



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:33 PM UTC

PDB ID : 2W75 / pdb_00002w75
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

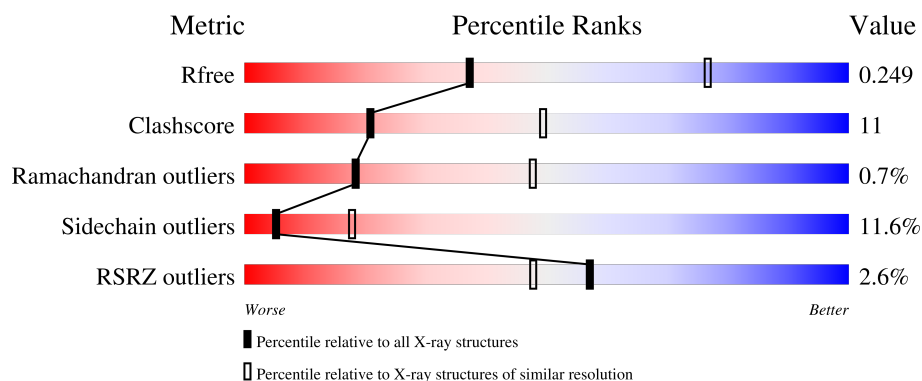
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	772	2% 68% 25% 6%
1	B	772	3% 69% 24% ...

2 Entry composition [i](#)

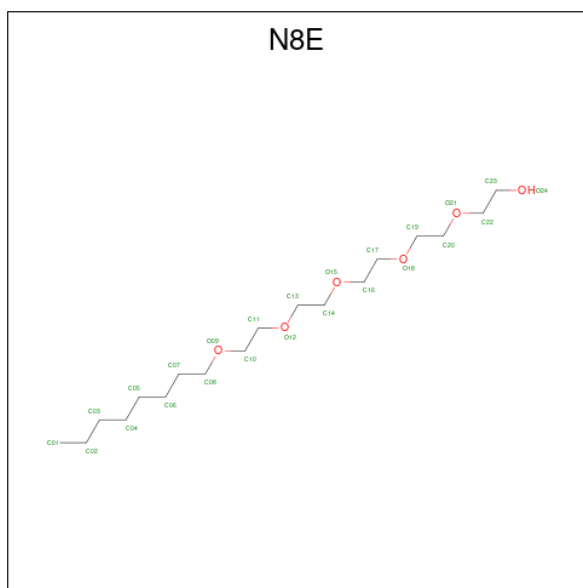
There are 3 unique types of molecules in this entry. The entry contains 12230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: N8E) (formula: $C_{18}H_{38}O_6$).

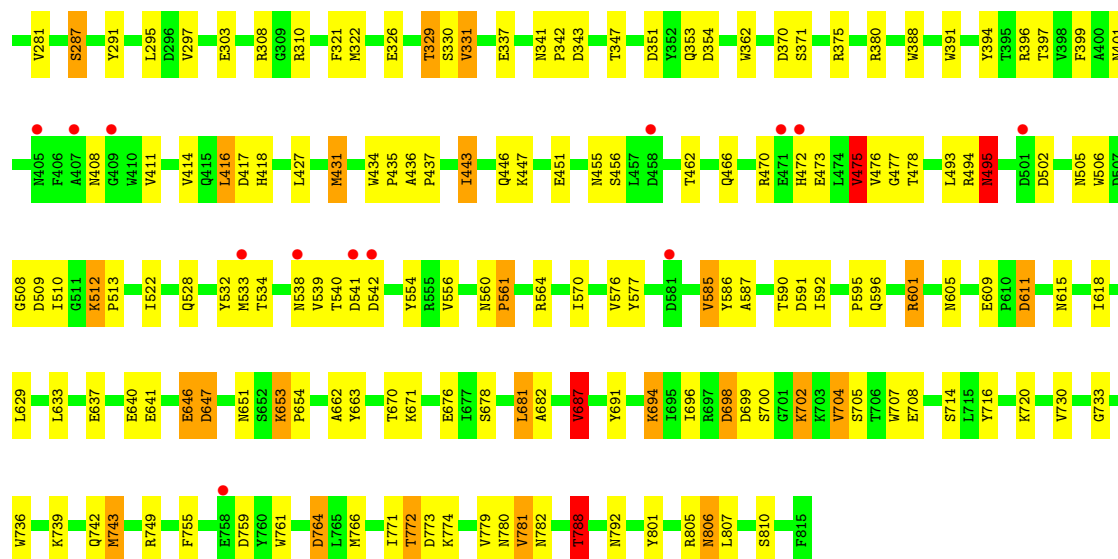


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			24	18	6		
2	A	1	Total	C	O	0	1
			48	36	12		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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		



