



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:10 AM GMT

PDB ID : 2W75
Title : STRUCTURES OF P. AERUGINOSA FPVA BOUND TO HETEROLOGOUS PYOVERDINES: APO-FPVA
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

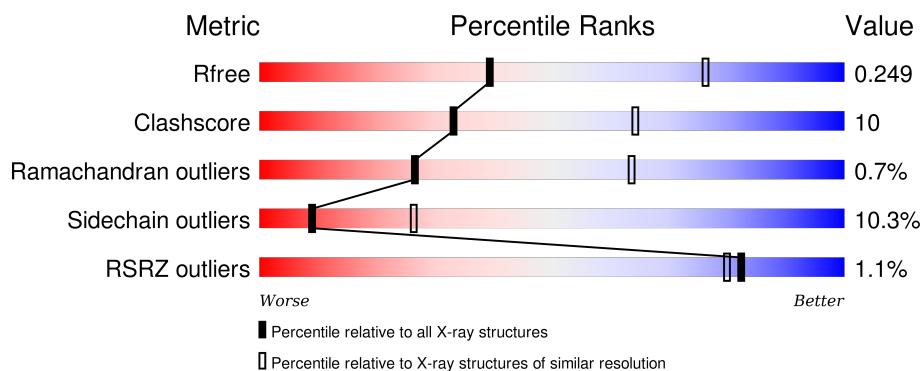
1 Overall quality at a glance

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	772	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 69%, yellow 23%, orange 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 70% 24% 5% </div> </div>
1	B	772	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 70%, yellow 23%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 72% 23% • • </div> </div>

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
2	N8E	A	1816	-	-	-	X
2	N8E	A	1817[A]	-	-	-	X
3	PO4	A	1820	-	-	-	X
3	PO4	A	1822	-	-	-	X
3	PO4	A	1823	-	-	-	X
3	PO4	B	1818	-	-	-	X

2 Entry composition [i](#)

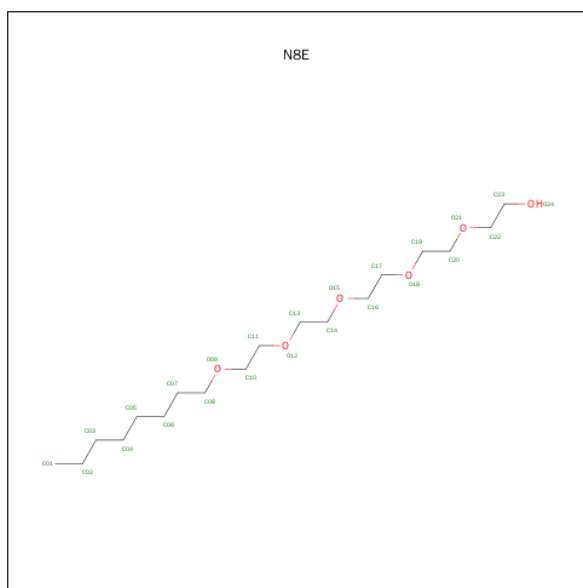
There are 3 unique types of molecules in this entry. The entry contains 12230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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



