



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:30 PM UTC

PDB ID : 2W77 / pdb_00002w77
Title : Structures of *P. aeruginosa* FpvA bound to heterologous pyoverdines: FpvA-Pvd(Pfl18.1)-Fe complex
Authors : Greenwald, J.; Nader, M.; Celia, H.; Gruffaz, C.; Meyer, J.-M.; Schalk, I.J.; Pattus, F.
Deposited on : 2008-12-20
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

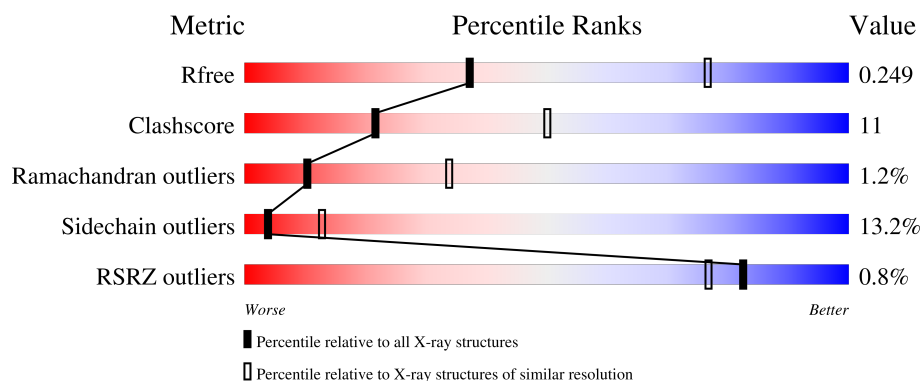
1 Overall quality at a glance

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	69% 24% 6% .
1	B	772	70% 23% 5% .
2	C	10	50% 20% 30%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12329 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

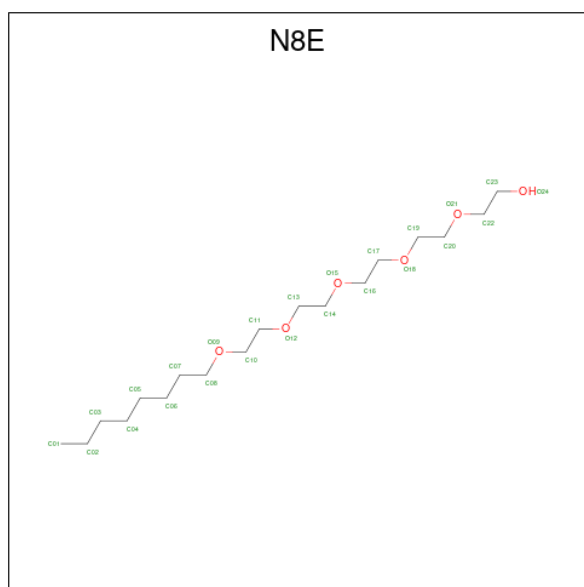
- Molecule 1 is a protein called FERRIPYOVERDINE RECEPTOR.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			72	40	14	18			

- Molecule 3 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (CCD ID: N8E) (formula: C₁₈H₃₈O₆).



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

Continued on next page...

Continued from previous page...

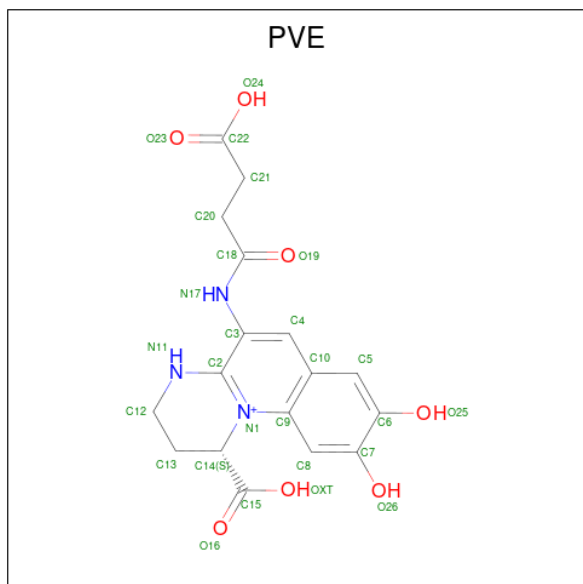
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			48	36	12		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

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



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

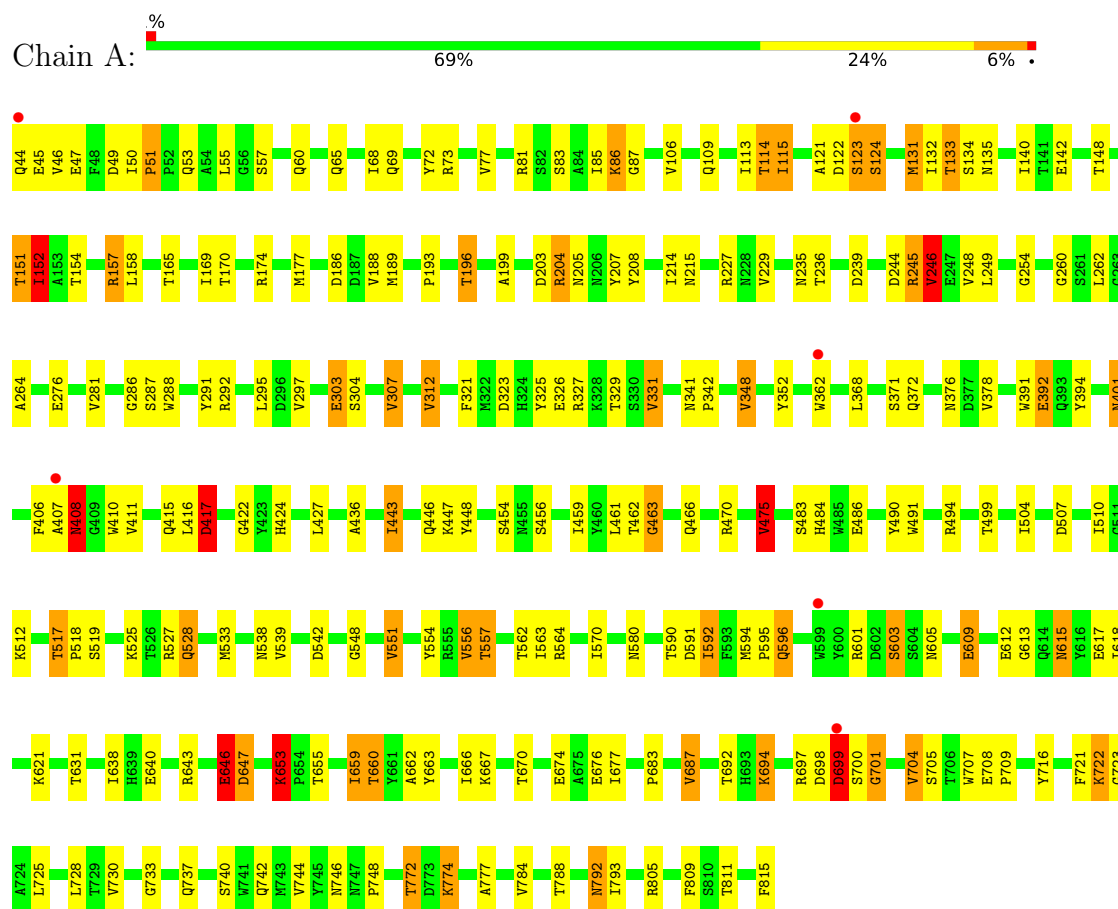
- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