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 – 2.90 107.07 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.0 (107.21-2.90) 92.0 (107.07-2.90)	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 (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 14.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.002 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	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, 0.333 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: PO4, N8E

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	1.19	5/6266 (0.1%)	1.28	40/8514 (0.5%)
1	B	1.10	9/6145 (0.1%)	1.18	15/8347 (0.2%)
All	All	1.14	14/12411 (0.1%)	1.23	55/16861 (0.3%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	679	GLY	C-O	-7.29	1.19	1.24
1	B	68	ILE	CA-CB	6.44	1.64	1.54
1	A	551	VAL	CA-CB	6.43	1.62	1.54
1	B	788	THR	CA-CB	6.21	1.62	1.53
1	B	139	THR	CA-CB	5.67	1.61	1.53
1	A	104	ALA	CA-CB	-5.51	1.45	1.53
1	B	331	VAL	CA-CB	5.44	1.61	1.54
1	B	248	VAL	CA-CB	-5.26	1.47	1.53
1	B	443	ILE	CA-CB	5.21	1.61	1.54
1	B	781	VAL	CA-CB	-5.15	1.47	1.54
1	A	763	VAL	CA-CB	5.14	1.60	1.54
1	B	743	MET	N-CA	-5.12	1.39	1.46
1	A	398	VAL	CA-CB	-5.07	1.48	1.54
1	B	730	VAL	CA-CB	5.03	1.60	1.54

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	687	VAL	CB-CA-C	-8.42	97.21	110.69
1	A	517	THR	CA-C-N	-8.28	110.88	119.83
1	A	517	THR	C-N-CA	-8.28	110.88	119.83
1	A	687	VAL	CB-CA-C	-7.96	96.84	110.30
1	A	594	MET	CA-C-N	-6.72	112.86	119.78
1	A	594	MET	C-N-CA	-6.72	112.86	119.78
1	A	248	VAL	N-CA-C	6.69	117.50	107.80
1	B	676	GLU	N-CA-C	6.66	119.45	108.99
1	A	281	VAL	N-CA-C	-6.60	98.68	108.85
1	A	79	ASN	N-CA-C	-6.55	102.49	110.88
1	A	502	ASP	N-CA-C	6.27	119.55	107.44
1	B	475	VAL	CB-CA-C	-6.24	101.22	110.33
1	A	362	TRP	N-CA-C	-6.12	103.23	112.04
1	B	473	GLU	N-CA-C	6.10	118.56	108.99
1	B	653	LYS	CA-C-N	6.03	125.99	119.78
1	B	653	LYS	C-N-CA	6.03	125.99	119.78
1	A	503	PHE	N-CA-C	5.88	117.49	111.14
1	A	475	VAL	CB-CA-C	-5.87	101.76	110.33
1	A	77	VAL	CB-CA-C	-5.79	104.76	112.46
1	A	482	PHE	N-CA-C	-5.76	99.02	108.76
1	B	682	ALA	N-CA-C	-5.70	103.00	108.07
1	A	683	PRO	CA-C-N	-5.63	110.37	121.41
1	A	683	PRO	C-N-CA	-5.63	110.37	121.41
1	A	741	TRP	N-CA-C	5.53	116.67	108.60
1	B	353	GLN	N-CA-C	5.53	117.43	108.26
1	A	264	ALA	N-CA-C	5.45	116.43	108.14
1	B	287	SER	N-CA-C	5.45	117.92	110.24
1	A	68	ILE	CA-C-N	-5.41	114.56	122.19
1	A	68	ILE	C-N-CA	-5.41	114.56	122.19
1	A	83	SER	CB-CA-C	5.39	118.73	109.51
1	A	307	VAL	CB-CA-C	5.38	118.63	110.62
1	A	245	ARG	CA-C-N	-5.36	116.12	123.14
1	A	245	ARG	C-N-CA	-5.36	116.12	123.14
1	A	286	GLY	N-CA-C	5.34	120.92	112.06
1	A	512	LYS	CA-C-N	-5.30	113.22	119.84
1	A	512	LYS	C-N-CA	-5.30	113.22	119.84
1	A	323	ASP	N-CA-C	5.29	117.54	110.35
1	A	660	THR	N-CA-C	-5.25	107.42	113.88
1	B	806	ASN	N-CA-C	5.22	117.19	108.99
1	A	321	PHE	N-CA-C	-5.21	105.72	111.71
1	A	507	ASP	N-CA-CB	-5.15	104.05	110.90
1	A	664	LYS	N-CA-C	-5.10	99.67	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	THR	CA-C-N	-5.10	116.49	123.12
1	B	196	THR	C-N-CA	-5.10	116.49	123.12
1	A	747	ASN	CA-C-N	5.07	126.18	119.84
1	A	747	ASN	C-N-CA	5.07	126.18	119.84
1	A	417	ASP	N-CA-C	5.07	117.71	109.24
1	A	659	ILE	CB-CA-C	-5.06	103.03	110.82
1	A	777	ALA	N-CA-C	5.06	117.81	109.72
1	A	252	ALA	CA-C-N	-5.03	115.68	123.17
1	A	252	ALA	C-N-CA	-5.03	115.68	123.17
1	A	73	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	B	528	GLN	N-CA-C	5.03	116.58	108.34
1	B	512	LYS	CA-C-N	-5.00	115.21	120.66
1	B	512	LYS	C-N-CA	-5.00	115.21	120.66