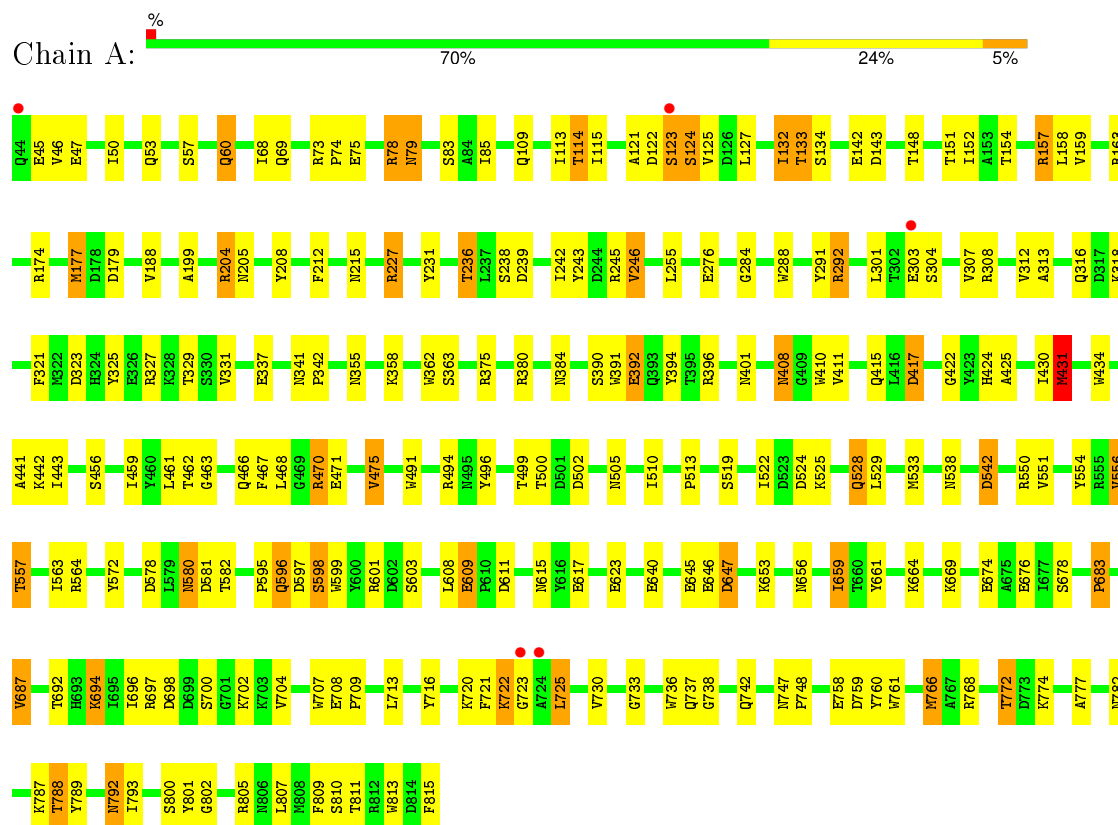


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

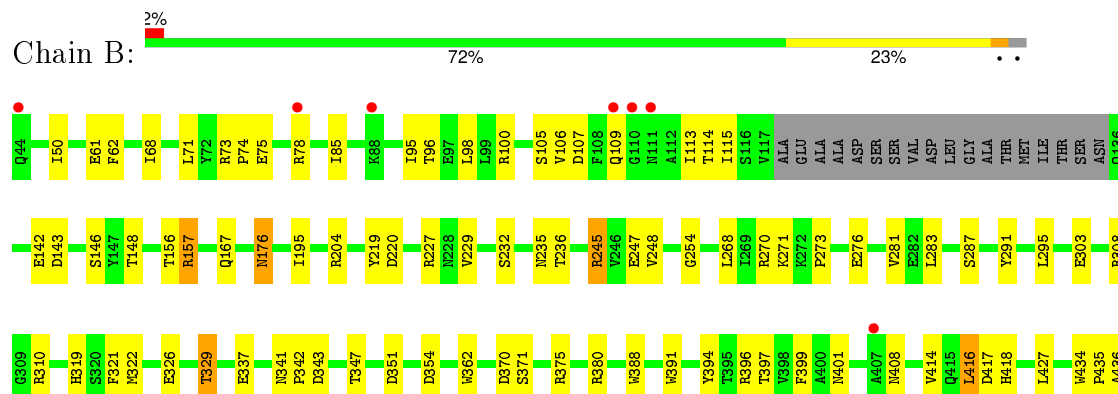
3 Residue-property plots

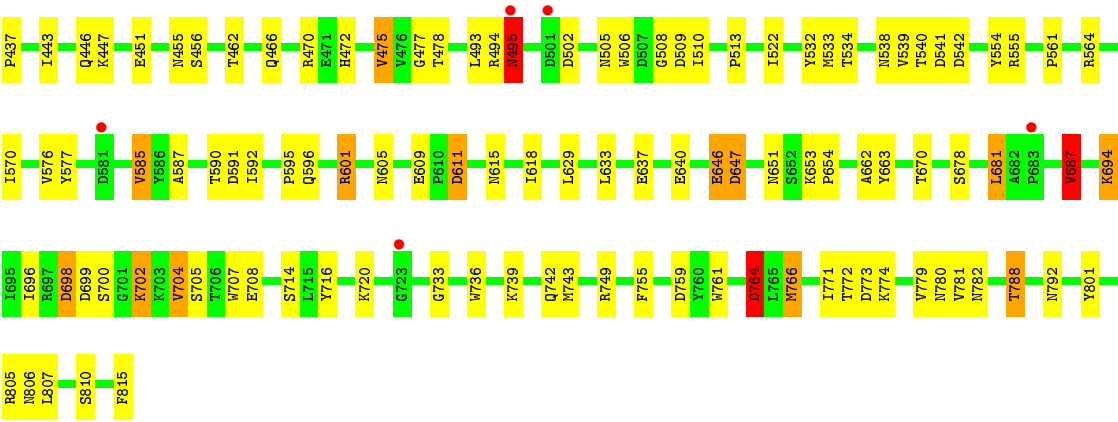
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



• Molecule 1: FERRIPYOVERDINE RECEPTOR





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.79Å 129.53Å 140.95Å 90.00° 130.57° 90.00°	Depositor
Resolution (Å)	107.21 – 2.90 30.83 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.0 (107.21-2.90) 92.1 (30.83-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.4.0054	Depositor
R, R_{free}	0.212 , 0.254 0.212 , 0.249	Depositor DCC
R_{free} test set	2742 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.3	EDS
Estimated twinning fraction	0.002 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 53996 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12230	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: N8E, PO4