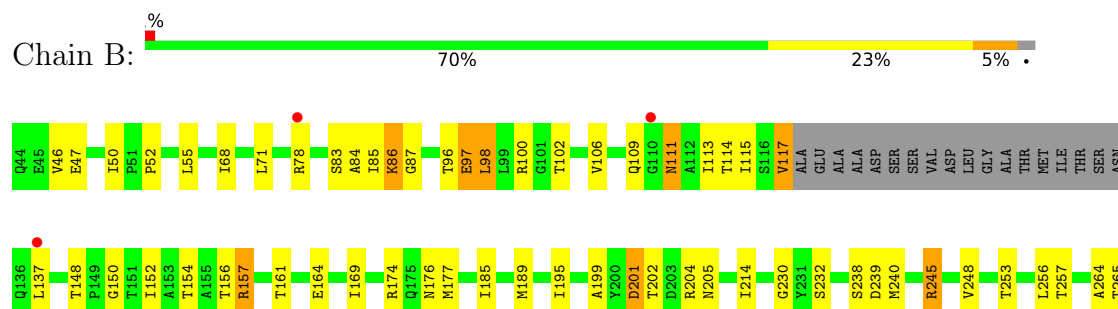
3 Residue-property plots

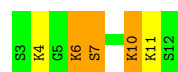
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	194.77Å 130.02Å 141.33Å 90.00° 130.92° 90.00°	Depositor
Resolution (Å)	25.57 – 2.90 25.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (25.57-2.90) 96.8 (25.57-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.253 0.202 , 0.249	Depositor DCC
R_{free} test set	2892 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12329	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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: FE, DSN, FHO, FH7, N8E, PO4, PVE

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	1.11	8/6266 (0.1%)	1.25	33/8514 (0.4%)
1	B	1.01	1/6145 (0.0%)	1.17	22/8347 (0.3%)
2	C	0.79	0/34	1.03	0/36
All	All	1.06	9/12445 (0.1%)	1.21	55/16897 (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	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	VAL	CA-CB	6.68	1.62	1.54
1	A	551	VAL	CA-CB	6.43	1.62	1.54
1	A	699	ASP	CA-C	6.04	1.60	1.52
1	A	504	ILE	CA-CB	6.02	1.61	1.54
1	B	551	VAL	CA-CB	5.64	1.61	1.54
1	A	115	ILE	CA-CB	5.63	1.60	1.54
1	A	312	VAL	CA-CB	5.40	1.62	1.54
1	A	348	VAL	CA-CB	5.20	1.62	1.54
1	A	647	ASP	N-CA	5.16	1.52	1.46

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	VAL	CB-CA-C	-8.94	96.95	110.55
1	A	660	THR	N-CA-C	-7.60	104.03	113.38
1	A	512	LYS	CA-C-N	-7.40	113.20	120.52
1	A	512	LYS	C-N-CA	-7.40	113.20	120.52
1	A	152	ILE	N-CA-CB	-7.33	101.29	111.19
1	A	475	VAL	CB-CA-C	-6.89	100.43	110.63
1	B	764	ASP	N-CA-C	6.85	120.14	109.52
1	A	517	THR	CA-C-N	-6.84	112.44	119.83
1	A	517	THR	C-N-CA	-6.84	112.44	119.83
1	A	51	PRO	CA-C-N	6.81	127.22	119.93
1	A	51	PRO	C-N-CA	6.81	127.22	119.93
1	A	87	GLY	N-CA-C	6.74	120.35	111.52
1	B	150	GLY	N-CA-C	-6.71	97.28	113.18
1	A	45	GLU	N-CA-C	6.69	120.08	110.24
1	B	687	VAL	CB-CA-C	-6.65	100.57	110.82
1	A	113	ILE	CA-C-N	-6.56	112.87	122.65
1	A	113	ILE	C-N-CA	-6.56	112.87	122.65
1	B	320	SER	N-CA-C	6.54	117.21	108.38
1	B	672	GLY	N-CA-C	6.46	120.56	111.19
1	B	272	LYS	CA-C-N	-6.41	114.12	120.98
1	B	272	LYS	C-N-CA	-6.41	114.12	120.98
1	A	463	GLY	CA-C-N	6.22	127.44	120.66
1	A	463	GLY	C-N-CA	6.22	127.44	120.66
1	A	653	LYS	CA-C-N	6.16	126.51	119.92
1	A	653	LYS	C-N-CA	6.16	126.51	119.92
1	A	507	ASP	N-CA-CB	-6.09	102.94	110.98
1	B	399	PHE	N-CA-C	6.08	118.02	108.96
1	B	642	ASN	N-CA-C	5.86	119.72	111.52
1	A	417	ASP	N-CA-C	5.81	118.94	109.24
1	B	436	ALA	CA-C-N	-5.75	112.95	119.28
1	B	436	ALA	C-N-CA	-5.75	112.95	119.28
1	A	106	VAL	CB-CA-C	-5.74	102.14	110.63
1	A	235	ASN	N-CA-C	5.59	117.38	111.28
1	B	509	ASP	N-CA-C	5.46	117.61	108.23
1	B	646	GLU	N-CA-C	5.45	117.30	111.36
1	A	151	THR	N-CA-C	-5.41	101.53	109.81
1	A	208	TYR	CA-CB-CG	5.33	123.50	113.90
1	A	50	ILE	CA-C-N	5.25	125.79	120.38
1	A	50	ILE	C-N-CA	5.25	125.79	120.38
1	B	475	VAL	CB-CA-C	-5.23	104.44	110.41
1	B	487	GLY	N-CA-C	5.23	118.70	110.91
1	A	246	VAL	CB-CA-C	5.22	118.36	110.63
1	B	743	MET	N-CA-C	-5.18	100.07	108.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	473	GLU	N-CA-C	5.18	117.25	109.23
1	A	551	VAL	CB-CA-C	5.13	118.60	110.81
1	A	307	VAL	CB-CA-C	5.13	117.81	110.33
1	A	683	PRO	CA-C-N	-5.12	109.41	122.78
1	A	683	PRO	C-N-CA	-5.12	109.41	122.78
1	A	704	VAL	CB-CA-C	5.08	118.15	111.19
1	A	362	TRP	N-CA-C	-5.07	104.70	111.24
1	B	230	GLY	N-CA-C	-5.05	106.62	113.24
1	B	137	LEU	N-CA-C	-5.05	106.71	112.92
1	B	560	ASN	CA-C-N	5.05	126.15	119.84
1	B	560	ASN	C-N-CA	5.05	126.15	119.84
1	B	493	LEU	N-CA-C	5.02	117.80	109.46