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 [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	141	0
1	B	5994	0	5675	128	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	265	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 (265) 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:260:GLY:HA2	1:A:594:MET:HE2	1.74	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:174:ARG:CZ	1:A:177:MET:HE3	2.25	0.67
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLN:OE1	1:A:114:THR:HG22	1.99	0.61
1:B:646:GLU:O	1:B:663:TYR:HA	1.99	0.61
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.34	0.61
1:A:525:LYS:HB2	1:A:557:THR:HG22	1.81	0.61
1:B:646:GLU:O	1:B:647:ASP:HB3	2.00	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:A:362:TRP:CD2	1:A:431:MET:HE1	2.39	0.57
1:B:698:ASP:HB3	1:B:700:SER:H	1.70	0.57
1:A:174:ARG:NH1	1:A:177:MET:HE3	2.19	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:394:TYR:CE1	1:A:422:GLY:HA3	2.41	0.56
1:A:805:ARG:HH11	2:A:1817[A]:N8E:H012	1.69	0.56
1:A:554:TYR:CD2	1:A:595:PRO:HG2	2.41	0.56
1:A:698:ASP:OD1	1:A:698:ASP:C	2.49	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:A:580:ASN:HB2	1:A:582:THR:H	1.72	0.55
1:B:375:ARG:NE	1:B:755:PHE:CZ	2.74	0.55
1:A:596:GLN:NE2	1:A:609:GLU:O	2.39	0.55
1:A:760:TYR:HB2	1:A:787:LYS:HE2	1.87	0.55
1:B:470:ARG:O	1:B:472:HIS:CE1	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:TRP:CE3	1:A:431:MET:HE1	2.42	0.55
1:B:189:MET:HE2	1:B:189:MET:HA	1.88	0.55
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:B:694:LYS:HD2	1:B:694:LYS:C	2.33	0.54
1:A:694:LYS:HE3	1:A:708:GLU:CD	2.32	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:A:709:PRO:HG3	1:A:737:GLN:NE2	2.23	0.53
1:B:772:THR:HG22	1:B:773:ASP:N	2.23	0.53
1:A:707:TRP:CH2	1:A:793:ILE:HG13	2.44	0.53
1:A:204:ARG:HG3	1:A:391:TRP:CH2	2.43	0.53
1:B:506:TRP:CE2	1:B:508:GLY:HA2	2.43	0.53
1:A:563:ILE:HD11	1:A:598:SER:HB2	1.90	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:A:142:GLU:HG3	3:A:1820:PO4:O2	2.09	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:B:646:GLU:O	1:B:662:ALA:O	2.28	0.52
1:A:417:ASP:HB2	1:A:456:SER:HB2	1.91	0.52
1:B:74:PRO:HG3	1:B:303:GLU:HG3	1.92	0.52
1:A:255:LEU:HD22	1:A:572:TYR:CD2	2.45	0.52
1:B:204:ARG:HG3	1:B:391:TRP:CH2	2.44	0.52
1:A:46:VAL:CG1	1:A:47:GLU:N	2.73	0.52
1:A:74:PRO:HG3	1:A:132:ILE:HG12	1.92	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:B:540:THR:CG2	1:B:541:ASP:N	2.74	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:A:813:TRP:CD1	1:A:813:TRP:C	2.89	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:A:239:ASP:CG	1:A:292:ARG:HH22	2.19	0.50
1:B:554:TYR:CD2	1:B:595:PRO:HG2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:434:TRP:CZ2	1:A:442:LYS:HB2	2.47	0.50
1:A:308:ARG:NH1	1:A:337:GLU:OE1	2.46	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:494:ARG:O	1:B:495:ASN:C	2.55	0.48
1:A:809:PHE:CD1	1:B:771:ILE:HG12	2.48	0.48
1:B:329:THR:HA	1:B:354:ASP:O	2.14	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:B:766:MET:SD	1:B:766:MET:C	2.98	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:A:491:TRP:CE2	1:A:519:SER:HB3	2.50	0.47
1:B:176:ASN:C	1:B:176:ASN:HD22	2.23	0.47
1:B:570:ILE:HG23	1:B:591:ASP:HB3	1.97	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