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	1.00	2/6266 (0.0%)	1.01	17/8514 (0.2%)
1	B	0.90	1/6145 (0.0%)	0.92	5/8347 (0.1%)
All	All	0.95	3/12411 (0.0%)	0.96	22/16861 (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	3
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	758	GLU	CG-CD	7.09	1.62	1.51
1	A	125	VAL	CB-CG2	6.21	1.65	1.52
1	B	555	ARG	CG-CD	5.02	1.64	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	555	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	292	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	A	687	VAL	CB-CA-C	-7.66	96.84	111.40
1	A	73	ARG	NE-CZ-NH1	-7.65	116.47	120.30
1	B	687	VAL	CB-CA-C	-7.47	97.21	111.40
1	A	292	ARG	NE-CZ-NH1	6.42	123.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	550	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	713	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	647	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	73	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	683	PRO	C-N-CA	-5.68	110.37	122.30
1	A	78	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	475	VAL	CB-CA-C	-5.36	101.22	111.40
1	A	396	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	764	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	B	283	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	766	MET	CG-SD-CE	-5.13	92.00	100.20
1	A	323	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	A	431	MET	CG-SD-CE	5.08	108.32	100.20
1	A	475	VAL	CB-CA-C	-5.08	101.76	111.40
1	A	529	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	TYR	Peptide
1	B	611	ASP	Peptide
1	B	687	VAL	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	6114	0	5788	131	0
1	B	5994	0	5675	117	0
2	A	72	0	114	12	0
3	A	30	0	0	1	0
3	B	20	0	0	1	0
All	All	12230	0	11577	244	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 (244) 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	1.04	1.21
1:A:777:ALA:HB1	2:A:1817[B]:N8E:H192	1.38	1.05
1:A:772:THR:HG21	1:B:291:TYR:OH	1.60	1.02
1:A:694:LYS:HE3	1:A:708:GLU:OE1	1.62	0.99
1:A:53:GLN:OE1	1:A:57:SER:HB3	1.69	0.91
2:A:1817[B]:N8E:H031	1:B:805:ARG:HH11	1.35	0.90
1:A:151:THR:O	1:A:152:ILE:HD13	1.75	0.87
1:B:418:HIS:CD2	1:B:455:ASN:HD21	1.92	0.86
1:B:772:THR:HG22	1:B:774:LYS:N	1.89	0.86
1:B:540:THR:HG22	1:B:541:ASP:H	1.40	0.85
1:A:772:THR:HG22	1:A:774:LYS:H	1.44	0.83
1:B:418:HIS:HD2	1:B:455:ASN:HD21	1.24	0.83
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.61	0.81
1:B:71:LEU:HD12	1:B:114:THR:HG22	1.62	0.81
1:A:556:VAL:HG13	1:A:563:ILE:HB	1.61	0.81
1:B:694:LYS:HE3	1:B:708:GLU:OE1	1.84	0.77
2:A:1817[B]:N8E:H031	1:B:805:ARG:HD2	1.66	0.76
1:B:764:ASP:HB3	1:B:782:ASN:HA	1.66	0.76
1:A:239:ASP:OD2	1:A:292:ARG:NH2	2.19	0.76
1:A:291:TYR:OH	1:B:772:THR:HG21	1.86	0.76
1:B:418:HIS:HD2	1:B:455:ASN:ND2	1.84	0.75
1:A:69:GLN:HE21	1:A:133:THR:HG23	1.52	0.74
2:A:1817[B]:N8E:C03	1:B:805:ARG:HD2	2.19	0.73
1:B:540:THR:HG22	1:B:541:ASP:N	2.04	0.71
1:A:174:ARG:CZ	1:A:177:MET:HE3	2.21	0.70
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.27	0.69
1:B:707:TRP:HB2	1:B:742:GLN:HE21	1.58	0.69
1:A:325:TYR:OH	1:A:327:ARG:NH1	2.27	0.67
1:A:133:THR:HG21	1:A:159:VAL:HG21	1.77	0.67