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts

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	137	0
1	B	5994	0	5675	124	0
2	C	72	0	65	2	0
3	A	72	0	114	8	0
4	A	30	0	0	0	0
4	B	20	0	0	2	0
5	C	26	0	14	0	0
6	C	1	0	0	0	0
All	All	12329	0	11656	260	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 (260) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:772:THR:HG22	1:B:774:LYS:H	1.07	1.16
1:A:722:LYS:HE2	1:A:723:GLY:H	1.21	1.01
1:A:742:GLN:HG3	1:A:793:ILE:O	1.63	0.97
1:B:446:GLN:HE21	1:B:491:TRP:HB2	1.27	0.97
1:A:772:THR:HG22	1:A:774:LYS:H	1.29	0.96
1:B:772:THR:HG22	1:B:774:LYS:N	1.87	0.89
1:B:694:LYS:HE3	1:B:708:GLU:OE1	1.74	0.87
1:A:60:GLN:NE2	1:A:134:SER:HA	1.90	0.85
1:B:744:VAL:HG22	1:B:755:PHE:HE1	1.40	0.83
1:A:556:VAL:HG13	1:A:563:ILE:HB	1.60	0.83
1:B:744:VAL:CG2	1:B:755:PHE:HE1	1.92	0.82
1:A:772:THR:HG21	1:B:291:TYR:OH	1.79	0.81
1:A:53:GLN:OE1	1:A:57:SER:HB2	1.81	0.81
1:B:698:ASP:HB3	1:B:700:SER:H	1.43	0.81
1:B:446:GLN:HE21	1:B:491:TRP:CB	1.94	0.80
1:A:73:ARG:CG	1:A:131:MET:HE3	2.12	0.80
1:B:472:HIS:HD2	1:B:538:ASN:H	1.25	0.80
1:A:470:ARG:NH1	1:A:538:ASN:OD1	2.15	0.79
1:B:646:GLU:O	1:B:662:ALA:O	2.00	0.79
1:B:764:ASP:HB3	1:B:782:ASN:HA	1.65	0.79
1:A:73:ARG:HG3	1:A:131:MET:HE3	1.64	0.78
1:A:777:ALA:HB1	3:A:1817[B]:N8E:H192	1.63	0.78
1:A:73:ARG:HG3	1:A:131:MET:CE	2.13	0.78
1:B:744:VAL:HG22	1:B:755:PHE:CE1	2.18	0.77
1:A:805:ARG:HD2	3:A:1817[A]:N8E:H031	1.66	0.77
1:A:151:THR:O	1:A:152:ILE:HD13	1.85	0.76
1:A:722:LYS:HE2	1:A:723:GLY:N	2.00	0.76
1:B:744:VAL:CG2	1:B:755:PHE:CE1	2.69	0.76
1:B:446:GLN:NE2	1:B:491:TRP:HB2	2.01	0.73
1:B:772:THR:CG2	1:B:774:LYS:H	1.96	0.73
1:B:446:GLN:NE2	1:B:491:TRP:CB	2.51	0.73
1:A:239:ASP:OD2	1:A:292:ARG:NH2	2.20	0.72
1:B:681:LEU:HD13	1:B:687:VAL:HG22	1.69	0.72
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.72	0.72
1:B:341:ASN:HB2	1:B:342:PRO:CD	2.21	0.70
1:A:410:TRP:CD2	1:A:463:GLY:HA3	2.27	0.70
1:A:694:LYS:HE3	1:A:708:GLU:OE1	1.92	0.69
1:A:443:ILE:HD13	1:A:443:ILE:N	2.08	0.68
1:A:371:SER:OG	1:A:436:ALA:HA	1.94	0.67
1:B:111:ASN:N	1:B:111:ASN:HD22	1.91	0.67
1:A:408:ASN:HB3	1:A:410:TRP:H	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TRP:CE2	1:A:463:GLY:HA3	2.30	0.66
1:B:540:THR:HG22	1:B:541:ASP:N	2.11	0.66
1:B:472:HIS:CD2	1:B:538:ASN:H	2.11	0.66
1:A:707:TRP:CH2	1:A:793:ILE:HG13	2.31	0.65
1:B:542:ASP:O	1:B:577:TYR:HA	1.95	0.65
1:A:406:PHE:C	1:A:408:ASN:H	2.05	0.65
1:B:204:ARG:HD3	1:B:391:TRP:CH2	2.31	0.65
1:A:53:GLN:OE1	1:A:57:SER:CB	2.44	0.65
1:A:239:ASP:CG	1:A:292:ARG:HH22	2.05	0.65
1:B:177:MET:HE3	1:B:240:MET:HB3	1.78	0.64
1:B:614:GLN:OE1	1:B:641:GLU:OE2	2.15	0.64
1:A:260:GLY:HA2	1:A:594:MET:HE2	1.79	0.64
1:B:587:ALA:HB2	1:B:618:ILE:HG13	1.80	0.62
1:B:97:GLU:OE2	1:B:100:ARG:HD2	2.00	0.61
1:B:111:ASN:HD22	1:B:111:ASN:H	1.47	0.60
1:A:109:GLN:OE1	1:A:114:THR:HG22	2.01	0.60
1:B:744:VAL:HG21	1:B:755:PHE:CE1	2.36	0.60
1:B:681:LEU:HD13	1:B:687:VAL:CG2	2.30	0.60
1:B:161:THR:OG1	1:B:164:GLU:HG3	2.01	0.60
1:A:443:ILE:HG12	1:A:510:ILE:CD1	2.32	0.60
1:B:540:THR:HG22	1:B:541:ASP:H	1.67	0.60
1:A:443:ILE:CG1	1:A:510:ILE:HD12	2.31	0.59
1:A:72:TYR:C	1:A:131:MET:HE2	2.28	0.59
1:A:73:ARG:HG2	1:A:131:MET:HE3	1.84	0.59
1:B:71:LEU:HD12	1:B:114:THR:HG22	1.85	0.58
1:A:188:VAL:HG11	1:A:246:VAL:CG1	2.32	0.58
1:A:443:ILE:HG12	1:A:510:ILE:HD12	1.85	0.58
1:A:615:ASN:HD21	1:A:617:GLU:HB2	1.68	0.58
1:A:188:VAL:HG11	1:A:246:VAL:HG13	1.86	0.58
1:A:325:TYR:OH	1:A:327:ARG:NH1	2.36	0.58
1:B:694:LYS:HD2	1:B:694:LYS:C	2.29	0.58
1:B:418:HIS:CD2	1:B:455:ASN:HD21	2.21	0.57
1:B:156:THR:O	1:B:157:ARG:HB2	2.04	0.57
1:A:262:LEU:HD23	1:A:592:ILE:HG22	1.86	0.57
1:A:199:ALA:HA	1:A:205:ASN:HD22	1.68	0.57
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.86	0.57
1:B:111:ASN:N	1:B:111:ASN:ND2	2.53	0.56
1:A:157:ARG:HB3	1:A:475:VAL:HG11	1.87	0.56
1:A:203:ASP:OD1	1:A:325:TYR:OH	2.23	0.56
1:B:176:ASN:C	1:B:176:ASN:HD22	2.13	0.56
1:B:276:GLU:N	1:B:276:GLU:OE1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:ARG:HH12	1:B:540:THR:CA	2.17	0.56
1:A:406:PHE:C	1:A:408:ASN:N	2.63	0.56
1:A:570:ILE:HG23	1:A:591:ASP:HB3	1.87	0.56
1:A:73:ARG:HG3	1:A:131:MET:HE1	1.88	0.55
1:B:52:PRO:HD3	1:B:84:ALA:HB2	1.88	0.55