1:A:151:THR:C	1:A:152:ILE:HD13	2.40	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:113:ILE:HD12	1:A:115:ILE:HD11	1.97	0.46
1:A:760:TYR:CB	1:A:787:LYS:HE2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:HD23	1:B:98:LEU:C	2.41	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
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:A:141:THR:O	1:A:142:GLU:C	2.60	0.45
1:A:73:ARG:HG3	1:A:131:MET:HE3	1.97	0.44
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:B:186:ASP:O	1:B:187:ASP:C	2.60	0.44
1:A:766:MET:SD	1:A:766:MET:C	3.01	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:A:174:ARG:CZ	1:A:177:MET:CE	2.94	0.44
1:A:208:TYR:HA	1:A:212:PHE:O	2.17	0.44
1:A:341:ASN:HB2	1:A:342:PRO:CD	2.42	0.44
1:A:443:ILE:HG13	1:A:510:ILE:CD1	2.48	0.44
1:B:227:ARG:HG2	1:B:227:ARG:NH1	2.30	0.44
1:B:418:HIS:HE1	3:B:1819:PO4:O1	2.00	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:227:ARG:NH2	1:A:597:ASP:HA	2.32	0.43
1:A:288:TRP:CE2	1:A:321:PHE:HB3	2.53	0.43
1:B:156:THR:O	1:B:157:ARG:CB	2.66	0.43
1:A:608:LEU:HD23	1:A:608:LEU:HA	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:268:LEU:N	1:B:268:LEU:HD12	2.33	0.43
1:B:477:GLY:HA3	1:B:532:TYR:CZ	2.53	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:A:517:THR:O	1:A:518:PRO:C	2.60	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:370:ASP:HA	1:B:434:TRP:O	2.18	0.42
1:B:380:ARG:HA	1:B:801:TYR:CE2	2.54	0.42
1:B:388:TRP:CZ2	1:B:513:PRO:HD3	2.54	0.42
1:B:321:PHE:CE1	1:B:322:MET:HG3	2.54	0.42
1:B:431:MET:HB3	1:B:431:MET:HE2	1.42	0.42
1:B:646:GLU:HG3	1:B:651:ASN:HD22	1.84	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:B:370:ASP:HA	1:B:434:TRP:C	2.45	0.42
1:A:127:LEU:HD11	1:A:581:ASP:HA	2.01	0.42
1:A:646:GLU:HG3	1:A:661:TYR:OH	2.19	0.42
1:A:158:LEU:HD21	1:A:475:VAL:HG22	2.02	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:B:401:ASN:HA	1:B:414:VAL:O	2.19	0.42
1:A:496:TYR:CG	1:A:513:PRO:HB3	2.55	0.41
1:A:736:TRP:HB2	1:A:761:TRP:CE3	2.55	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:775:LEU:HD23	1:A:775:LEU:C	2.46	0.41
1:A:46:VAL:HG12	1:A:47:GLU:N	2.36	0.41
1:B:341:ASN:C	1:B:343:ASP:H	2.29	0.41
1:B:653:LYS:HA	1:B:654:PRO:HD2	1.76	0.41
1:A:647:ASP:HB2	1:A:664:LYS:HB2	2.03	0.41
1:B:276:GLU:OE1	1:B:276:GLU:N	2.51	0.41
1:A:410:TRP:CE2	1:A:463:GLY:HA3	2.56	0.41
1:B:475:VAL:O	1:B:533:MET:HA	2.20	0.41
1:B:502:ASP:CG	1:B:505:ASN:HB2	2.45	0.41
1:B:271:LYS:HD3	1:B:310:ARG:NH2	2.36	0.41
1:B:560:ASN:O	1:B:561:PRO:C	2.64	0.41
1:A:75:GLU:HB3	1:A:471:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:PRO:HG3	1:A:737:GLN:CD	2.46	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:B:470:ARG:NH1	1:B:539:VAL:C	2.79	0.41
1:B:586:TYR:CD2	1:B:586:TYR:C	2.98	0.41
1:A:380:ARG:HG2	1:A:801:TYR:CG	2.56	0.41
1:A:505:ASN:O	1:A:506:TRP:C	2.64	0.40
1:B:470:ARG:HH12	1:B:540:THR:C	2.29	0.40
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:691:TYR:C	1:B:691:TYR:CD1	2.99	0.40
1:B:696:ILE:HG23	1:B:704:VAL:HG12	2.03	0.40
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
1:B:472:HIS:CD2	1:B:538:ASN:H	2.34	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%)	21	51
1	B	750/772 (97%)	700 (93%)	45 (6%)	5 (1%)	18	48
All	All	1520/1544 (98%)	1417 (93%)	93 (6%)	10 (1%)	18	48

