



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:10 PM UTC

PDB ID : 2W6T / pdb_00002w6t
Title : Structures of *P. aeruginosa* FpvA bound to heterologous pyoverdines: FpvA-Pvd(DSM50106)-Fe complex
Authors : Greenwald, J.; Nader, M.; Celia, H.; Gruffaz, C.; Meyer, J.-M.; Schalk, I.J.; Pattus, F.
Deposited on : 2008-12-19
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

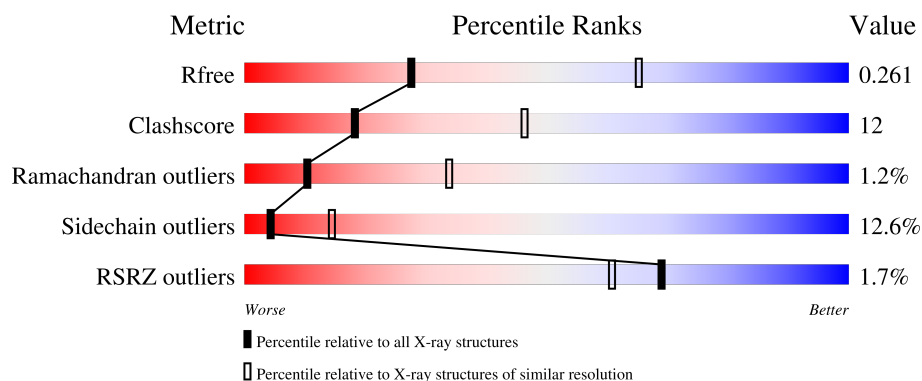
1 Overall quality at a glance

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% 66% 28% 6% .
1	B	772	2% 68% 24% 5% ..
2	C	10	60% 20% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	1823	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12342 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.

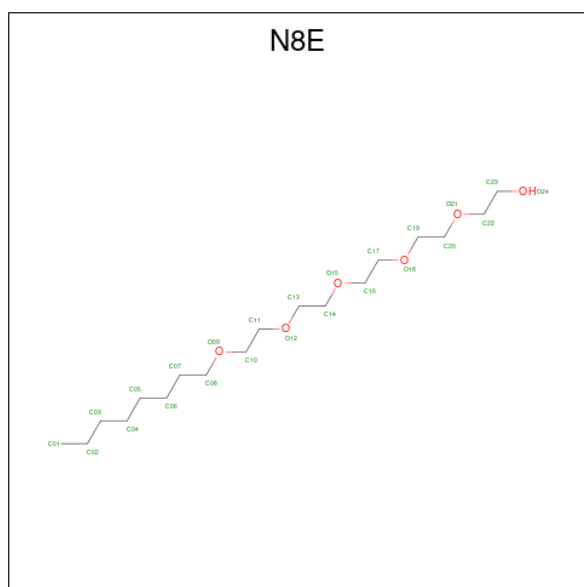
- Molecule 1 is a protein called FERRIPYOVERDINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	0	1	0
			6128	3856	1048	1212	12			
1	B	754	Total	C	N	O	S	0	0	0
			5994	3775	1027	1181	11			

- Molecule 2 is a protein called PYOVERDINE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			71	39	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		

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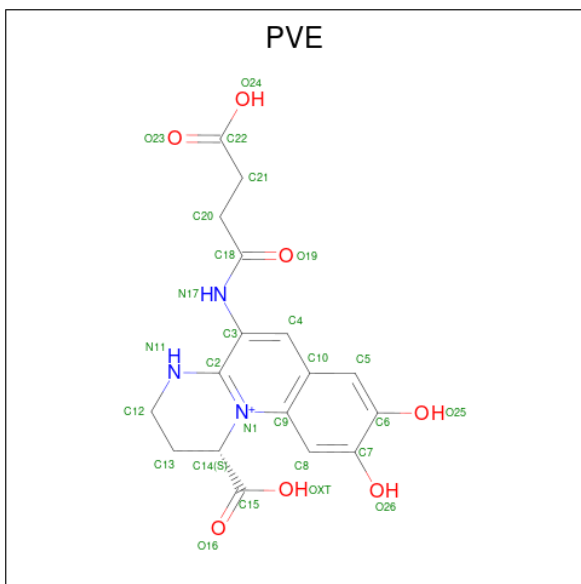
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			48	36	12		

- 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-TETRAHYDROPYRIMIDO[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		