1:B:418:HIS:HD2	1:B:455:ASN:HD21	1.54	0.55
1:A:239:ASP:CG	1:A:292:ARG:NH2	2.64	0.55
1:B:470:ARG:NH2	1:B:541:ASP:OD1	2.39	0.55
1:A:262:LEU:HD11	1:A:613:GLY:HA3	1.87	0.55
1:B:156:THR:O	1:B:157:ARG:CB	2.55	0.55
1:A:368:LEU:O	1:A:376:ASN:HB2	2.06	0.55
1:A:709:PRO:HG3	1:A:737:GLN:NE2	2.22	0.55
1:A:51:PRO:O	1:A:53:GLN:HG2	2.08	0.54
1:B:698:ASP:HB3	1:B:700:SER:N	2.18	0.54
2:C:10:LYS:O	2:C:10:LYS:HG3	2.03	0.54
1:A:55:LEU:HB3	1:A:77:VAL:HB	1.89	0.53
1:A:470:ARG:HD3	1:A:538:ASN:O	2.08	0.53
1:A:254:GLY:CA	1:A:592:ILE:HG13	2.38	0.53
1:B:55:LEU:HD22	1:B:102:THR:HG21	1.91	0.53
1:B:459:ILE:HG13	1:B:459:ILE:O	2.06	0.53
1:A:391:TRP:HB2	1:A:427:LEU:HD21	1.89	0.53
1:B:736:TRP:HB2	1:B:761:TRP:CE3	2.44	0.53
1:B:446:GLN:NE2	1:B:491:TRP:HB3	2.22	0.53
1:A:447:LYS:HB3	1:A:490:TYR:HB2	1.90	0.52
1:A:109:GLN:OE1	1:A:114:THR:CG2	2.57	0.52
1:A:291:TYR:OH	1:B:772:THR:HG21	2.09	0.52
1:B:174:ARG:CZ	1:B:177:MET:HE2	2.39	0.52
1:B:596:GLN:HG2	1:B:600:TYR:HB2	1.92	0.52
1:A:254:GLY:HA2	1:A:592:ILE:HG13	1.90	0.52
1:B:775:LEU:HD12	1:B:813:TRP:HB2	1.90	0.52
1:B:792:ASN:HB3	1:B:800:SER:HB2	1.91	0.52
1:A:525:LYS:HB2	1:A:557:THR:HG22	1.92	0.52
1:A:214:ILE:HG12	1:A:264:ALA:HB3	1.92	0.52
1:B:98:LEU:HD23	1:B:98:LEU:C	2.34	0.52
1:B:772:THR:CG2	1:B:773:ASP:N	2.72	0.51
1:A:204:ARG:NH1	1:A:229:VAL:HG12	2.26	0.51
1:A:174:ARG:CZ	1:A:177:MET:CE	2.89	0.51
1:A:288:TRP:CZ2	1:A:321:PHE:HB3	2.44	0.51
1:B:199:ALA:HA	1:B:205:ASN:HD22	1.76	0.51
1:B:50:ILE:HD12	1:B:85:ILE:HD11	1.93	0.51
1:A:694:LYS:HE3	1:A:708:GLU:CD	2.34	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:LYS:O	1:A:653:LYS:HG3	2.11	0.51
1:A:262:LEU:CD2	1:A:592:ILE:HG22	2.41	0.51
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.46	0.51
1:A:60:GLN:HE22	1:A:134:SER:HA	1.74	0.51
1:B:506:TRP:CE2	1:B:508:GLY:HA2	2.45	0.51
1:B:689:ALA:HA	1:B:714:SER:O	2.10	0.51
1:A:174:ARG:HB2	1:A:244:ASP:O	2.11	0.50
1:A:596:GLN:NE2	1:A:609:GLU:O	2.44	0.50
2:C:6:FHO:O	2:C:7:SER:HB2	2.10	0.50
1:A:446:GLN:OE1	1:A:448:TYR:OH	2.17	0.50
1:B:152:ILE:HD12	1:B:169:ILE:HG12	1.94	0.50
1:A:72:TYR:C	1:A:131:MET:CE	2.84	0.50
1:B:506:TRP:CZ2	1:B:508:GLY:HA2	2.46	0.50
1:B:426:PRO:HB3	1:B:447:LYS:HG3	1.93	0.49
1:A:640:GLU:CD	1:A:643:ARG:HB2	2.37	0.49
1:A:809:PHE:HD2	3:A:1817[B]:N8E:H201	1.77	0.49
1:A:725:LEU:HD22	3:A:1817[B]:N8E:H062	1.93	0.49
3:A:1817[B]:N8E:H031	1:B:805:ARG:HD2	1.95	0.49
1:A:158:LEU:HD21	1:A:475:VAL:HG22	1.95	0.48
1:A:165:THR:O	1:A:621:LYS:NZ	2.45	0.48
1:A:638:ILE:HB	1:A:670:THR:HB	1.95	0.48
1:A:772:THR:HG21	1:B:291:TYR:HH	1.76	0.48
1:B:470:ARG:NH1	1:B:539:VAL:C	2.71	0.48
1:B:410:TRP:CD1	1:B:464:PRO:HD2	2.48	0.48
1:A:260:GLY:CA	1:A:594:MET:HE2	2.42	0.48
1:A:646:GLU:O	1:A:662:ALA:O	2.32	0.48
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.49	0.48
1:B:762:LEU:HD21	1:B:789:TYR:CE1	2.49	0.48
1:A:123:SER:O	1:A:124:SER:HB3	2.14	0.48
1:A:484:HIS:CE1	1:A:486:GLU:OE2	2.66	0.48
1:B:363:SER:OG	1:B:431:MET:CE	2.62	0.47
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.49	0.47
1:B:86:LYS:HG3	1:B:87:GLY:N	2.30	0.47
1:A:631:THR:HG22	1:A:677:ILE:HG13	1.96	0.47
1:B:602:ASP:HA	1:B:663:TYR:O	2.14	0.47
1:A:666:ILE:HD12	1:A:698:ASP:HB2	1.97	0.47
1:B:371:SER:OG	1:B:436:ALA:HA	2.15	0.47
1:A:805:ARG:HH11	3:A:1817[A]:N8E:H031	1.78	0.47
1:A:196:THR:HG21	1:A:709:PRO:CD	2.45	0.47
1:A:605:ASN:HA	1:A:659:ILE:HG12	1.96	0.47
1:B:696:ILE:HG23	1:B:704:VAL:HG12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ARG:HD3	1:B:788:THR:HB	1.96	0.46
1:B:214:ILE:HD13	1:B:264:ALA:HB3	1.97	0.46
1:A:417:ASP:HB2	1:A:456:SER:HB2	1.96	0.46
1:A:491:TRP:CE2	1:A:519:SER:HB3	2.51	0.46
1:B:540:THR:CG2	1:B:541:ASP:N	2.77	0.46
1:A:443:ILE:N	1:A:443:ILE:CD1	2.78	0.46
1:B:647:ASP:HB2	1:B:664:LYS:HG2	1.97	0.46
1:B:556:VAL:HG13	1:B:563:ILE:HB	1.98	0.46
1:B:638:ILE:O	1:B:669:LYS:HA	2.16	0.46
1:A:454:SER:OG	1:A:483:SER:HB3	2.16	0.46
1:A:700:SER:OG	1:A:701:GLY:N	2.48	0.45
1:B:418:HIS:HE1	4:B:1819:PO4:O1	1.98	0.45
1:B:467:PHE:HB3	1:B:472:HIS:HE1	1.80	0.45
1:B:470:ARG:HH12	1:B:540:THR:N	2.14	0.45
1:B:189:MET:HE1	1:B:248:VAL:HG21	1.98	0.45
1:B:625:LEU:O	1:B:628:ARG:HD3	2.17	0.45
1:A:170:THR:HG21	1:A:193:PRO:HD2	1.98	0.45
1:A:286:GLY:O	1:A:287:SER:C	2.59	0.45