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 ⓘ

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%)	574 (88%)	76 (12%)	5	17
1	B	637/650 (98%)	564 (88%)	73 (12%)	5	18
All	All	1287/1300 (99%)	1138 (88%)	149 (12%)	5	18

All (149) 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	152	ILE
1	A	154	THR
1	A	157	ARG

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Mol	Chain	Res	Type
1	A	177	MET
1	A	204	ARG
1	A	215	ASN
1	A	236	THR
1	A	238	SER
1	A	245	ARG
1	A	246	VAL
1	A	248	VAL
1	A	276	GLU
1	A	297	VAL
1	A	301	LEU
1	A	303	GLU
1	A	304	SER
1	A	307	VAL
1	A	312	VAL
1	A	329	THR
1	A	331	VAL
1	A	355	ASN
1	A	358	LYS
1	A	392	GLU
1	A	408	ASN
1	A	431	MET
1	A	459	ILE
1	A	461	LEU
1	A	466	GLN
1	A	468	LEU
1	A	475	VAL
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	603	SER
1	A	606	LYS

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Mol	Chain	Res	Type
1	A	609	GLU
1	A	618	ILE
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	725	LEU
1	A	730	VAL
1	A	744	VAL
1	A	771	ILE
1	A	772	THR
1	A	774	LYS
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
1	B	75	GLU
1	B	96	THR
1	B	98	LEU
1	B	105	SER
1	B	106	VAL
1	B	107	ASP
1	B	109	GLN
1	B	113	ILE
1	B	115	ILE
1	B	117	VAL
1	B	140	ILE
1	B	146	SER
1	B	148	THR
1	B	152	ILE
1	B	154	THR
1	B	157	ARG
1	B	160	LEU
1	B	195	ILE
1	B	229	VAL
1	B	236	THR

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Mol	Chain	Res	Type
1	B	245	ARG
1	B	265	THR
1	B	297	VAL
1	B	326	GLU
1	B	329	THR
1	B	330	SER
1	B	331	VAL
1	B	396	ARG
1	B	397	THR
1	B	411	VAL
1	B	416	LEU
1	B	431	MET
1	B	447	LYS
1	B	462	THR
1	B	466	GLN
1	B	475	VAL
1	B	476	VAL
1	B	478	THR
1	B	493	LEU
1	B	495	ASN
1	B	509	ASP
1	B	512	LYS
1	B	522	ILE
1	B	556	VAL
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	641	GLU
1	B	646	GLU
1	B	671	LYS
1	B	681	LEU
1	B	687	VAL
1	B	694	LYS
1	B	702	LYS
1	B	704	VAL
1	B	705	SER
1	B	714	SER
1	B	720	LYS

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Mol	Chain	Res	Type
1	B	739	LYS
1	B	743	MET
1	B	749	ARG
1	B	759	ASP
1	B	764	ASP
1	B	772	THR
1	B	788	THR
1	B	792	ASN
1	B	810	SER