1:A:656:ASN:HB3	1:A:659:ILE:HD12	1.78	0.66
1:B:681:LEU:HD22	1:B:687:VAL:HG22	1.78	0.66
1:A:157:ARG:HB3	1:A:475:VAL:HG11	1.76	0.65
1:A:470:ARG:NH1	1:A:538:ASN:OD1	2.26	0.65
1:B:646:GLU:O	1:B:647:ASP:CB	2.44	0.65
1:B:245:ARG:NH1	1:B:247:GLU:OE2	2.29	0.64
1:B:772:THR:CG2	1:B:773:ASP:N	2.61	0.63
1:A:401:ASN:ND2	1:A:415:GLN:HG2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ASP:HB3	1:A:578:ASP:HB2	1.79	0.63
1:B:232:SER:O	1:B:235:ASN:HB2	1.99	0.63
1:A:747:ASN:HB3	1:A:748:PRO:HD3	1.81	0.62
1:B:646:GLU:O	1:B:663:TYR:HA	1.99	0.61
1:A:109:GLN:OE1	1:A:114:THR:HG22	1.99	0.61
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.34	0.61
1:B:646:GLU:O	1:B:647:ASP:HB3	2.00	0.61
1:A:525:LYS:HB2	1:A:557:THR:HG22	1.81	0.61
1:B:698:ASP:OD2	1:B:702:LYS:HG2	2.01	0.61
1:B:472:HIS:HD2	1:B:538:ASN:H	1.48	0.61
1:B:443:ILE:HG13	1:B:510:ILE:HD13	1.81	0.60
1:A:777:ALA:HB1	2:A:1817[B]:N8E:C19	2.25	0.60
1:B:601:ARG:NH1	1:B:605:ASN:O	2.35	0.60
1:B:540:THR:CG2	1:B:541:ASP:H	2.14	0.59
1:B:470:ARG:NH2	1:B:541:ASP:OD1	2.35	0.59
1:A:362:TRP:HE3	1:A:363:SER:HB3	1.67	0.59
1:A:69:GLN:NE2	1:A:133:THR:HG23	2.16	0.59
1:A:694:LYS:CE	1:A:708:GLU:OE1	2.44	0.58
1:B:380:ARG:HD3	1:B:788:THR:HB	1.84	0.58
1:A:380:ARG:HD3	1:A:788:THR:HB	1.86	0.58
1:A:410:TRP:CD2	1:A:463:GLY:HA3	2.39	0.58
1:B:394:TYR:OH	1:B:451:GLU:HG3	2.04	0.58
1:B:698:ASP:HB3	1:B:700:SER:H	1.70	0.57
1:B:341:ASN:HB2	1:B:342:PRO:CD	2.35	0.57
1:A:502:ASP:OD2	1:A:505:ASN:HB2	2.04	0.57
1:A:738:GLY:HA2	1:A:759:ASP:HB3	1.85	0.57
1:B:142:GLU:O	1:B:143:ASP:HB2	2.04	0.56
1:A:694:LYS:NZ	1:A:708:GLU:O	2.38	0.56
1:B:362:TRP:HH2	1:B:446:GLN:OE1	1.89	0.56
1:A:188:VAL:HG11	1:A:246:VAL:HG13	1.88	0.56
1:A:199:ALA:HA	1:A:205:ASN:HD22	1.70	0.56
1:A:805:ARG:HH11	2:A:1817[A]:N8E:H012	1.69	0.56
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.41	0.56
1:A:554:TYR:CD2	1:A:595:PRO:HG2	2.41	0.56
1:A:669:LYS:O	1:A:696:ILE:HG13	2.06	0.55
1:A:288:TRP:CZ2	1:A:321:PHE:HB3	2.40	0.55
1:B:375:ARG:NE	1:B:755:PHE:CZ	2.74	0.55
1:A:580:ASN:HB2	1:A:582:THR:H	1.72	0.55
1:B:470:ARG:O	1:B:472:HIS:CE1	2.60	0.55
1:A:760:TYR:HB2	1:A:787:LYS:HE2	1.87	0.55
1:A:596:GLN:NE2	1:A:609:GLU:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:SER:OG	1:B:436:ALA:HA	2.07	0.55
1:A:188:VAL:HG11	1:A:246:VAL:CG1	2.36	0.54
1:A:722:LYS:HG3	1:A:723:GLY:H	1.73	0.54
1:B:341:ASN:OD1	1:B:343:ASP:HB2	2.07	0.54
1:B:772:THR:HG22	1:B:773:ASP:N	2.23	0.53
1:A:709:PRO:HG3	1:A:737:GLN:NE2	2.23	0.53
1:A:707:TRP:CH2	1:A:793:ILE:HG13	2.44	0.53
1:B:506:TRP:CE2	1:B:508:GLY:HA2	2.43	0.53
1:A:204:ARG:HG3	1:A:391:TRP:CH2	2.43	0.53
1:A:563:ILE:HD11	1:A:598:SER:HB2	1.90	0.53
1:A:174:ARG:NH1	1:A:177:MET:HE3	2.24	0.53
1:B:436:ALA:HB1	1:B:437:PRO:HD2	1.90	0.53
1:A:805:ARG:HD3	2:A:1817[A]:N8E:H052	1.90	0.53
1:B:646:GLU:HG2	1:B:647:ASP:N	2.23	0.53
1:B:417:ASP:HB2	1:B:456:SER:HB2	1.91	0.53
1:B:646:GLU:O	1:B:662:ALA:O	2.28	0.52
1:A:722:LYS:HG3	1:A:723:GLY:N	2.23	0.52
1:B:542:ASP:O	1:B:577:TYR:HA	2.09	0.52
1:A:142:GLU:HG3	3:A:1820:PO4:O2	2.09	0.52
1:B:74:PRO:HG3	1:B:303:GLU:HG3	1.92	0.52
1:A:417:ASP:HB2	1:A:456:SER:HB2	1.91	0.52
1:B:204:ARG:HG3	1:B:391:TRP:CH2	2.44	0.52
1:A:255:LEU:HD22	1:A:572:TYR:CD2	2.45	0.52
1:A:74:PRO:HG3	1:A:132:ILE:HG12	1.92	0.52