1:A:186:ASP:OD1	1:A:207:TYR:OH	2.33	0.45
1:B:467:PHE:HB3	1:B:472:HIS:CE1	2.51	0.45
1:A:655:THR:O	1:A:655:THR:HG22	2.17	0.45
1:A:443:ILE:CG1	1:A:510:ILE:CD1	2.91	0.45
1:A:746:ASN:OD1	1:A:748:PRO:HD2	2.16	0.45
1:B:201:ASP:O	1:B:202:THR:C	2.59	0.45
1:A:392:GLU:HG3	1:A:424:HIS:HB3	1.98	0.45
1:B:394:TYR:OH	1:B:451:GLU:HG3	2.16	0.45
1:A:281:VAL:HG23	1:A:815:PHE:CZ	2.52	0.44
1:A:517:THR:O	1:A:518:PRO:C	2.57	0.44
1:B:388:TRP:CZ2	1:B:513:PRO:HD3	2.52	0.44
1:B:540:THR:CG2	1:B:541:ASP:H	2.29	0.44
1:A:694:LYS:CE	1:A:708:GLU:OE1	2.62	0.44
1:B:425:ALA:O	1:B:447:LYS:HA	2.18	0.44
1:B:431:MET:HB3	1:B:431:MET:HE2	1.56	0.44
1:A:698:ASP:OD1	1:A:698:ASP:C	2.60	0.44
1:A:196:THR:HG21	1:A:709:PRO:HD3	1.99	0.44
1:B:380:ARG:HA	1:B:801:TYR:CE2	2.52	0.44
1:A:262:LEU:HD23	1:A:592:ILE:CG2	2.47	0.44
1:A:554:TYR:CD2	1:A:595:PRO:HG2	2.53	0.44
1:B:117:VAL:O	1:B:117:VAL:HG12	2.18	0.44
1:B:157:ARG:HD3	1:B:256:LEU:HD13	1.99	0.44
3:A:1817[A]:N8E:H062	1:B:725:LEU:HD23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:CG1	1:A:47:GLU:N	2.80	0.43
1:A:667:LYS:HB2	1:A:699:ASP:OD2	2.19	0.43
1:A:189:MET:HA	1:A:189:MET:HE2	1.98	0.43
1:B:590:THR:O	1:B:614:GLN:HA	2.17	0.43
1:A:249:LEU:O	1:A:264:ALA:HA	2.19	0.43
1:A:596:GLN:HE21	1:A:596:GLN:HB2	1.55	0.43
1:A:709:PRO:HG3	1:A:737:GLN:CD	2.44	0.43
1:A:140:ILE:HG23	1:A:244:ASP:OD1	2.17	0.43
1:A:158:LEU:CD2	1:A:475:VAL:HG22	2.49	0.43
1:A:533:MET:O	1:A:548:GLY:HA3	2.19	0.43
1:B:410:TRP:CD2	1:B:463:GLY:HA3	2.54	0.43
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.54	0.42
1:A:443:ILE:HG13	1:A:510:ILE:HD12	2.00	0.42
1:B:780:ASN:O	1:B:807:LEU:HA	2.19	0.42
1:A:49:ASP:CG	1:A:86:LYS:HE3	2.45	0.42
1:A:352:TYR:CD1	1:A:352:TYR:C	2.97	0.42
1:B:648:ALA:HA	1:B:651:ASN:HB2	2.00	0.42
1:B:812:ARG:NH2	4:B:1818:PO4:O4	2.35	0.42
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.55	0.42
1:A:674:GLU:HG3	1:A:692:THR:OG1	2.20	0.42
1:B:245:ARG:NH1	1:B:269:ILE:HG13	2.33	0.42
1:B:239:ASP:OD2	1:B:292:ARG:NH2	2.52	0.42
1:B:438:ASP:OD1	1:B:438:ASP:N	2.53	0.42
1:B:691:TYR:CD1	1:B:691:TYR:C	2.98	0.42
1:A:281:VAL:HG22	1:A:295:LEU:HD13	2.00	0.42
1:B:485:TRP:CD1	1:B:485:TRP:C	2.95	0.42
1:A:772:THR:HG22	1:A:774:LYS:N	2.13	0.41
1:A:615:ASN:ND2	1:A:617:GLU:HB2	2.35	0.41
1:A:408:ASN:CB	1:A:410:TRP:HB2	2.50	0.41
1:A:528:GLN:HG2	1:A:554:TYR:HD1	1.86	0.41
1:B:682:ALA:O	1:B:683:PRO:C	2.63	0.41
1:A:244:ASP:O	1:A:245:ARG:HB3	2.20	0.41
1:B:413:LYS:HE2	1:B:460:TYR:OH	2.20	0.41
1:B:609:GLU:HG3	1:B:610:PRO:HD2	2.03	0.41
1:A:721:PHE:CD2	1:A:728:LEU:HD23	2.56	0.41
3:A:1817[A]:N8E:H201	1:B:777:ALA:HB1	2.02	0.41
1:B:347:THR:HB	1:B:401:ASN:HB2	2.02	0.41
1:A:69:GLN:NE2	1:A:133:THR:HG23	2.36	0.41
1:A:199:ALA:O	1:A:792:ASN:HB2	2.21	0.41
1:A:590:THR:OG1	1:A:615:ASN:HB3	2.21	0.41
1:B:46:VAL:HG12	1:B:47:GLU:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:GLU:O	1:B:647:ASP:HB3	2.21	0.41
1:A:406:PHE:O	1:A:408:ASN:N	2.54	0.41
1:A:401:ASN:ND2	1:A:415:GLN:HG2	2.36	0.40
1:B:649:LEU:O	1:B:649:LEU:HD12	2.22	0.40
1:B:253:THR:O	1:B:257:THR:HB	2.22	0.40
1:A:331:VAL:HA	1:A:352:TYR:O	2.21	0.40
1:B:694:LYS:HE3	1:B:708:GLU:CD	2.45	0.40
1:A:135:ASN:OD1	1:A:135:ASN:C	2.64	0.40
1:B:199:ALA:HA	1:B:205:ASN:ND2	2.37	0.40
1:B:445:ALA:O	1:B:446:GLN:CG	2.69	0.40
1:B:531:SER:O	1:B:550:ARG:HA	2.21	0.40
1:A:646:GLU:O	1:A:663:TYR:HA	2.21	0.40
1:B:185:ILE:N	1:B:238:SER:O	2.49	0.40
1:B:653:LYS:HA	1:B:654:PRO:HD2	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	770/772 (100%)	716 (93%)	42 (6%)	12 (2%)	7	27
1	B	750/772 (97%)	702 (94%)	43 (6%)	5 (1%)	18	48
2	C	5/10 (50%)	4 (80%)	0	1 (20%)	0	0
All	All	1525/1554 (98%)	1422 (93%)	85 (6%)	18 (1%)	10	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
1	A	124	SER
1	A	603	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	646	GLU
1	A	122	ASP
1	A	407	ALA
1	A	647	ASP
1	A	699	ASP
1	B	363	SER
1	B	408	ASN
1	B	699	ASP
1	A	227	ARG
2	C	7	SER
1	A	303	GLU
1	A	562	THR
1	B	495	ASN
1	A	701	GLY
1	B	610	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	650/650 (100%)	560 (86%)	90 (14%)	3	12
1	B	637/650 (98%)	558 (88%)	79 (12%)	4	15
2	C	4/4 (100%)	2 (50%)	2 (50%)	0	0
All	All	1291/1304 (99%)	1120 (87%)	171 (13%)	4	13