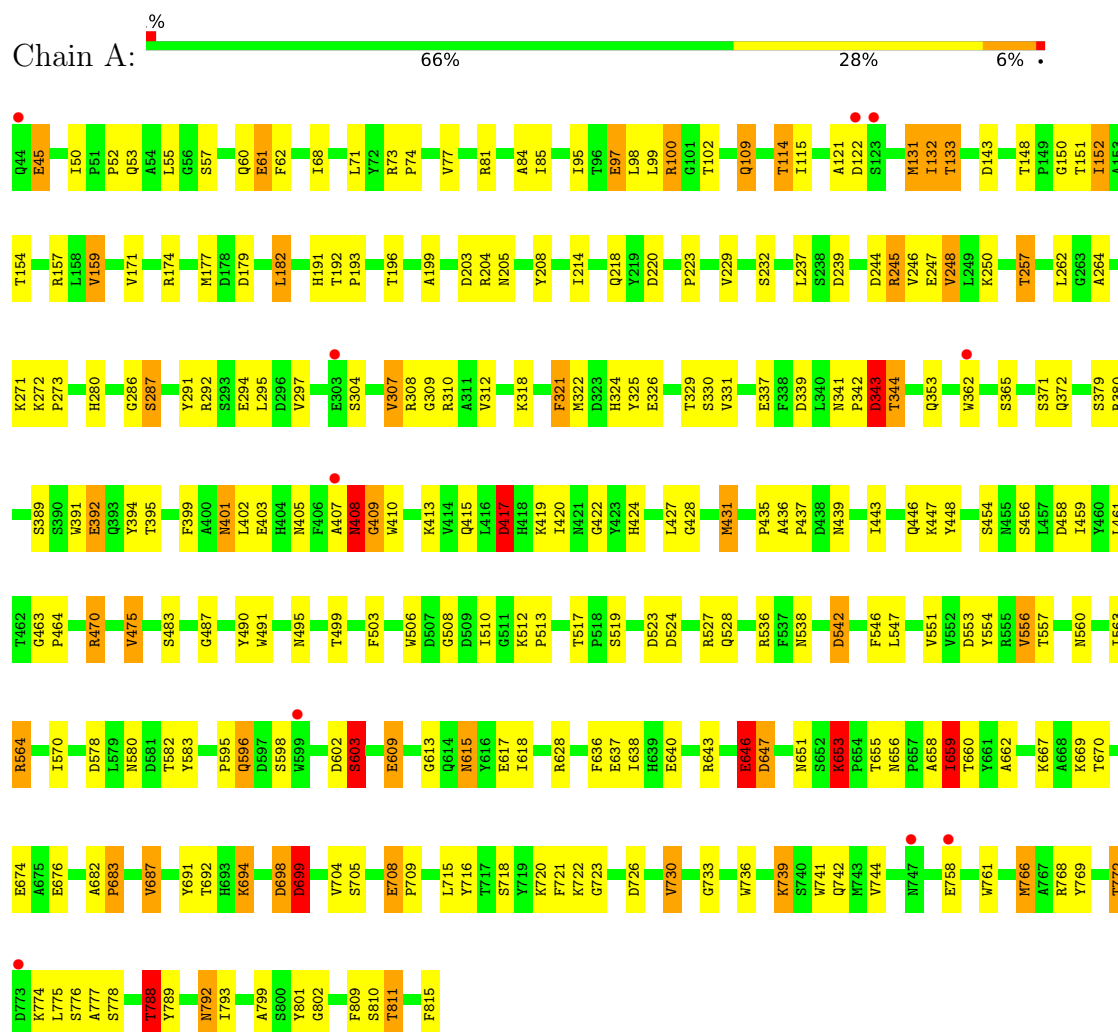
- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