1:A:46:VAL:CG1	1:A:47:GLU:N	2.73	0.52
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.44	0.52
1:A:50:ILE:HD12	1:A:85:ILE:HD11	1.91	0.52
1:B:418:HIS:CD2	1:B:455:ASN:ND2	2.64	0.51
1:A:362:TRP:CD2	1:A:431:MET:HE3	2.46	0.51
1:B:540:THR:CG2	1:B:541:ASP:N	2.74	0.51
1:A:698:ASP:OD1	1:A:698:ASP:C	2.49	0.51
1:B:227:ARG:HG2	1:B:227:ARG:HH11	1.75	0.51
1:A:53:GLN:OE1	1:A:57:SER:CB	2.53	0.51
1:B:50:ILE:HD12	1:B:85:ILE:HD11	1.92	0.51
1:B:472:HIS:HD2	1:B:538:ASN:N	2.09	0.51
1:A:60:GLN:HE21	1:A:134:SER:HA	1.76	0.50
1:A:615:ASN:HD21	1:A:617:GLU:HB2	1.75	0.50
1:B:554:TYR:CD2	1:B:595:PRO:HG2	2.47	0.50
1:B:629:LEU:HD12	1:B:678:SER:O	2.11	0.50
1:B:470:ARG:NH1	1:B:539:VAL:O	2.44	0.50
1:A:109:GLN:OE1	1:A:114:THR:CG2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TRP:CZ2	1:A:442:LYS:HB2	2.47	0.50
1:B:694:LYS:HD2	1:B:694:LYS:C	2.33	0.49
1:A:308:ARG:NH1	1:A:337:GLU:OE1	2.46	0.49
1:A:694:LYS:HE3	1:A:708:GLU:CD	2.32	0.49
1:A:408:ASN:HB3	1:A:410:TRP:HD1	1.77	0.49
1:B:195:ILE:HD11	1:B:248:VAL:HG11	1.94	0.49
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.48	0.49
1:A:60:GLN:NE2	1:A:133:THR:O	2.46	0.49
1:B:807:LEU:HD12	1:B:807:LEU:N	2.27	0.49
1:A:807:LEU:HD11	2:A:1817[A]:N8E:H041	1.94	0.49
1:A:772:THR:HG21	1:B:291:TYR:HH	1.74	0.49
1:B:329:THR:HA	1:B:354:ASP:O	2.14	0.48
1:A:809:PHE:CD1	1:B:771:ILE:HG12	2.48	0.48
1:A:742:GLN:HG3	1:A:793:ILE:O	2.12	0.48
1:A:528:GLN:HG2	1:A:554:TYR:CD1	2.49	0.48
1:B:399:PHE:HA	1:B:416:LEU:O	2.14	0.48
1:A:79:ASN:OD1	1:A:79:ASN:N	2.46	0.47
1:A:384:ASN:HB2	1:A:430:ILE:HB	1.96	0.47
1:B:587:ALA:HB2	1:B:618:ILE:HG13	1.94	0.47
1:A:700:SER:OG	1:A:702:LYS:HG2	2.13	0.47
1:B:50:ILE:HG12	1:B:61:GLU:HG2	1.96	0.47
1:B:570:ILE:HG23	1:B:591:ASP:HB3	1.97	0.47
1:A:491:TRP:CE2	1:A:519:SER:HB3	2.50	0.47
1:A:123:SER:O	1:A:124:SER:HB3	2.14	0.47
1:B:637:GLU:HA	1:B:670:THR:O	2.14	0.47
1:B:270:ARG:NH1	1:B:351:ASP:OD2	2.48	0.47
1:A:772:THR:HG22	1:A:774:LYS:N	2.23	0.46
1:B:577:TYR:HB3	1:B:585:VAL:HG23	1.97	0.46
2:A:1817[B]:N8E:H052	1:B:805:ARG:CD	2.45	0.46
1:B:780:ASN:O	1:B:807:LEU:HA	2.16	0.46
1:A:760:TYR:CB	1:A:787:LYS:HE2	2.46	0.46
1:A:113:ILE:HD12	1:A:115:ILE:HD11	1.97	0.46
1:A:813:TRP:C	1:A:813:TRP:CD1	2.89	0.46
1:A:411:VAL:HG12	1:A:462:THR:HG22	1.98	0.46
1:B:781:VAL:HG22	1:B:807:LEU:HG	1.97	0.46
1:A:362:TRP:CE3	1:A:363:SER:HB3	2.49	0.46
1:A:443:ILE:HG13	1:A:510:ILE:HD12	1.98	0.46
1:B:254:GLY:CA	1:B:592:ILE:HG13	2.46	0.46
1:A:163:ARG:HD2	1:A:623:GLU:HB2	1.98	0.46
1:B:273:PRO:HG2	1:B:337:GLU:HG3	1.98	0.46
1:A:242:ILE:HD11	1:A:243:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:PHE:HB2	1:A:725:LEU:O	2.16	0.45
1:B:308:ARG:NH1	1:B:337:GLU:OE1	2.49	0.45
1:B:443:ILE:HD11	1:B:506:TRP:CH2	2.51	0.45
1:B:736:TRP:HB2	1:B:761:TRP:CE3	2.51	0.45
1:B:281:VAL:HG22	1:B:295:LEU:HD13	1.99	0.45
1:B:287:SER:HB2	1:B:806:ASN:HB2	1.99	0.45
1:B:494:ARG:O	1:B:495:ASN:C	2.55	0.45
1:B:113:ILE:O	1:B:113:ILE:HG13	2.17	0.44
1:A:291:TYR:O	1:A:316:GLN:HA	2.18	0.44
1:A:792:ASN:HB3	1:A:800:SER:HB2	1.98	0.44
1:A:789:TYR:CZ	1:A:802:GLY:HA3	2.52	0.44
1:A:408:ASN:HB3	1:A:410:TRP:CD1	2.52	0.44
1:A:467:PHE:CE2	1:A:468:LEU:HD12	2.52	0.44
1:A:528:GLN:HG2	1:A:554:TYR:HD1	1.80	0.44
1:B:502:ASP:OD2	1:B:505:ASN:HB2	2.17	0.44