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	65	GLN
1	A	68	ILE
1	A	81	ARG
1	A	83	SER
1	A	85	ILE
1	A	86	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	114	THR
1	A	115	ILE
1	A	123	SER
1	A	131	MET
1	A	132	ILE
1	A	133	THR
1	A	142	GLU
1	A	148	THR
1	A	152	ILE
1	A	154	THR
1	A	157	ARG
1	A	169	ILE
1	A	196	THR
1	A	204	ARG
1	A	215	ASN
1	A	236	THR
1	A	245	ARG
1	A	246	VAL
1	A	248	VAL
1	A	276	GLU
1	A	297	VAL
1	A	303	GLU
1	A	304	SER
1	A	307	VAL
1	A	312	VAL
1	A	323	ASP
1	A	326	GLU
1	A	329	THR
1	A	331	VAL
1	A	348	VAL
1	A	372	GLN
1	A	378	VAL
1	A	392	GLU
1	A	401	ASN
1	A	408	ASN
1	A	411	VAL
1	A	416	LEU
1	A	417	ASP
1	A	443	ILE
1	A	459	ILE
1	A	461	LEU
1	A	462	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	466	GLN
1	A	475	VAL
1	A	494	ARG
1	A	499	THR
1	A	527	ARG
1	A	528	GLN
1	A	539	VAL
1	A	542	ASP
1	A	551	VAL
1	A	556	VAL
1	A	557	THR
1	A	564	ARG
1	A	580	ASN
1	A	592	ILE
1	A	596	GLN
1	A	601	ARG
1	A	603	SER
1	A	609	GLU
1	A	612	GLU
1	A	615	ASN
1	A	618	ILE
1	A	646	GLU
1	A	653	LYS
1	A	659	ILE
1	A	660	THR
1	A	676	GLU
1	A	687	VAL
1	A	694	LYS
1	A	697	ARG
1	A	704	VAL
1	A	705	SER
1	A	722	LYS
1	A	730	VAL
1	A	740	SER
1	A	744	VAL
1	A	772	THR
1	A	774	LYS
1	A	784	VAL
1	A	788	THR
1	A	792	ASN
1	A	811	THR
1	B	68	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	78	ARG
1	B	83	SER
1	B	86	LYS
1	B	96	THR
1	B	97	GLU
1	B	98	LEU
1	B	106	VAL
1	B	109	GLN
1	B	111	ASN
1	B	113	ILE
1	B	115	ILE
1	B	117	VAL
1	B	148	THR
1	B	154	THR
1	B	157	ARG
1	B	195	ILE
1	B	201	ASP
1	B	232	SER
1	B	245	ARG
1	B	265	THR
1	B	329	THR
1	B	331	VAL
1	B	360	SER
1	B	379	SER
1	B	396	ARG
1	B	411	VAL
1	B	447	LYS
1	B	454	SER
1	B	459	ILE
1	B	462	THR
1	B	466	GLN
1	B	473	GLU
1	B	478	THR
1	B	493	LEU
1	B	495	ASN
1	B	509	ASP
1	B	512	LYS
1	B	533	MET
1	B	545	LEU
1	B	551	VAL
1	B	556	VAL
1	B	564	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	576	VAL
1	B	596	GLN
1	B	603	SER
1	B	609	GLU
1	B	615	ASN
1	B	618	ILE
1	B	641	GLU
1	B	646	GLU
1	B	649	LEU
1	B	660	THR
1	B	671	LYS
1	B	681	LEU
1	B	683	PRO
1	B	687	VAL
1	B	694	LYS
1	B	699	ASP
1	B	702	LYS
1	B	704	VAL
1	B	705	SER
1	B	713	LEU
1	B	720	LYS
1	B	722	LYS
1	B	727	LYS
1	B	730	VAL
1	B	739	LYS
1	B	744	VAL
1	B	758	GLU
1	B	759	ASP
1	B	764	ASP
1	B	771	ILE
1	B	772	THR
1	B	774	LYS
1	B	775	LEU
1	B	788	THR
1	B	792	ASN
1	B	815	PHE
2	C	4	LYS
2	C	10	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	79	ASN
1	A	136	GLN
1	A	176	ASN
1	A	183	ASN
1	A	205	ASN
1	A	408	ASN
1	A	415	GLN
1	A	439	ASN
1	A	455	ASN
1	A	466	GLN
1	A	505	ASN
1	A	580	ASN
1	A	596	GLN
1	A	615	ASN
1	A	710	GLN
1	A	737	GLN
1	A	747	ASN
1	B	60	GLN
1	B	109	GLN
1	B	111	ASN
1	B	167	GLN
1	B	176	ASN
1	B	183	ASN
1	B	205	ASN
1	B	215	ASN
1	B	405	ASN
1	B	418	HIS
1	B	455	ASN
1	B	466	GLN
1	B	472	HIS
1	B	495	ASN
1	B	544	ASN
1	B	596	GLN
1	B	614	GLN
1	B	615	ASN
1	B	688	GLN
1	B	710	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FH7	C	11	2,6	9,10,11	5.15	2 (22%)	4,11,13	2.18	2 (50%)
2	FHO	C	6	2,6	9,10,11	5.01	2 (22%)	4,11,13	2.56	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FH7	C	11	2,6	-	1/7/10/12	-
2	FHO	C	6	2,6	-	5/7/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	FH7	OZ-NE	-14.55	1.22	1.39
2	C	6	FHO	OZ-NE	-14.14	1.22	1.39
2	C	11	FH7	CZ-NE	-5.09	1.26	1.34
2	C	6	FHO	CZ-NE	-4.83	1.27	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	FHO	OZ-NE-CD	4.13	123.38	113.81
2	C	11	FH7	OZ-NE-CD	3.24	121.30	113.81
2	C	11	FH7	CG-CD-NE	2.36	115.94	111.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6	FHO	CG-CD-NE-OZ
2	C	6	FHO	CG-CD-NE-CZ
2	C	11	FH7	O-C-CA-CB
2	C	6	FHO	CA-CB-CG-CD
2	C	6	FHO	C-CA-CB-CG
2	C	6	FHO	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	A	1822	-	4,4,4	0.82	0	6,6,6	0.67	0
4	PO4	B	1818	-	4,4,4	0.83	0	6,6,6	1.09	0
4	PO4	A	1823	-	4,4,4	1.02	0	6,6,6	0.90	0
5	PVE	C	1	2,6	26,28,29	1.97	4 (15%)	30,40,42	1.48	5 (16%)
3	N8E	A	1817[B]	-	23,23,23	0.85	0	22,22,22	0.95	1 (4%)
4	PO4	B	1819	-	4,4,4	0.97	0	6,6,6	0.45	0
4	PO4	A	1820	-	4,4,4	1.17	0	6,6,6	0.50	0
4	PO4	A	1818	-	4,4,4	0.74	0	6,6,6	1.41	1 (16%)
3	N8E	A	1816	-	23,23,23	0.55	0	22,22,22	0.49	0
4	PO4	A	1821	-	4,4,4	0.97	0	6,6,6	0.62	0
4	PO4	B	1817	-	4,4,4	0.73	0	6,6,6	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	B	1816	-	4,4,4	0.64	0	6,6,6	1.21	1 (16%)
3	N8E	A	1817[A]	-	23,23,23	0.90	0	22,22,22	0.91	0
4	PO4	A	1819	-	4,4,4	0.97	0	6,6,6	1.66	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N8E	A	1816	-	-	9/21/21/21	-
3	N8E	A	1817[A]	-	-	10/21/21/21	-
3	N8E	A	1817[B]	-	-	12/21/21/21	-
5	PVE	C	1	2,6	-	8/10/21/23	0/2/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	PVE	C20-C18	-6.76	1.37	1.51
5	C	1	PVE	C5-C6	4.52	1.41	1.37
5	C	1	PVE	C8-C7	4.10	1.41	1.37
5	C	1	PVE	C4-C3	2.48	1.42	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	PVE	C21-C20-C18	-3.64	105.17	112.67
5	C	1	PVE	C20-C18-N17	-3.52	108.47	114.59
4	A	1819	PO4	O4-P-O2	3.35	118.34	107.91
5	C	1	PVE	C15-C14-N1	-2.78	107.87	111.53
3	A	1817[B]	N8E	O18-C19-C20	2.73	122.78	110.35
4	A	1818	PO4	O4-P-O1	-2.31	102.77	110.95
5	C	1	PVE	C3-C2-N11	-2.24	117.14	122.87
5	C	1	PVE	C13-C12-N11	-2.23	106.73	110.04
4	B	1816	PO4	O3-P-O1	-2.16	103.33	110.95
4	A	1819	PO4	O2-P-O1	-2.06	103.66	110.95

