Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 01:43 PM EDT

PDB ID	:	2O5P
Title	:	Crystal structure of the full length ferric pyoverdine outer membrane receptor FpvA of Pseudomonas aeruginosa in its apo form
Authors	:	Cobessi, D.
Deposited on	:	2006-12-06
Resolution	:	2.77 Å(reported)

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

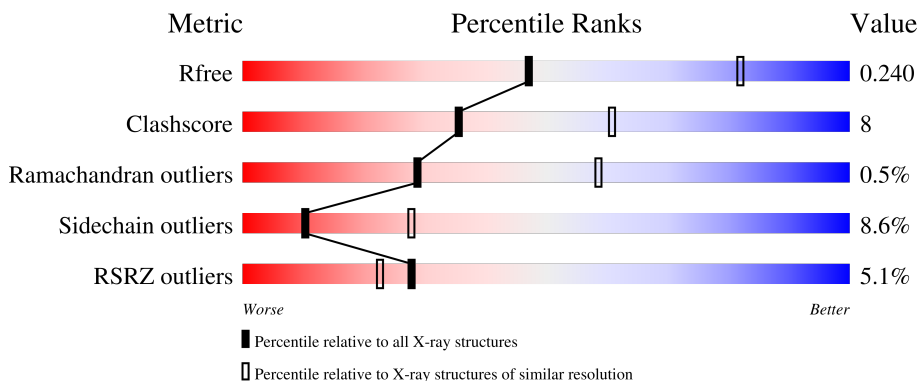|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.77 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	Percentile Ranks	Value
Rfree		0.240
Clashscore		8
Ramachandran outliers		0.5%
Sidechain outliers		8.6%
RSRZ outliers		5.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 <=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	3% 74% 23% •
1	B	772	7% 76% 20% ••

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 12184 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
			6115	3845	1046	1212	12			
1	B	754	Total	C	N	O	S	0	0	0
			5995	3775	1027	1182	11			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