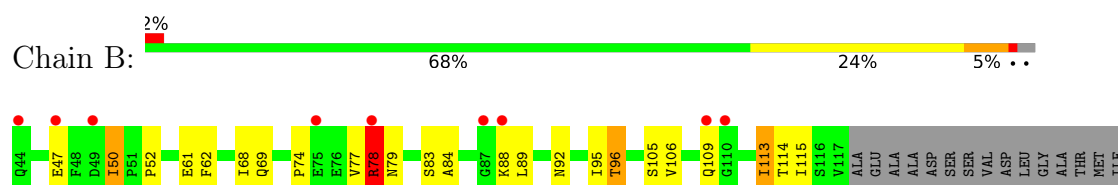
3 Residue-property plots

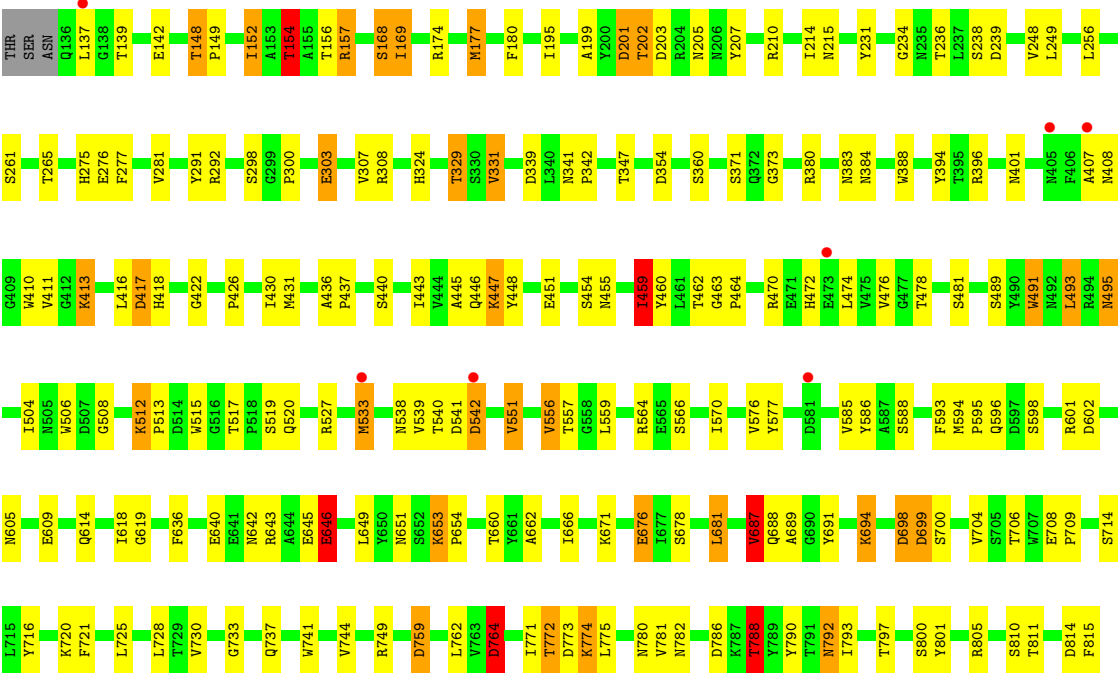
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





• Molecule 2: PYOVERDINE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	194.56Å 129.13Å 141.82Å 90.00° 131.65° 90.00°	Depositor
Resolution (Å)	106.00 – 2.90 105.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (106.00-2.90) 93.4 (105.97-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.263 0.204 , 0.261	Depositor DCC
R_{free} test set	2785 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 17.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12342	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, PO4, DSN, PVE, N8E, ORN, FHO, FH7