There are no chirality outliers.

All (39) torsion outliers are listed below:

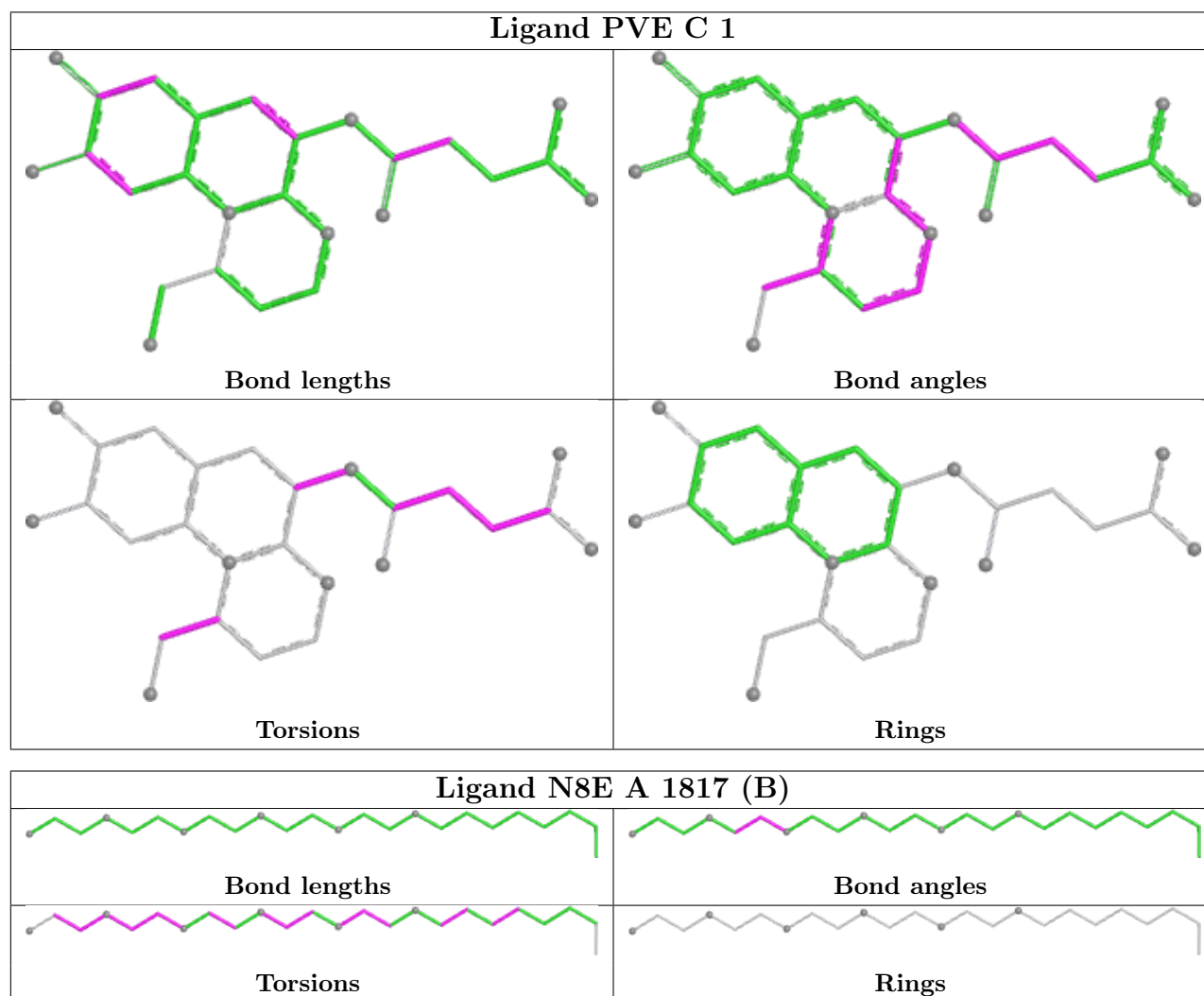
Mol	Chain	Res	Type	Atoms
5	C	1	PVE	C13-C14-C15-O16
3	A	1817[B]	N8E	O09-C10-C11-O12
3	A	1817[A]	N8E	O15-C16-C17-O18
3	A	1817[A]	N8E	O18-C19-C20-O21
3	A	1817[B]	N8E	O18-C19-C20-O21
3	A	1817[B]	N8E	C06-C07-C08-O09
3	A	1817[A]	N8E	O12-C13-C14-O15
3	A	1817[A]	N8E	C02-C03-C04-C05
5	C	1	PVE	O19-C18-C20-C21
5	C	1	PVE	C2-C3-N17-C18
3	A	1817[B]	N8E	O21-C22-C23-O24
3	A	1817[B]	N8E	O15-C16-C17-O18
5	C	1	PVE	C18-C20-C21-C22
5	C	1	PVE	C4-C3-N17-C18
5	C	1	PVE	N17-C18-C20-C21
3	A	1817[B]	N8E	C13-C14-O15-C16
3	A	1817[A]	N8E	C11-C10-O09-C08
3	A	1816	N8E	O15-C16-C17-O18
3	A	1817[A]	N8E	C17-C16-O15-C14
3	A	1817[A]	N8E	C10-C11-O12-C13
3	A	1817[A]	N8E	C23-C22-O21-C20
3	A	1817[B]	N8E	C19-C20-O21-C22
3	A	1817[B]	N8E	C04-C05-C06-C07
3	A	1817[A]	N8E	O21-C22-C23-O24
3	A	1817[A]	N8E	C04-C05-C06-C07
3	A	1816	N8E	C19-C20-O21-C22
3	A	1816	N8E	C23-C22-O21-C20
3	A	1817[B]	N8E	C10-C11-O12-C13
3	A	1817[B]	N8E	C20-C19-O18-C17
5	C	1	PVE	C20-C21-C22-O23
5	C	1	PVE	C20-C21-C22-O24
3	A	1816	N8E	C04-C05-C06-C07
3	A	1816	N8E	C13-C14-O15-C16
3	A	1816	N8E	C01-C02-C03-C04
3	A	1816	N8E	O21-C22-C23-O24
3	A	1816	N8E	C11-C10-O09-C08
3	A	1816	N8E	C02-C03-C04-C05
3	A	1817[B]	N8E	O12-C13-C14-O15
3	A	1817[B]	N8E	C23-C22-O21-C20

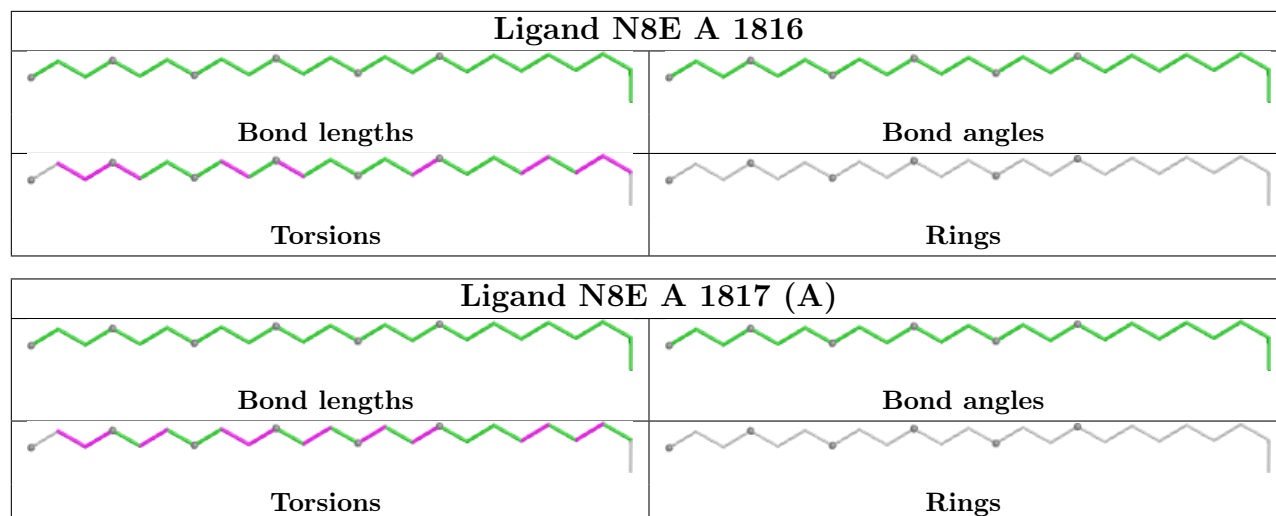
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1818	PO4	1	0
3	A	1817[B]	N8E	4	0
4	B	1819	PO4	1	0
3	A	1817[A]	N8E	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.39	6 (0%) 82 77	7, 19, 34, 52	0
1	B	754/772 (97%)	-0.25	7 (0%) 81 75	11, 24, 43, 60	0
2	C	6/10 (60%)	0.56	0 100 100	29, 38, 40, 43	0
All	All	1532/1554 (98%)	-0.32	13 (0%) 82 77	7, 21, 39, 60	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	SER	5.1
1	A	44	GLN	4.4
1	B	407	ALA	3.8
1	B	78	ARG	3.5
1	A	699	ASP	3.3
1	B	533	MET	3.0
1	B	110	GLY	2.9
1	A	362	TRP	2.4
1	A	407	ALA	2.4
1	A	599	TRP	2.3
1	B	137	LEU	2.3
1	B	538	ASN	2.2
1	B	471	GLU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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($\text{\AA}^2$)	Q<0.9
2	DSN	C	3	6/7	0.84	0.11	39,40,40,41	0
2	DSN	C	8	6/7	0.88	0.12	40,42,42,42	0
2	FHO	C	6	11/12	0.92	0.10	38,41,43,44	0
2	FH7	C	11	11/12	0.97	0.07	29,29,32,32	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