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

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

- Molecule 3 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (three-letter code: N8E) (formula: $C_{18}H_{38}O_6$).
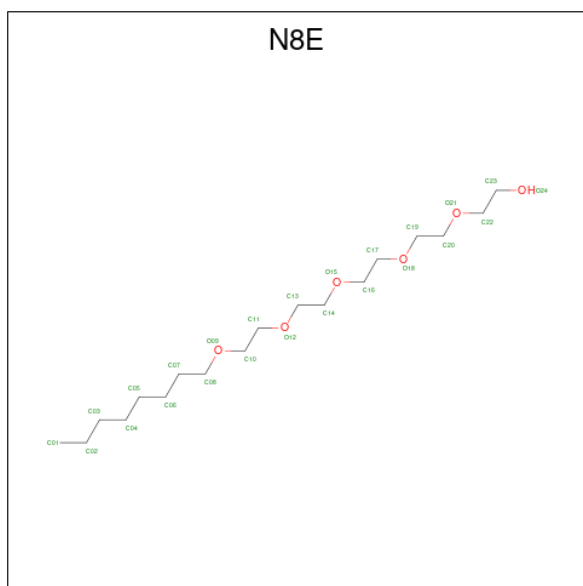
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 24	C 18	O 6	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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
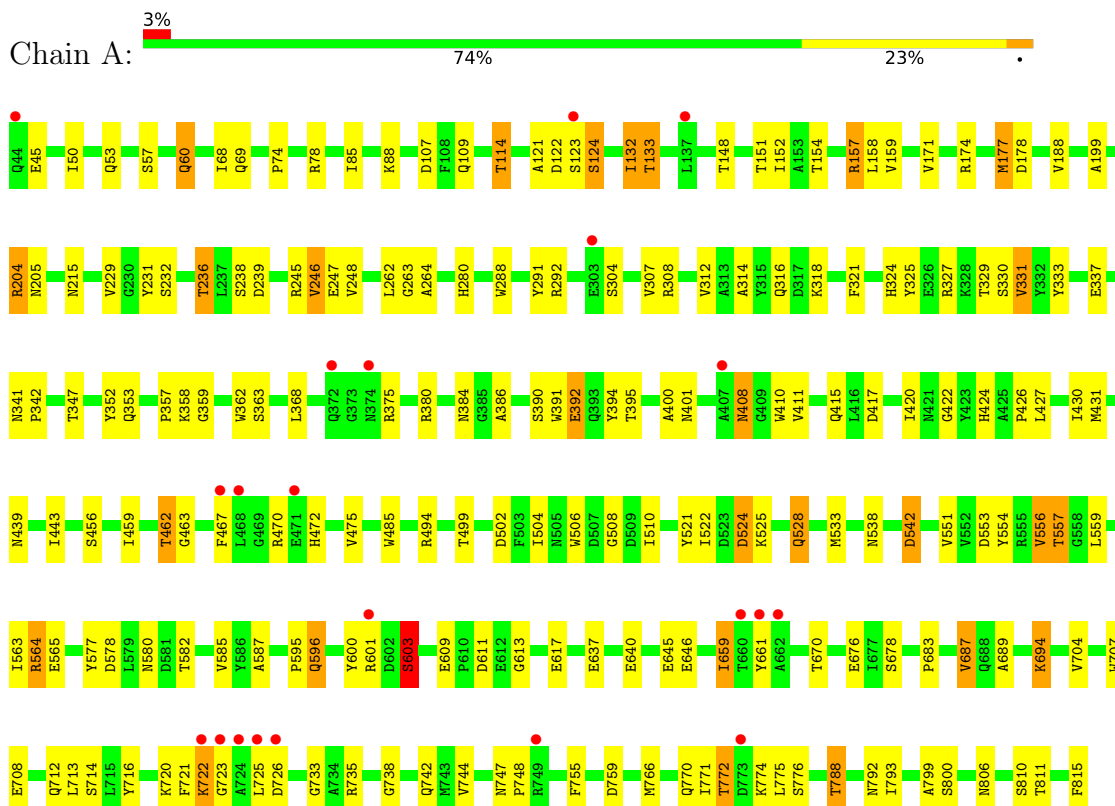
• Molecule 1: Ferripyoverdine receptor
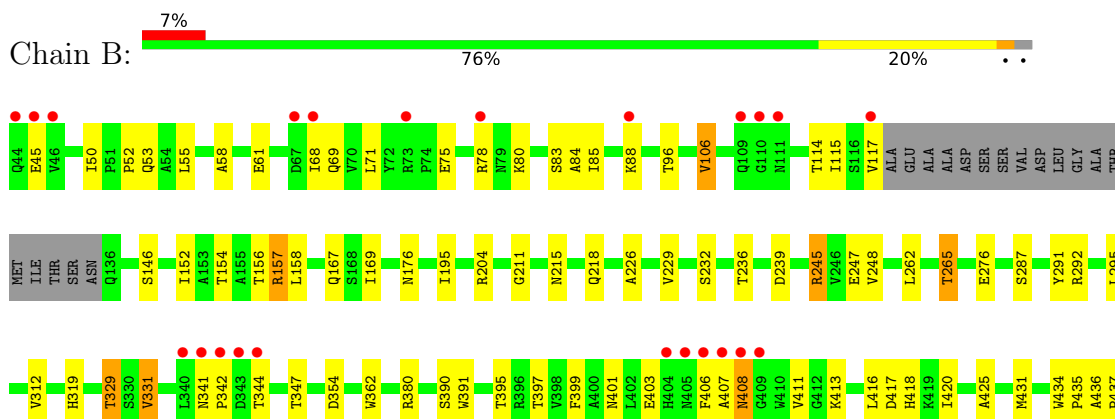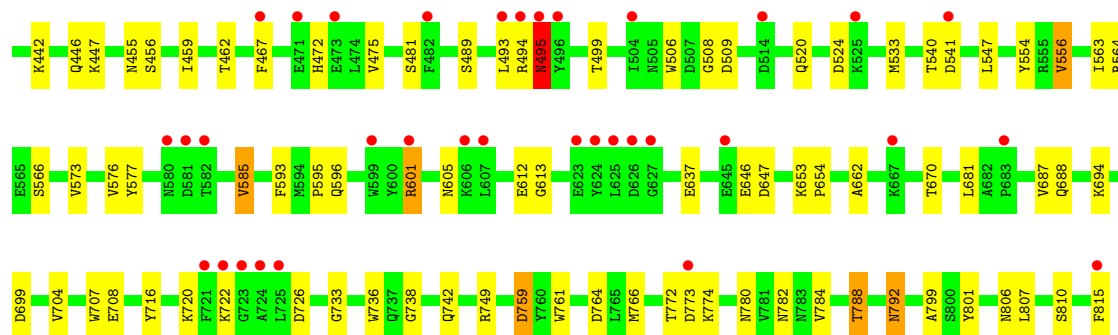
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	189.88Å 128.78Å 139.15Å 90.00° 130.55° 90.00°	Depositor
Resolution (Å)	30.47 – 2.77 30.47 – 2.77	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.47-2.77) 97.5 (30.47-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	8.00	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.247 0.203 , 0.240	Depositor DCC
R_{free} test set	3195 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 43.1	EDS
L-test for twinning [2]	$< \lvert L \rvert > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12184	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.59	0/6267	0.72	2/8514 (0.0%)
1	B	0.52	0/6146	0.65	0/8347
All	All	0.56	0/12413	0.68	2/16861 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	687	VAL	CB-CA-C	-6.05	99.90	111.40
1	A	713	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

There are no planarity outliers.

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	6115	0	5788	114	0
1	B	5995	0	5675	79	0
2	A	30	0	0	2	0
2	B	20	0	0	0	0
3	A	24	0	38	0	0
All	All	12184	0	11501	191	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 8.