1:A:782:ASN:O	1:A:805:ARG:HA	2.18	0.44
1:B:418:HIS:HE1	3:B:1819:PO4:O1	2.00	0.44
1:A:341:ASN:HB2	1:A:342:PRO:CD	2.42	0.44
1:A:174:ARG:CZ	1:A:177:MET:CE	2.94	0.44
1:B:227:ARG:HG2	1:B:227:ARG:NH1	2.30	0.44
1:A:443:ILE:HG13	1:A:510:ILE:CD1	2.48	0.44
1:A:208:TYR:HA	1:A:212:PHE:O	2.17	0.44
1:B:590:THR:OG1	1:B:615:ASN:HB3	2.18	0.44
1:A:678:SER:HA	1:A:687:VAL:O	2.17	0.44
1:A:313:ALA:HA	1:A:331:VAL:O	2.18	0.44
1:B:62:PHE:CZ	1:B:95:ILE:HB	2.52	0.44
1:A:284:GLY:HA2	1:A:809:PHE:O	2.18	0.43
1:A:288:TRP:CE2	1:A:321:PHE:HB3	2.53	0.43
1:A:227:ARG:NH2	1:A:597:ASP:HA	2.32	0.43
1:B:156:THR:O	1:B:157:ARG:CB	2.66	0.43
1:A:722:LYS:HE2	1:A:723:GLY:H	1.84	0.43
1:B:156:THR:HB	1:B:534:THR:HG21	2.00	0.43
1:A:608:LEU:HD23	1:A:608:LEU:HA	1.86	0.43
1:A:475:VAL:O	1:A:533:MET:HA	2.19	0.43
1:A:467:PHE:CD2	1:A:468:LEU:HD12	2.54	0.43
1:B:477:GLY:HA3	1:B:532:TYR:CZ	2.53	0.43
1:B:268:LEU:N	1:B:268:LEU:HD12	2.33	0.43
1:A:392:GLU:HG3	1:A:424:HIS:HB3	2.01	0.43
1:A:179:ASP:OD1	1:A:768:ARG:NH1	2.34	0.43
1:B:766:MET:C	1:B:766:MET:SD	2.98	0.42
1:B:380:ARG:HA	1:B:801:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ASP:HA	1:B:434:TRP:O	2.18	0.42
1:B:388:TRP:CZ2	1:B:513:PRO:HD3	2.54	0.42
1:B:219:TYR:O	1:B:220:ASP:HB2	2.20	0.42
1:B:347:THR:HB	1:B:401:ASN:HB2	2.00	0.42
1:B:321:PHE:CE1	1:B:322:MET:HG3	2.54	0.42
1:B:646:GLU:HG3	1:B:651:ASN:HD22	1.84	0.42
1:B:176:ASN:C	1:B:176:ASN:HD22	2.23	0.42
1:A:491:TRP:CZ2	1:A:519:SER:HB3	2.55	0.42
1:A:674:GLU:HG3	1:A:692:THR:OG1	2.19	0.42
1:A:646:GLU:HG3	1:A:661:TYR:OH	2.19	0.42
1:A:127:LEU:HD11	1:A:581:ASP:HA	2.01	0.42
1:A:805:ARG:HD2	2:A:1817[A]:N8E:H032	2.02	0.42
2:A:1817[B]:N8E:H032	1:B:805:ARG:HD2	1.99	0.42
1:A:158:LEU:HD21	1:A:475:VAL:HG22	2.02	0.42
1:B:401:ASN:HA	1:B:414:VAL:O	2.19	0.42
1:A:736:TRP:HB2	1:A:761:TRP:CE3	2.55	0.41
1:A:496:TYR:CG	1:A:513:PRO:HB3	2.55	0.41
1:A:151:THR:C	1:A:152:ILE:HD13	2.40	0.41
1:A:236:THR:H	1:A:236:THR:HG22	1.53	0.41
1:A:390:SER:O	1:A:425:ALA:HA	2.20	0.41
1:A:611:ASP:OD1	1:A:640:GLU:OE2	2.37	0.41
1:A:46:VAL:HG12	1:A:47:GLU:N	2.36	0.41
1:B:653:LYS:HA	1:B:654:PRO:HD2	1.76	0.41
1:B:276:GLU:N	1:B:276:GLU:OE1	2.51	0.41
1:A:647:ASP:HB2	1:A:664:LYS:HB2	2.03	0.41
1:A:410:TRP:CE2	1:A:463:GLY:HA3	2.56	0.41
1:B:98:LEU:HD23	1:B:98:LEU:C	2.41	0.41
1:B:475:VAL:O	1:B:533:MET:HA	2.20	0.41
1:B:271:LYS:HD3	1:B:310:ARG:NH2	2.36	0.41
1:A:738:GLY:HA2	1:A:759:ASP:CB	2.51	0.41
1:B:74:PRO:HG3	1:B:303:GLU:CG	2.51	0.41
1:B:254:GLY:HA3	1:B:592:ILE:HG13	2.03	0.41
1:A:75:GLU:HB3	1:A:471:GLU:HG3	2.03	0.41
1:A:380:ARG:HG2	1:A:801:TYR:CG	2.56	0.41
1:B:611:ASP:OD1	1:B:640:GLU:OE2	2.40	0.40
1:B:779:VAL:O	1:B:779:VAL:HG13	2.21	0.40
1:A:441:ALA:HB3	1:A:500:THR:HG22	2.03	0.40
1:A:597:ASP:HB3	1:A:599:TRP:CZ3	2.56	0.40
2:A:1817[B]:N8E:H052	1:B:805:ARG:HD2	2.02	0.40
1:B:696:ILE:HG23	1:B:704:VAL:HG12	2.03	0.40
1:B:472:HIS:CD2	1:B:538:ASN:H	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:TRP:HB2	1:B:427:LEU:HD21	2.04	0.40
1:B:434:TRP:HB3	1:B:435:PRO:HA	2.04	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%)	717 (93%)	48 (6%)	5 (1%)	30	67
1	B	750/772 (97%)	700 (93%)	45 (6%)	5 (1%)	26	63
All	All	1520/1544 (98%)	1417 (93%)	93 (6%)	10 (1%)	26	63