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

Mol	Chain	Res	Type
1	A	60	GLN
1	A	176	ASN
1	A	183	ASN
1	A	191	HIS
1	A	205	ASN
1	A	408	ASN
1	A	421	ASN
1	A	455	ASN
1	A	505	ASN
1	A	615	ASN
1	A	780	ASN
1	B	109	GLN
1	B	176	ASN
1	B	183	ASN
1	B	205	ASN
1	B	405	ASN
1	B	418	HIS
1	B	455	ASN
1	B	472	HIS
1	B	528	GLN
1	B	560	ASN
1	B	688	GLN
1	B	710	GLN
1	B	742	GLN
1	B	806	ASN

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 oligosaccharides 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	$\# Z > 2$
3	PO4	A	1819	-	4,4,4	0.84	0	6,6,6	0.77	0
3	PO4	A	1818	-	4,4,4	0.86	0	6,6,6	0.85	0
2	N8E	A	1816	-	23,23,23	0.62	0	22,22,22	0.56	0
2	N8E	A	1817[B]	-	23,23,23	0.78	0	22,22,22	0.85	1 (4%)
2	N8E	A	1817[A]	-	23,23,23	0.70	0	22,22,22	0.53	0
3	PO4	B	1817	-	4,4,4	0.99	0	6,6,6	1.27	1 (16%)
3	PO4	A	1820	-	4,4,4	0.85	0	6,6,6	0.64	0
3	PO4	A	1821	-	4,4,4	0.56	0	6,6,6	1.14	1 (16%)
3	PO4	B	1816	-	4,4,4	0.56	0	6,6,6	1.33	0
3	PO4	B	1818	-	4,4,4	0.86	0	6,6,6	0.70	0
3	PO4	B	1819	-	4,4,4	0.75	0	6,6,6	0.48	0
3	PO4	A	1822	-	4,4,4	0.94	0	6,6,6	0.63	0
3	PO4	A	1823	-	4,4,4	1.04	0	6,6,6	0.68	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	1817[B]	-	-	12/21/21/21	-
2	N8E	A	1817[A]	-	-	10/21/21/21	-
2	N8E	A	1816	-	-	10/21/21/21	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1817	PO4	O3-P-O2	2.43	115.48	107.91
3	A	1821	PO4	O4-P-O2	2.14	114.58	107.91
2	A	1817[B]	N8E	O18-C19-C20	2.14	120.11	110.35

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1817[B]	N8E	O18-C19-C20-O21
2	A	1817[B]	N8E	O09-C10-C11-O12
2	A	1817[A]	N8E	O18-C19-C20-O21
2	A	1816	N8E	O21-C22-C23-O24
2	A	1816	N8E	O12-C13-C14-O15
2	A	1816	N8E	O09-C10-C11-O12
2	A	1816	N8E	C04-C05-C06-C07
2	A	1817[A]	N8E	O21-C22-C23-O24
2	A	1817[A]	N8E	C02-C03-C04-C05
2	A	1817[B]	N8E	C02-C03-C04-C05
2	A	1816	N8E	C14-C13-O12-C11
2	A	1816	N8E	C16-C17-O18-C19
2	A	1817[A]	N8E	C23-C22-O21-C20
2	A	1816	N8E	C13-C14-O15-C16
2	A	1817[B]	N8E	C10-C11-O12-C13
2	A	1817[A]	N8E	C17-C16-O15-C14
2	A	1817[B]	N8E	C03-C04-C05-C06
2	A	1817[B]	N8E	O15-C16-C17-O18
2	A	1817[A]	N8E	C20-C19-O18-C17
2	A	1817[B]	N8E	C13-C14-O15-C16
2	A	1817[B]	N8E	C20-C19-O18-C17
2	A	1817[B]	N8E	C05-C06-C07-C08
2	A	1817[A]	N8E	O09-C10-C11-O12
2	A	1816	N8E	C17-C16-O15-C14