All (191) 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	1.02	1.11
1:A:772:THR:HG21	1:B:291:TYR:OH	1.64	0.96
1:A:772:THR:HG22	1:A:774:LYS:H	1.33	0.90
1:A:694:LYS:HE3	1:A:708:GLU:OE1	1.73	0.89
1:B:772:THR:HG22	1:B:774:LYS:N	1.88	0.88
1:A:556:VAL:HG13	1:A:563:ILE:HB	1.57	0.86
1:A:470:ARG:NH1	1:A:538:ASN:OD1	2.08	0.85
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.59	0.83
1:B:764:ASP:HB3	1:B:782:ASN:HA	1.61	0.82
1:B:52:PRO:HD3	1:B:84:ALA:HB2	1.63	0.80
1:A:151:THR:O	1:A:152:ILE:HD13	1.86	0.76
1:A:291:TYR:OH	1:B:772:THR:HG21	1.86	0.75
1:A:109:GLN:OE1	1:A:114:THR:HG22	1.88	0.74
1:A:792:ASN:HB3	1:A:800:SER:HB2	1.71	0.73
1:A:384:ASN:HB2	1:A:430:ILE:HB	1.71	0.70
1:B:50:ILE:HG12	1:B:61:GLU:HG2	1.73	0.70
1:B:694:LYS:HE3	1:B:708:GLU:OE1	1.92	0.69
1:A:542:ASP:HB3	1:A:578:ASP:HB2	1.75	0.69
1:A:239:ASP:OD2	1:A:292:ARG:NH2	2.27	0.68
1:A:603:SER:O	1:A:659:ILE:HD11	1.95	0.67
1:B:245:ARG:NH1	1:B:247:GLU:OE2	2.27	0.67
1:A:53:GLN:OE1	1:A:57:SER:HB3	1.95	0.66
1:A:123:SER:O	1:A:124:SER:HB3	1.92	0.66
1:A:772:THR:HG22	1:A:774:LYS:N	2.11	0.65
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.31	0.65
1:B:601:ARG:NH1	1:B:605:ASN:O	2.30	0.65
1:A:109:GLN:OE1	1:A:114:THR:CG2	2.45	0.64
1:A:262:LEU:HD21	1:A:613:GLY:HA3	1.78	0.64
1:A:401:ASN:ND2	1:A:415:GLN:HG2	2.14	0.63
1:B:362:TRP:HH2	1:B:446:GLN:OE1	1.82	0.63
1:A:204:ARG:HG3	1:A:391:TRP:CH2	2.34	0.63
1:B:442:LYS:HG2	1:B:499:THR:HG22	1.82	0.62
1:B:417:ASP:HB2	1:B:456:SER:HB2	1.82	0.62
1:B:195:ILE:HD11	1:B:248:VAL:HG11	1.80	0.62
1:B:69:GLN:HG2	1:B:276:GLU:HA	1.81	0.61
1:B:204:ARG:HG3	1:B:391:TRP:CH2	2.36	0.61
1:A:231:TYR:OH	1:A:524:ASP:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HD12	1:A:85:ILE:HD11	1.81	0.61
1:A:443:ILE:HG13	1:A:510:ILE:HD13	1.81	0.61
1:B:646:GLU:O	1:B:662:ALA:O	2.18	0.61
1:A:392:GLU:HG3	1:A:424:HIS:HB3	1.83	0.61
1:A:755:PHE:HB3	1:A:793:ILE:HG21	1.82	0.61
1:B:152:ILE:HD12	1:B:169:ILE:HG12	1.82	0.61
1:B:347:THR:HB	1:B:401:ASN:HB2	1.81	0.60
1:A:45:GLU:HG2	1:A:88:LYS:HG2	1.84	0.60
1:A:178:ASP:OD2	2:A:4:PO4:O1	2.19	0.60
1:A:171:VAL:HG22	1:A:247:GLU:HB3	1.84	0.59
1:B:50:ILE:HD12	1:B:85:ILE:HD11	1.84	0.59
1:B:554:TYR:CD2	1:B:595:PRO:HG2	2.38	0.58
1:A:554:TYR:CD2	1:A:595:PRO:HG2	2.38	0.58
1:B:380:ARG:HD3	1:B:788:THR:HB	1.84	0.58
1:B:418:HIS:CD2	1:B:455:ASN:HD21	2.22	0.57
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.38	0.57
1:B:540:THR:HG22	1:B:541:ASP:H	1.69	0.57
1:B:556:VAL:HG13	1:B:563:ILE:HB	1.87	0.57
1:A:341:ASN:HB2	1:A:342:PRO:CD	2.35	0.56
1:A:742:GLN:HG3	1:A:793:ILE:O	2.05	0.56
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.87	0.56
1:B:362:TRP:HB3	1:B:431:MET:HE1	1.87	0.56
1:B:764:ASP:HA	1:B:784:VAL:HG23	1.88	0.56
1:A:410:TRP:CD2	1:A:463:GLY:HA3	2.41	0.56
1:B:646:GLU:O	1:B:647:ASP:HB3	2.06	0.56
1:A:325:TYR:OH	1:A:327:ARG:NH1	2.36	0.55
1:B:540:THR:HG22	1:B:541:ASP:N	2.21	0.55