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
1	A	124	SER
1	A	45	GLU
1	B	408	ASN
1	B	495	ASN
1	B	647	ASP
1	B	699	ASP
1	A	122	ASP
1	A	653	LYS
1	B	561	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	650/650 (100%)	577 (89%)	73 (11%)	7	22
1	B	637/650 (98%)	578 (91%)	59 (9%)	11	32
All	All	1287/1300 (99%)	1155 (90%)	132 (10%)	9	26

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	68	ILE
1	A	78	ARG
1	A	79	ASN
1	A	83	SER
1	A	114	THR
1	A	123	SER
1	A	132	ILE
1	A	133	THR
1	A	143	ASP
1	A	148	THR
1	A	154	THR
1	A	157	ARG
1	A	177	MET
1	A	204	ARG
1	A	215	ASN
1	A	227	ARG
1	A	236	THR
1	A	238	SER
1	A	245	ARG
1	A	246	VAL
1	A	276	GLU
1	A	301	LEU
1	A	303	GLU
1	A	304	SER
1	A	307	VAL
1	A	312	VAL
1	A	318	LYS
1	A	329	THR
1	A	355	ASN
1	A	358	LYS
1	A	375	ARG
1	A	392	GLU

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Mol	Chain	Res	Type
1	A	408	ASN
1	A	417	ASP
1	A	431	MET
1	A	459	ILE
1	A	461	LEU
1	A	466	GLN
1	A	470	ARG
1	A	494	ARG
1	A	499	THR
1	A	522	ILE
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	580	ASN
1	A	596	GLN
1	A	598	SER
1	A	601	ARG
1	A	603	SER
1	A	609	GLU
1	A	645	GLU
1	A	659	ILE
1	A	676	GLU
1	A	683	PRO
1	A	694	LYS
1	A	704	VAL
1	A	720	LYS
1	A	722	LYS
1	A	725	LEU
1	A	730	VAL
1	A	766	MET
1	A	772	THR
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	73	ARG