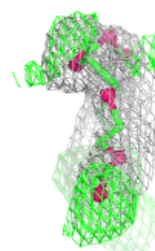
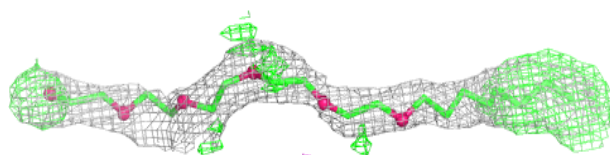
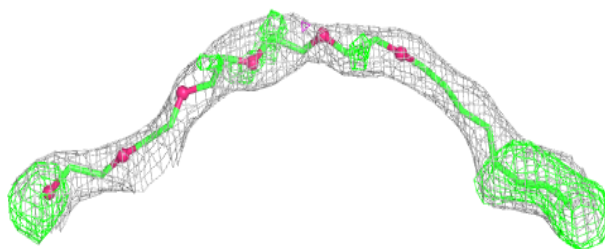
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	N8E	A	1817[A]	24/24	0.75	0.26	2,2,7,8	24
3	N8E	A	1817[B]	24/24	0.75	0.26	2,2,4,6	24
5	PVE	C	1	26/27	0.86	0.12	38,40,59,62	5
4	PO4	A	1822	5/5	0.90	0.14	79,79,81,81	0
4	PO4	B	1816	5/5	0.90	0.16	43,43,44,45	0
4	PO4	B	1818	5/5	0.90	0.14	53,54,55,57	0
3	N8E	A	1816	24/24	0.90	0.15	36,48,68,70	0
4	PO4	A	1821	5/5	0.91	0.15	59,60,60,61	0
4	PO4	A	1823	5/5	0.94	0.17	62,62,63,63	0
4	PO4	B	1819	5/5	0.96	0.08	43,44,45,46	0
4	PO4	A	1818	5/5	0.97	0.07	28,31,31,32	0
4	PO4	B	1817	5/5	0.98	0.07	21,22,23,24	0
4	PO4	A	1820	5/5	0.98	0.07	46,48,48,49	0
4	PO4	A	1819	5/5	0.99	0.06	17,20,24,25	0
6	FE	C	2	1/1	1.00	0.03	36,36,36,36	0

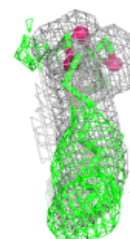
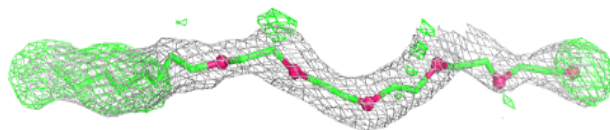
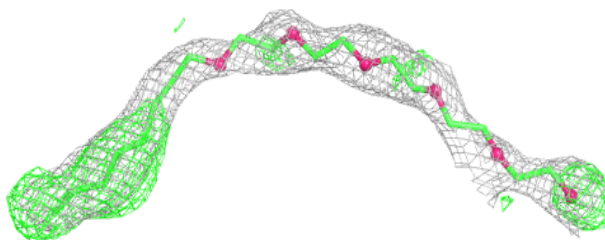
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

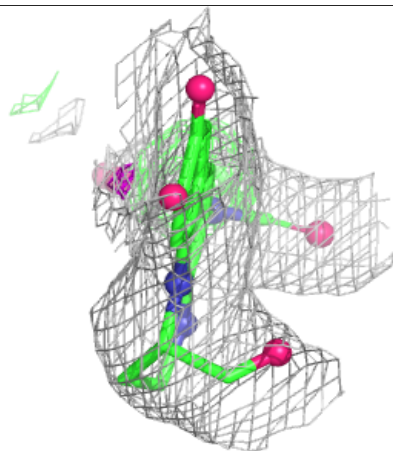
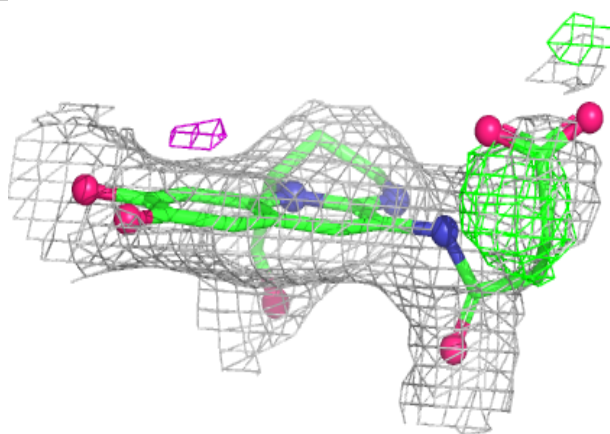
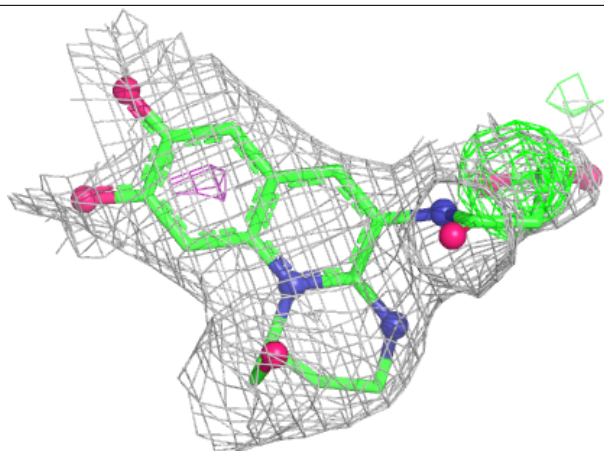
**Electron density around N8E A 1817 (B):**

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

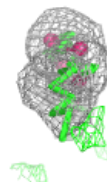
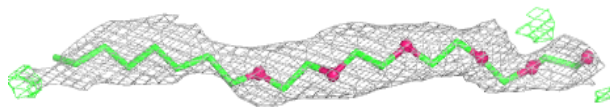
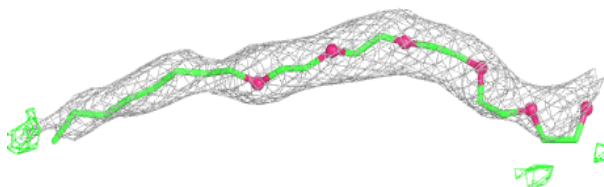


Electron density around PVE C 1:

$2mF_o-DF_c$ (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.