1:A:69:GLN:HE21	1:A:133:THR:HG23	1.70	0.55
1:A:74:PRO:HG3	1:A:132:ILE:HG12	1.89	0.54
1:A:380:ARG:HD3	1:A:788:THR:HB	1.90	0.54
1:B:694:LYS:HD2	1:B:694:LYS:C	2.27	0.54
1:B:436:ALA:HB1	1:B:437:PRO:HD2	1.89	0.54
1:A:362:TRP:HE3	1:A:363:SER:HB3	1.72	0.54
1:B:211:GLY:HA2	1:B:708:GLU:OE1	2.07	0.54
1:A:359:GLY:HA2	1:A:386:ALA:O	2.08	0.54
1:B:780:ASN:O	1:B:807:LEU:HA	2.08	0.54
1:B:792:ASN:O	1:B:799:ALA:HA	2.08	0.54
1:A:174:ARG:CZ	1:A:177:MET:HE3	2.38	0.53
1:B:71:LEU:HD12	1:B:114:THR:HG22	1.91	0.53
1:A:411:VAL:HG12	1:A:462:THR:HG22	1.90	0.53
1:A:772:THR:CG2	1:A:774:LYS:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ARG:NH1	1:A:337:GLU:OE1	2.42	0.52
1:A:707:TRP:CH2	1:A:793:ILE:HG13	2.45	0.52
1:B:106:VAL:HG13	1:B:115:ILE:HD13	1.90	0.52
1:A:229:VAL:HA	1:A:232:SER:HB3	1.90	0.52
1:B:406:PHE:O	1:B:408:ASN:N	2.42	0.52
1:A:280:HIS:NE2	2:A:10:PO4:O4	2.43	0.52
1:A:363:SER:O	1:A:363:SER:OG	2.28	0.52
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.44	0.52
1:B:418:HIS:CD2	1:B:455:ASN:ND2	2.79	0.51
1:A:712:GLN:OE1	1:A:735:ARG:NH1	2.44	0.51
1:A:475:VAL:O	1:A:533:MET:HA	2.12	0.50
1:A:60:GLN:NE2	1:A:133:THR:O	2.44	0.49
1:A:199:ALA:HA	1:A:205:ASN:HD22	1.77	0.49
1:B:329:THR:HA	1:B:354:ASP:O	2.12	0.49
1:A:443:ILE:HG13	1:A:510:ILE:CD1	2.42	0.49
1:A:580:ASN:HB2	1:A:582:THR:H	1.78	0.49
1:B:156:THR:C	1:B:158:LEU:H	2.16	0.49
1:A:611:ASP:OD1	1:A:640:GLU:OE2	2.31	0.49
1:A:755:PHE:CB	1:A:793:ILE:HG21	2.43	0.48
1:A:722:LYS:HG3	1:A:723:GLY:N	2.28	0.48
1:A:564:ARG:HD3	1:A:565:GLU:N	2.29	0.47
1:B:262:LEU:HD21	1:B:613:GLY:HA3	1.97	0.47
1:A:188:VAL:HG11	1:A:246:VAL:CG1	2.45	0.47
1:A:528:GLN:HG2	1:A:554:TYR:CD1	2.49	0.47
1:A:646:GLU:HG3	1:A:661:TYR:OH	2.14	0.47
1:A:158:LEU:CD2	1:A:475:VAL:HG22	2.45	0.47
1:A:439:ASN:HD21	1:A:504:ILE:HG13	1.80	0.47
1:B:55:LEU:HB2	1:B:80:LYS:HB2	1.97	0.46
1:B:157:ARG:HB3	1:B:475:VAL:HG11	1.97	0.46
1:B:239:ASP:HB3	1:B:331:VAL:HG11	1.96	0.46
1:A:239:ASP:CG	1:A:292:ARG:HH22	2.17	0.46
1:A:553:ASP:OD1	1:A:564:ARG:NH2	2.49	0.46
1:A:188:VAL:HG11	1:A:246:VAL:HG13	1.97	0.46
1:A:722:LYS:HG3	1:A:723:GLY:H	1.81	0.46
1:B:494:ARG:O	1:B:495:ASN:C	2.53	0.46
1:B:738:GLY:HA2	1:B:759:ASP:HB2	1.98	0.46
1:B:418:HIS:HD2	1:B:455:ASN:ND2	2.13	0.46
1:A:107:ASP:HB3	1:A:114:THR:HG23	1.97	0.45
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.50	0.45
1:B:399:PHE:HA	1:B:416:LEU:O	2.16	0.45
1:B:462:THR:HB	1:B:475:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:653:LYS:HA	1:B:654:PRO:HD2	1.76	0.45
1:A:288:TRP:CH2	1:A:806:ASN:HB3	2.51	0.45
1:B:287:SER:HB2	1:B:806:ASN:HB2	1.99	0.45
1:A:347:THR:O	1:A:400:ALA:HA	2.17	0.45
1:B:736:TRP:HB2	1:B:761:TRP:CE3	2.52	0.45
1:A:417:ASP:HB2	1:A:456:SER:HB2	1.98	0.45
1:B:506:TRP:CZ2	1:B:508:GLY:HA2	2.52	0.45
1:A:157:ARG:HB3	1:A:475:VAL:HG11	1.99	0.45
1:A:204:ARG:NH1	1:A:229:VAL:HG12	2.31	0.45
1:A:263:GLY:O	1:A:264:ALA:HB2	2.17	0.45