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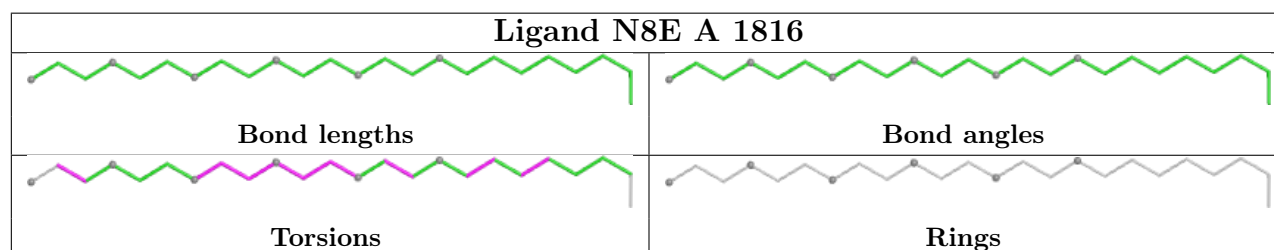
Mol	Chain	Res	Type	Atoms
2	A	1817[B]	N8E	C04-C05-C06-C07
2	A	1817[A]	N8E	C14-C13-O12-C11
2	A	1817[B]	N8E	C19-C20-O21-C22
2	A	1816	N8E	C06-C07-C08-O09
2	A	1817[A]	N8E	O15-C16-C17-O18
2	A	1817[A]	N8E	O12-C13-C14-O15
2	A	1816	N8E	O15-C16-C17-O18
2	A	1817[B]	N8E	C23-C22-O21-C20

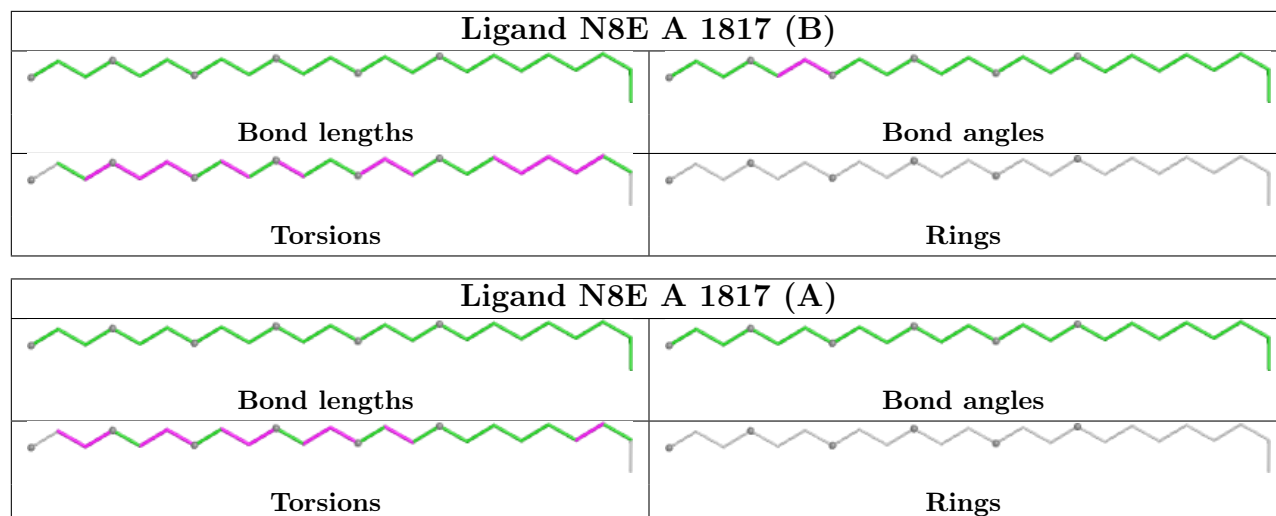
There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1817[B]	N8E	8	0
2	A	1817[A]	N8E	4	0
3	A	1820	PO4	1	0
3	B	1819	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	0.18	18 (2%) 61 52	2, 9, 19, 34	0
1	B	754/772 (97%)	0.26	21 (2%) 55 46	2, 8, 17, 29	0
All	All	1526/1544 (98%)	0.22	39 (2%) 57 48	2, 8, 18, 34	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	ALA	5.0
1	B	110	GLY	4.6
1	A	123	SER	4.3
1	B	109	GLN	4.1
1	B	44	GLN	3.7
1	A	44	GLN	3.6
1	B	541	ASP	3.6
1	B	78	ARG	3.4
1	A	79	ASN	3.3
1	A	303	GLU	3.2
1	A	124	SER	3.1
1	B	538	ASN	2.8
1	B	88	LYS	2.8
1	A	724	ALA	2.7
1	A	143	ASP	2.7
1	B	67	ASP	2.7
1	A	93	GLN	2.6
1	A	501	ASP	2.6
1	B	542	ASP	2.6
1	B	472	HIS	2.5
1	B	581	ASP	2.5
1	B	533	MET	2.5
1	A	599	TRP	2.5
1	A	276	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	122	ASP	2.4
1	B	409	GLY	2.4
1	B	405	ASN	2.4
1	A	645	GLU	2.4
1	B	458	ASP	2.3
1	B	229	VAL	2.3
1	A	597	ASP	2.3
1	B	758	GLU	2.2
1	A	507	ASP	2.2
1	B	111	ASN	2.1
1	A	407	ALA	2.1
1	A	125	VAL	2.1
1	A	609	GLU	2.0
1	B	471	GLU	2.0
1	B	501	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
2	N8E	A	1817[A]	24/24	0.70	0.35	2,2,5,7	24
2	N8E	A	1817[B]	24/24	0.70	0.35	2,2,7,8	24
3	PO4	A	1822	5/5	0.80	0.22	70,71,71,72	0
3	PO4	B	1816	5/5	0.85	0.22	41,42,43,43	0
2	N8E	A	1816	24/24	0.88	0.19	24,41,47,49	0
3	PO4	A	1823	5/5	0.89	0.27	52,53,53,54	0
3	PO4	B	1819	5/5	0.89	0.10	40,42,42,43	0
3	PO4	B	1818	5/5	0.90	0.17	60,60,61,62	0