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Mol	Chain	Res	Type
1	B	75	GLU
1	B	78	ARG
1	B	96	THR
1	B	100	ARG
1	B	105	SER
1	B	106	VAL
1	B	107	ASP
1	B	109	GLN
1	B	115	ILE
1	B	146	SER
1	B	148	THR
1	B	157	ARG
1	B	167	GLN
1	B	176	ASN
1	B	229	VAL
1	B	236	THR
1	B	245	ARG
1	B	319	HIS
1	B	326	GLU
1	B	329	THR
1	B	396	ARG
1	B	397	THR
1	B	416	LEU
1	B	447	LYS
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	522	ILE
1	B	564	ARG
1	B	576	VAL
1	B	585	VAL
1	B	596	GLN
1	B	601	ARG
1	B	609	GLU
1	B	633	LEU
1	B	646	GLU
1	B	681	LEU
1	B	687	VAL
1	B	694	LYS

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Mol	Chain	Res	Type
1	B	702	LYS
1	B	704	VAL
1	B	705	SER
1	B	714	SER
1	B	720	LYS
1	B	739	LYS
1	B	743	MET
1	B	749	ARG
1	B	759	ASP
1	B	764	ASP
1	B	766	MET
1	B	788	THR
1	B	792	ASN
1	B	810	SER
1	B	815	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	205	ASN
1	A	218	GLN
1	A	401	ASN
1	A	408	ASN
1	A	455	ASN
1	A	505	ASN
1	A	615	ASN
1	A	780	ASN
1	B	53	GLN
1	B	176	ASN
1	B	183	ASN
1	B	418	HIS
1	B	455	ASN
1	B	472	HIS
1	B	688	GLN
1	B	742	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 ⓘ

13 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	$\# Z > 2$
2	N8E	A	1816	-	23,23,23	0.62	0	22,22,22	0.58	0
2	N8E	A	1817[A]	-	23,23,23	0.70	0	22,22,22	0.55	0
2	N8E	A	1817[B]	-	23,23,23	0.79	0	22,22,22	0.86	1 (4%)
3	PO4	A	1818	-	4,4,4	0.40	0	6,6,6	0.29	0
3	PO4	A	1819	-	4,4,4	0.32	0	6,6,6	0.29	0
3	PO4	A	1820	-	4,4,4	0.38	0	6,6,6	0.28	0
3	PO4	A	1821	-	4,4,4	0.16	0	6,6,6	0.31	0
3	PO4	A	1822	-	4,4,4	0.50	0	6,6,6	0.28	0
3	PO4	A	1823	-	4,4,4	0.51	0	6,6,6	0.28	0
3	PO4	B	1816	-	4,4,4	0.29	0	6,6,6	0.33	0
3	PO4	B	1817	-	4,4,4	0.34	0	6,6,6	0.31	0
3	PO4	B	1818	-	4,4,4	0.43	0	6,6,6	0.28	0
3	PO4	B	1819	-	4,4,4	0.29	0	6,6,6	0.26	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	N8E	A	1816	-	-	0/21/21/21	0/0/0/0
2	N8E	A	1817[A]	-	-	0/21/21/21	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	N8E	A	1817[B]	-	-	0/21/21/21	0/0/0/0
3	PO4	A	1818	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1819	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1820	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1821	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1822	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1823	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1816	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1817	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1818	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1819	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1817[B]	N8E	O18-C19-C20	2.19	120.11	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1817[A]	N8E	4	0
2	A	1817[B]	N8E	8	0
3	A	1820	PO4	1	0
3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	772/772 (100%)	-0.45	5 (0%) 90 89	2, 9, 19, 34	0
1	B	754/772 (97%)	-0.29	12 (1%) 74 72	2, 8, 17, 29	0
All	All	1526/1544 (98%)	-0.37	17 (1%) 82 80	2, 8, 18, 34	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	GLN	4.9
1	B	407	ALA	4.5
1	A	44	GLN	4.1
1	B	78	ARG	3.9
1	B	109	GLN	3.5
1	A	123	SER	3.2
1	B	110	GLY	3.1
1	B	88	LYS	3.1
1	B	581	ASP	2.6
1	A	724	ALA	2.6
1	B	723	GLY	2.6
1	B	495	ASN	2.6
1	A	723	GLY	2.5
1	B	683	PRO	2.2
1	B	501	ASP	2.0
1	B	111	ASN	2.0
1	A	303	GLU	2.0

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	A	1822	5/5	0.91	0.28	6.04	70,71,71,72	0
3	PO4	B	1818	5/5	0.94	0.24	4.78	60,60,61,62	0
2	N8E	A	1816	24/24	0.86	0.34	3.78	24,41,47,49	0
3	PO4	A	1823	5/5	0.92	0.22	2.81	52,53,53,54	0
2	N8E	A	1817[A]	24/24	0.87	0.27	2.58	2,2,5,7	24
3	PO4	A	1820	5/5	0.98	0.18	2.46	40,40,42,43	0
2	N8E	A	1817[B]	24/24	0.87	0.27	1.86	2,2,7,8	24
3	PO4	A	1818	5/5	0.98	0.12	-1.45	16,18,20,21	0
3	PO4	B	1817	5/5	0.98	0.10	-1.64	7,7,8,8	0
3	PO4	A	1819	5/5	0.98	0.09	-2.44	12,14,15,15	0
3	PO4	B	1816	5/5	0.96	0.38	-	41,42,43,43	0
3	PO4	B	1819	5/5	0.96	0.22	-	40,42,42,43	0
3	PO4	A	1821	5/5	0.93	0.29	-	37,37,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.