1:A:747:ASN:HB3	1:A:748:PRO:HD3	2.00	0.44
1:B:593:PHE:HB3	1:B:612:GLU:HG3	1.99	0.44
1:A:357:PRO:O	1:A:358:LYS:HD2	2.17	0.44
1:B:434:TRP:HB3	1:B:435:PRO:HA	1.99	0.44
1:B:637:GLU:HA	1:B:670:THR:O	2.17	0.44
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.53	0.44
1:A:133:THR:HG21	1:A:159:VAL:HG21	1.98	0.44
1:B:53:GLN:HG3	1:B:58:ALA:HB2	1.98	0.44
1:A:721:PHE:O	1:A:726:ASP:HA	2.17	0.44
1:A:771:ILE:H	1:A:771:ILE:HG13	1.56	0.44
1:B:707:TRP:HB2	1:B:742:GLN:HE21	1.83	0.44
1:A:392:GLU:CG	1:A:424:HIS:HB3	2.46	0.44
1:A:467:PHE:HB3	1:A:472:HIS:HE2	1.81	0.44
1:A:502:ASP:C	1:A:502:ASP:OD1	2.56	0.44
1:B:218:GLN:OE1	1:B:265:THR:HG21	2.18	0.44
1:B:390:SER:O	1:B:425:ALA:HA	2.17	0.44
1:A:577:TYR:HB3	1:A:585:VAL:HG23	2.00	0.44
1:B:152:ILE:CD1	1:B:169:ILE:HG12	2.47	0.44
1:A:312:VAL:HG13	1:A:333:TYR:HD2	1.83	0.43
1:B:489:SER:HB2	1:B:520:GLN:HB3	2.00	0.43
1:B:807:LEU:N	1:B:807:LEU:HD12	2.33	0.43
1:B:726:ASP:OD1	1:B:726:ASP:C	2.57	0.43
1:A:288:TRP:CZ2	1:A:321:PHE:HB3	2.53	0.43
1:A:485:TRP:CD2	1:A:522:ILE:HG21	2.54	0.43
1:A:689:ALA:HA	1:A:714:SER:O	2.19	0.43
1:A:521:TYR:O	1:A:559:LEU:HD11	2.19	0.43
1:A:637:GLU:HA	1:A:670:THR:O	2.19	0.43
1:B:403:GLU:HB3	1:B:413:LYS:HG3	2.01	0.43
1:A:331:VAL:HA	1:A:352:TYR:O	2.19	0.42
1:B:694:LYS:HE3	1:B:708:GLU:CD	2.40	0.42
1:A:330:SER:O	1:A:353:GLN:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLN:HE22	1:A:159:VAL:HG11	1.84	0.42
1:B:341:ASN:HB2	1:B:342:PRO:CD	2.50	0.42
1:A:694:LYS:HE3	1:A:708:GLU:CD	2.37	0.42
1:A:69:GLN:HE21	1:A:133:THR:CG2	2.32	0.42
1:B:395:THR:HA	1:B:420:ILE:O	2.19	0.42
1:B:475:VAL:O	1:B:533:MET:HA	2.19	0.42
1:A:236:THR:H	1:A:236:THR:HG22	1.53	0.41
1:A:596:GLN:HG3	1:A:600:TYR:HD2	1.84	0.41
1:A:738:GLY:HA2	1:A:759:ASP:HB3	2.01	0.41
1:A:391:TRP:HB2	1:A:427:LEU:HD21	2.02	0.41
1:A:770:GLN:OE1	1:A:776:SER:HB3	2.21	0.41
1:A:587:ALA:HA	1:A:617:GLU:O	2.21	0.41
1:B:547:LEU:HD23	1:B:573:VAL:HG22	2.03	0.41
1:B:707:TRP:HB2	1:B:742:GLN:HG2	2.03	0.41
1:A:506:TRP:CZ2	1:A:508:GLY:HA2	2.56	0.41
1:A:123:SER:O	1:A:124:SER:CB	2.64	0.41
1:A:291:TYR:O	1:A:316:GLN:HA	2.21	0.41
1:A:528:GLN:HG2	1:A:554:TYR:HD1	1.85	0.41
1:A:678:SER:HA	1:A:687:VAL:O	2.21	0.41
1:A:395:THR:HA	1:A:420:ILE:O	2.20	0.41
1:B:215:ASN:ND2	1:B:226:ALA:O	2.51	0.41
1:B:577:TYR:HB3	1:B:585:VAL:HG23	2.02	0.41
1:A:158:LEU:HD23	1:A:475:VAL:HG22	2.03	0.40
1:A:368:LEU:HD21	1:A:799:ALA:HB2	2.03	0.40
1:A:408:ASN:HD22	1:A:408:ASN:HA	1.64	0.40
1:B:467:PHE:HB3	1:B:472:HIS:CE1	2.56	0.40
1:A:525:LYS:HB2	1:A:557:THR:HG22	2.04	0.40
1:A:314:ALA:HB3	1:A:331:VAL:HG13	2.03	0.40
1:A:390:SER:O	1:A:426:PRO:HD2	2.22	0.40
1:B:45:GLU:HB3	1:B:88:LYS:HG2	2.04	0.40
1:B:295:LEU:O	1:B:312:VAL:HA	2.21	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%)	724 (94%)	41 (5%)	5 (1%)	25	54
1	B	750/772 (97%)	717 (96%)	30 (4%)	3 (0%)	34	64
All	All	1520/1544 (98%)	1441 (95%)	71 (5%)	8 (0%)	29	58

