
2	C	6	FHO	CG-CD-NE	2.07	115.05	111.23
2	C	11	FH7	CG-CD-NE	2.56	115.94	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	FHO	1	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	0.55	0	22,22,22	0.51	0
3	N8E	A	1817[A]	-	23,23,23	0.90	0	22,22,22	0.92	0
3	N8E	A	1817[B]	-	23,23,23	0.86	0	22,22,22	0.95	1 (4%)
4	PO4	A	1818	-	4,4,4	0.25	0	6,6,6	0.33	0
4	PO4	A	1819	-	4,4,4	0.44	0	6,6,6	0.36	0
4	PO4	A	1820	-	4,4,4	0.67	0	6,6,6	0.27	0
4	PO4	A	1821	-	4,4,4	0.47	0	6,6,6	0.27	0
4	PO4	A	1822	-	4,4,4	0.35	0	6,6,6	0.28	0
4	PO4	A	1823	-	4,4,4	0.52	0	6,6,6	0.28	0
4	PO4	B	1816	-	4,4,4	0.23	0	6,6,6	0.31	0
4	PO4	B	1817	-	4,4,4	0.35	0	6,6,6	0.29	0
4	PO4	B	1818	-	4,4,4	0.52	0	6,6,6	0.31	0
4	PO4	B	1819	-	4,4,4	0.43	0	6,6,6	0.26	0
5	PVE	C	1	2,6	24,28,29	2.07	4 (16%)	24,40,42	1.43	4 (16%)

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	1816	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1817	-	-	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
5	PVE	C	1	2,6	-	0/7/21/23	0/2/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	PVE	C20-C18	-6.91	1.37	1.51
5	C	1	PVE	C14-C15	2.10	1.52	1.50
5	C	1	PVE	C8-C7	3.99	1.41	1.37
5	C	1	PVE	C5-C6	4.38	1.41	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1	PVE	C20-C18-N17	-3.58	108.47	114.52
5	C	1	PVE	C21-C20-C18	-3.20	105.17	113.01
5	C	1	PVE	C13-C12-N11	-2.31	106.73	110.29
5	C	1	PVE	C7-C8-C9	2.12	120.92	117.09
3	A	1817[B]	N8E	O18-C19-C20	2.79	122.78	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1817[A]	N8E	4	0
3	A	1817[B]	N8E	4	0
4	B	1818	PO4	1	0
4	B	1819	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%)	-0.63	5 (0%) 90 89	7, 19, 34, 52	0
1	B	754/772 (97%)	-0.51	7 (0%) 85 84	11, 24, 43, 60	0
2	C	6/10 (60%)	0.45	0 100 100	29, 38, 40, 43	0
All	All	1532/1554 (98%)	-0.57	12 (0%) 87 86	7, 21, 39, 60	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	SER	6.4
1	B	407	ALA	4.9
1	A	44	GLN	4.5
1	B	78	ARG	3.7
1	B	44	GLN	3.6
1	A	407	ALA	2.6
1	B	110	GLY	2.5
1	B	109	GLN	2.3
1	B	143	ASP	2.2
1	A	699	ASP	2.2
1	A	658	ALA	2.1
1	B	581	ASP	2.1

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

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	0.95	0.18	-	38,41,43,44	0
2	FH7	C	11	11/12	0.97	0.13	-	29,29,32,32	0
2	DSN	C	8	6/7	0.87	0.45	-	40,42,42,42	0
2	DSN	C	3	6/7	0.89	0.24	-	39,40,40,41	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
4	PO4	A	1823	5/5	0.95	0.27	6.51	62,62,63,63	0
4	PO4	A	1822	5/5	0.88	0.27	6.28	79,79,81,81	0
3	N8E	A	1816	24/24	0.90	0.29	5.33	36,48,68,70	0
3	N8E	A	1817[A]	24/24	0.85	0.29	4.69	2,2,7,8	24
3	N8E	A	1817[B]	24/24	0.85	0.29	4.00	2,2,4,6	24
4	PO4	A	1820	5/5	0.98	0.14	1.59	46,48,48,49	0
4	PO4	B	1816	5/5	0.96	0.22	1.50	43,43,44,45	0
5	PVE	C	1	26/27	0.93	0.16	1.02	38,40,59,62	5
4	PO4	A	1818	5/5	0.98	0.11	-0.41	28,31,31,32	0
4	PO4	B	1818	5/5	0.96	0.12	-0.50	53,54,55,57	0
4	PO4	B	1817	5/5	0.98	0.10	-0.73	21,22,23,24	0
4	PO4	A	1819	5/5	0.99	0.09	-1.75	17,20,24,25	0
4	PO4	A	1821	5/5	0.93	0.41	-	59,60,60,61	0
4	PO4	B	1819	5/5	0.98	0.24	-	43,44,45,46	0
6	FE	C	2	1/1	0.98	0.03	-	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.