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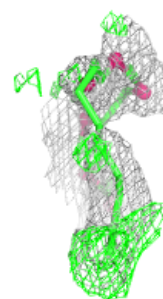
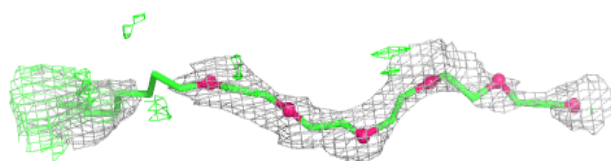
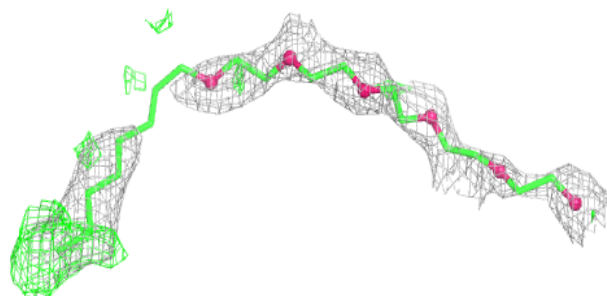
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	A	1821	5/5	0.91	0.13	37,37,38,39	0
3	PO4	A	1820	5/5	0.95	0.14	40,40,42,43	0
3	PO4	B	1817	5/5	0.97	0.07	7,7,8,8	0
3	PO4	A	1819	5/5	0.97	0.07	12,14,15,15	0
3	PO4	A	1818	5/5	0.97	0.07	16,18,20,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

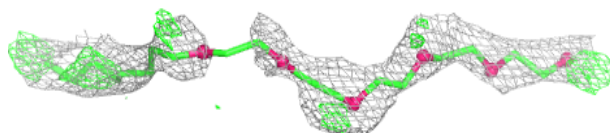
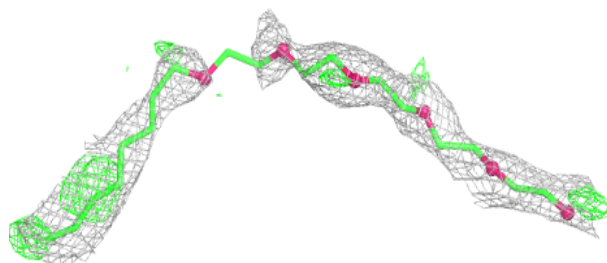
Electron density around N8E A 1817 (A):

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

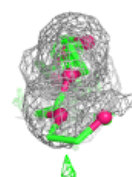
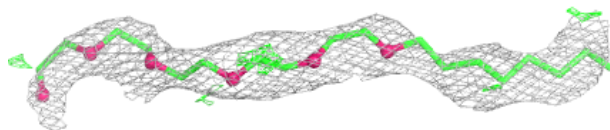
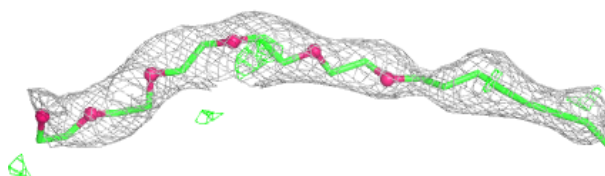


Electron density around N8E A 1817 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around N8E A 1816:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.