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	SER
1	A	121	ALA
1	B	407	ALA
1	B	495	ASN
1	A	122	ASP
1	A	603	SER
1	B	408	ASN
1	A	324	HIS

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%)	592 (91%)	58 (9%)	9	26
1	B	637/650 (98%)	584 (92%)	53 (8%)	11	29
All	All	1287/1300 (99%)	1176 (91%)	111 (9%)	10	28

All (111) 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	114	THR
1	A	132	ILE

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Mol	Chain	Res	Type
1	A	133	THR
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	236	THR
1	A	238	SER
1	A	245	ARG
1	A	246	VAL
1	A	248	VAL
1	A	304	SER
1	A	307	VAL
1	A	318	LYS
1	A	329	THR
1	A	331	VAL
1	A	375	ARG
1	A	392	GLU
1	A	408	ASN
1	A	431	MET
1	A	459	ILE
1	A	462	THR
1	A	494	ARG
1	A	499	THR
1	A	524	ASP
1	A	528	GLN
1	A	542	ASP
1	A	551	VAL
1	A	556	VAL
1	A	557	THR
1	A	564	ARG
1	A	596	GLN
1	A	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

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Mol	Chain	Res	Type
1	A	720	LYS
1	A	722	LYS
1	A	725	LEU
1	A	744	VAL
1	A	766	MET
1	A	772	THR
1	A	775	LEU
1	A	788	THR
1	A	810	SER
1	A	811	THR
1	A	815	PHE
1	B	68	ILE
1	B	75	GLU
1	B	78	ARG
1	B	83	SER
1	B	96	THR
1	B	106	VAL
1	B	117	VAL
1	B	146	SER
1	B	154	THR
1	B	157	ARG
1	B	167	GLN
1	B	176	ASN
1	B	229	VAL
1	B	232	SER
1	B	236	THR
1	B	245	ARG
1	B	265	THR
1	B	292	ARG
1	B	319	HIS
1	B	329	THR
1	B	331	VAL
1	B	344	THR
1	B	397	THR
1	B	411	VAL
1	B	447	LYS
1	B	459	ILE
1	B	481	SER
1	B	493	LEU
1	B	495	ASN
1	B	509	ASP
1	B	524	ASP

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Mol	Chain	Res	Type
1	B	556	VAL
1	B	564	ARG
1	B	566	SER
1	B	576	VAL
1	B	585	VAL
1	B	596	GLN
1	B	601	ARG
1	B	681	LEU
1	B	687	VAL
1	B	688	GLN
1	B	699	ASP
1	B	704	VAL
1	B	720	LYS
1	B	722	LYS
1	B	749	ARG
1	B	759	ASP
1	B	766	MET
1	B	773	ASP
1	B	788	THR
1	B	792	ASN
1	B	810	SER
1	B	815	PHE

Sometimes 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	183	ASN
1	A	218	GLN
1	A	401	ASN
1	A	408	ASN
1	A	455	ASN
1	A	505	ASN
1	A	580	ASN
1	A	596	GLN
1	A	615	ASN
1	A	642	ASN
1	B	109	GLN
1	B	176	ASN
1	B	401	ASN
1	B	408	ASN

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Mol	Chain	Res	Type
1	B	415	GLN
1	B	418	HIS
1	B	455	ASN
1	B	472	HIS
1	B	596	GLN
1	B	688	GLN
1	B	742	GLN
1	B	780	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 monosaccharides in this entry.

5.6　Ligand geometry ⓘ

11 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	PO4	A	3	-	4,4,4	0.97	0	6,6,6	0.45	0
2	PO4	A	1	-	4,4,4	0.97	0	6,6,6	1.18	0
3	N8E	A	11	-	23,23,23	0.78	1 (4%)	22,22,22	0.48	0
2	PO4	B	2	-	4,4,4	0.80	0	6,6,6	0.83	0
2	PO4	A	7	-	4,4,4	0.85	0	6,6,6	0.52	0
2	PO4	A	9	-	4,4,4	0.88	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	PO4	B	5	-	4,4,4	0.75	0	6,6,6	0.81	0
2	PO4	B	6	-	4,4,4	0.92	0	6,6,6	0.51	0
2	PO4	A	10	-	4,4,4	1.03	0	6,6,6	0.42	0
2	PO4	A	4	-	4,4,4	0.95	0	6,6,6	0.72	0
2	PO4	B	8	-	4,4,4	0.89	0	6,6,6	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N8E	A	11	-	-	11/21/21/21	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	11	N8E	C04-C03	-3.01	1.34	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	11	N8E	O09-C10-C11-O12
3	A	11	N8E	O12-C13-C14-O15
3	A	11	N8E	C01-C02-C03-C04
3	A	11	N8E	C13-C14-O15-C16
3	A	11	N8E	C17-C16-O15-C14
3	A	11	N8E	C14-C13-O12-C11
3	A	11	N8E	C19-C20-O21-C22
3	A	11	N8E	O18-C19-C20-O21
3	A	11	N8E	C16-C17-O18-C19
3	A	11	N8E	O15-C16-C17-O18
3	A	11	N8E	C04-C05-C06-C07

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	10	PO4	1	0
2	A	4	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 then 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.

Ligand N8E A 11

Bond lengths   Bond angles

Torsions   Rings
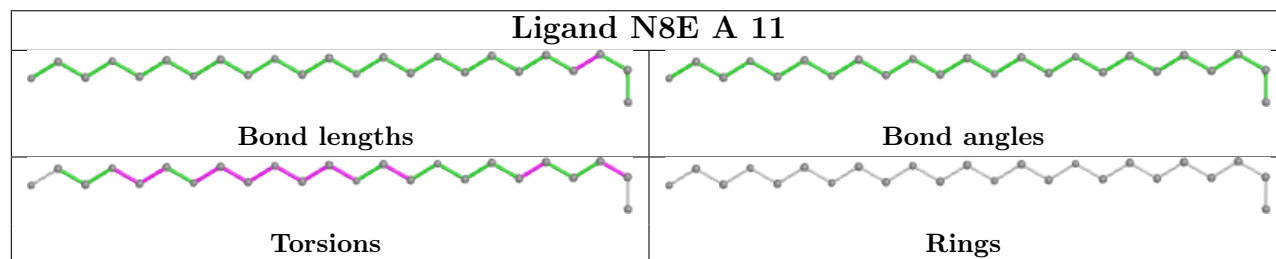
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.15	21 (2%)	54 49	32, 40, 48, 55	0
1	B	754/772 (97%)	0.37	57 (7%)	13 9	31, 40, 46, 53	0
All	All	1526/1544 (98%)	0.26	78 (5%)	28 22	31, 40, 47, 55	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	ALA	7.1
1	B	44	GLN	5.0
1	B	723	GLY	4.6
1	B	343	ASP	4.6
1	A	407	ALA	4.5
1	B	724	ALA	4.4
1	B	581	ASP	4.3
1	B	722	LYS	4.1
1	B	683	PRO	4.0
1	B	344	THR	4.0
1	B	342	PRO	4.0
1	B	626	ASP	4.0
1	A	44	GLN	3.9
1	B	406	PHE	3.9
1	B	340	LEU	3.7
1	B	109	GLN	3.6
1	B	78	ARG	3.6
1	B	606	LYS	3.5
1	B	117	VAL	3.4
1	A	724	ALA	3.3
1	A	723	GLY	3.3
1	B	495	ASN	3.2
1	B	625	LEU	3.2
1	B	815	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	627	GLY	3.2
1	B	110	GLY	3.1
1	B	111	ASN	3.1
1	B	493	LEU	3.1
1	B	541	ASP	3.1
1	A	773	ASP	3.0
1	A	662	ALA	2.9
1	B	88	LYS	2.8
1	A	303	GLU	2.8
1	A	374	ASN	2.8
1	B	624	TYR	2.7
1	B	504	ILE	2.7
1	B	473	GLU	2.7
1	B	405	ASN	2.6
1	A	722	LYS	2.6
1	B	471	GLU	2.6
1	B	45	GLU	2.6
1	A	661	TYR	2.5
1	B	341	ASN	2.5
1	B	721	PHE	2.5
1	A	123	SER	2.4
1	B	73	ARG	2.4
1	B	623	GLU	2.4
1	A	467	PHE	2.4
1	B	525	LYS	2.4
1	B	482	PHE	2.4
1	A	372	GLN	2.3
1	B	514	ASP	2.3
1	B	607	LEU	2.3
1	A	725	LEU	2.3
1	B	725	LEU	2.3
1	B	467	PHE	2.3
1	B	46	VAL	2.3
1	B	67	ASP	2.3
1	B	667	LYS	2.3
1	A	749	ARG	2.3
1	B	68	ILE	2.3
1	B	773	ASP	2.3
1	A	726	ASP	2.2
1	B	408	ASN	2.2
1	A	471	GLU	2.2
1	B	601	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	468	LEU	2.2
1	B	409	GLY	2.2
1	B	496	TYR	2.1
1	B	582	THR	2.1
1	B	404	HIS	2.1
1	A	660	THR	2.1
1	B	645	GLU	2.1
1	B	580	ASN	2.0
1	B	599	TRP	2.0
1	A	137	LEU	2.0
1	A	601	ARG	2.0
1	B	494	ARG	2.0

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

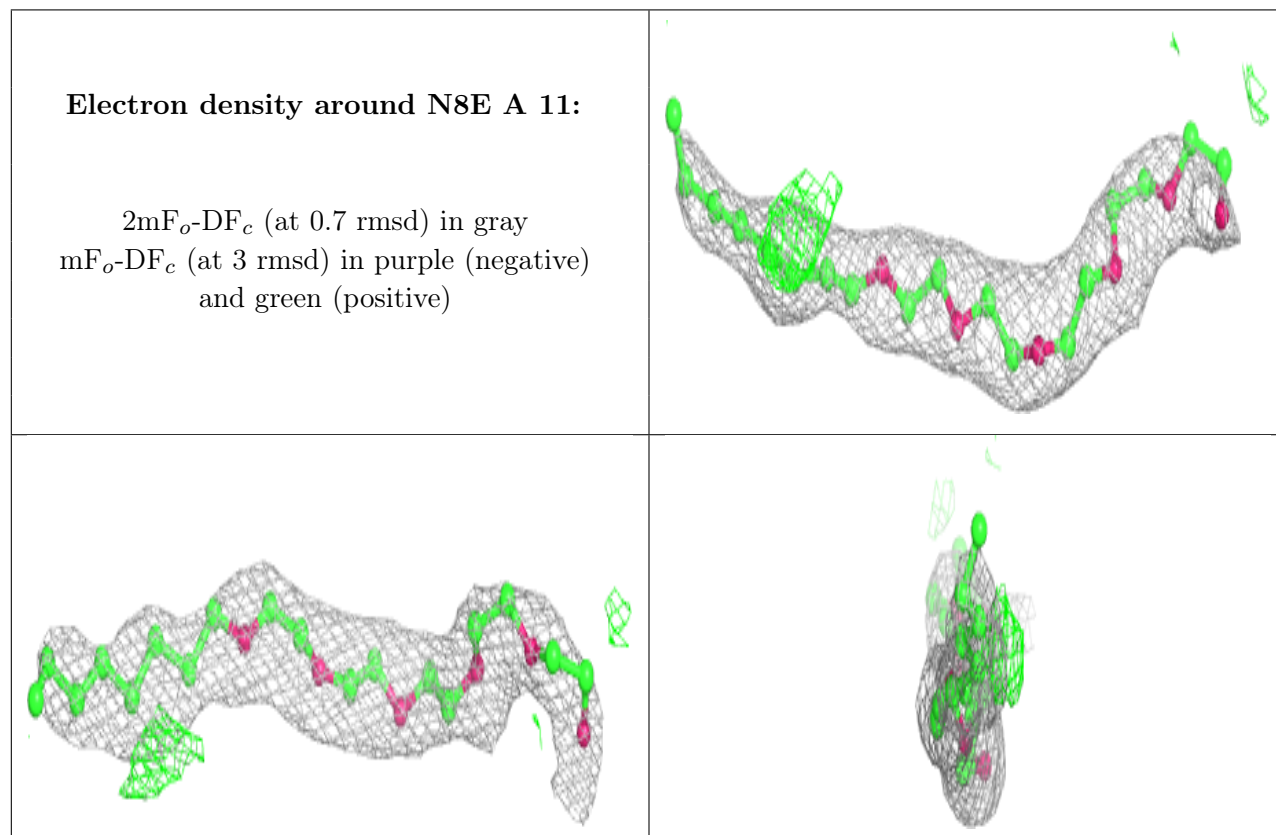There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	N8E	A	11	24/24	0.77	0.31	66,75,80,80	0
2	PO4	B	8	5/5	0.92	0.30	84,85,85,86	0
2	PO4	A	7	5/5	0.93	0.32	68,69,69,70	0
2	PO4	B	2	5/5	0.95	0.38	75,76,76,77	0
2	PO4	A	9	5/5	0.95	0.25	74,74,75,76	0
2	PO4	A	10	5/5	0.95	0.26	68,69,69,70	0
2	PO4	B	6	5/5	0.96	0.18	66,66,66,68	0
2	PO4	A	1	5/5	0.98	0.15	48,48,49,50	0
2	PO4	A	3	5/5	0.98	0.09	50,50,50,50	0
2	PO4	B	5	5/5	0.98	0.10	48,49,49,50	0
2	PO4	A	4	5/5	0.99	0.15	50,51,52,53	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 11:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.