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.15	9/6282 (0.1%)	1.26	29/8537 (0.3%)
1	B	1.07	7/6145 (0.1%)	1.21	28/8347 (0.3%)
2	C	0.76	0/25	0.96	0/25
All	All	1.11	16/12452 (0.1%)	1.24	57/16909 (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	B	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	PHE	CA-C	-6.78	1.44	1.52
1	A	788	THR	CA-CB	6.24	1.61	1.53
1	B	459	ILE	CA-CB	6.02	1.62	1.54
1	B	570	ILE	CA-CB	5.93	1.59	1.54
1	A	61	GLU	CG-CD	5.91	1.66	1.52
1	A	523	ASP	CA-C	5.80	1.59	1.53
1	A	159	VAL	CA-CB	-5.63	1.46	1.54
1	A	513	PRO	CA-C	5.58	1.59	1.52
1	B	551	VAL	CA-CB	5.56	1.61	1.54
1	B	556	VAL	CA-CB	5.43	1.61	1.54
1	A	417	ASP	CA-C	-5.32	1.46	1.52
1	A	439	ASN	CA-C	5.30	1.59	1.52
1	A	150	GLY	C-O	-5.24	1.18	1.24
1	B	788	THR	CA-CB	5.20	1.60	1.53
1	B	504	ILE	CA-CB	5.07	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	609	GLU	CA-C	5.05	1.58	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	646	GLU	N-CA-C	9.34	121.55	111.36
1	B	653	LYS	CA-C-N	9.02	128.96	119.85
1	B	653	LYS	C-N-CA	9.02	128.96	119.85
1	A	687	VAL	CB-CA-C	-8.26	98.00	110.55
1	B	687	VAL	CB-CA-C	-7.65	98.45	110.69
1	A	475	VAL	CB-CA-C	-7.47	99.42	110.33
1	B	642	ASN	N-CA-C	7.31	121.60	111.74
1	A	237	LEU	N-CA-C	6.86	122.61	112.94
1	B	551	VAL	N-CA-CB	6.84	117.99	110.53
1	A	248	VAL	N-CA-C	6.76	117.37	107.37
1	B	234	GLY	N-CA-C	6.48	123.64	115.21
1	A	257	THR	N-CA-C	-6.33	105.68	113.41
1	B	542	ASP	N-CA-C	-6.26	106.61	114.56
1	B	676	GLU	N-CA-C	6.26	118.81	108.99
1	A	708	GLU	N-CA-C	-6.25	101.78	109.65
1	A	495	ASN	N-CA-C	6.19	119.95	111.54
1	B	491	TRP	N-CA-C	5.98	123.06	114.39
1	B	281	VAL	N-CA-C	-5.89	99.99	108.48
1	A	637	GLU	CA-C-N	-5.89	115.89	123.19
1	A	637	GLU	C-N-CA	-5.89	115.89	123.19
1	A	653	LYS	CA-C-N	5.82	126.15	119.92
1	A	653	LYS	C-N-CA	5.82	126.15	119.92
1	A	487	GLY	N-CA-C	5.79	118.95	110.38
1	A	512	LYS	CA-C-N	-5.68	114.90	120.52
1	A	512	LYS	C-N-CA	-5.68	114.90	120.52
1	B	384	ASN	N-CA-C	5.61	119.63	112.34
1	A	682	ALA	N-CA-C	-5.60	103.18	108.22
1	B	50	ILE	CA-C-N	5.59	126.14	120.38
1	B	50	ILE	C-N-CA	5.59	126.14	120.38
1	B	460	TYR	N-CA-C	5.50	118.04	109.52
1	B	115	ILE	CB-CA-C	-5.49	103.38	110.84
1	A	659	ILE	CB-CA-C	-5.48	104.69	111.32
1	B	570	ILE	CB-CA-C	-5.45	105.90	111.08
1	B	764	ASP	N-CA-C	5.43	117.93	109.52
1	A	409	GLY	N-CA-C	-5.42	107.83	115.32
1	B	154	THR	CA-C-N	5.35	127.71	120.65
1	B	154	THR	C-N-CA	5.35	127.71	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	741	TRP	N-CA-C	5.34	117.10	109.14
1	A	517	THR	CA-C-N	-5.34	114.46	119.85
1	A	517	THR	C-N-CA	-5.34	114.46	119.85
1	B	588	SER	N-CA-C	5.28	116.55	108.42
1	A	45	GLU	N-CA-C	5.21	117.90	110.24
1	B	331	VAL	N-CA-C	5.21	116.22	108.46
1	B	307	VAL	N-CA-C	-5.21	100.57	108.17
1	A	321	PHE	N-CA-C	-5.20	106.20	112.54
1	A	171	VAL	N-CA-C	5.18	115.94	108.48
1	A	208	TYR	CA-CB-CG	5.16	123.19	113.90
1	A	245	ARG	CA-C-N	-5.15	116.40	123.14
1	A	245	ARG	C-N-CA	-5.15	116.40	123.14
1	A	570	ILE	N-CA-C	-5.14	103.06	108.15
1	A	121	ALA	N-CA-C	5.13	116.57	110.97
1	B	517	THR	CA-C-N	-5.10	114.32	119.83
1	B	517	THR	C-N-CA	-5.10	114.32	119.83
1	A	343	ASP	N-CA-C	5.06	119.18	112.30
1	B	148	THR	CA-C-N	5.02	125.00	120.03
1	B	148	THR	C-N-CA	5.02	125.00	120.03
1	B	602	ASP	N-CA-C	5.01	117.27	110.35

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	407	ALA	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	6128	0	5797	151	0
1	B	5994	0	5675	141	0
2	C	71	0	63	4	0
3	A	72	0	114	6	0
4	A	30	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	0	3	0
5	C	26	0	14	0	0
6	C	1	0	0	0	0
All	All	12342	0	11663	290	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 12.

All (290) 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:A:772:THR:HG21	1:B:291:TYR:OH	1.54	1.06
1:B:772:THR:HG22	1:B:774:LYS:H	1.24	1.01
1:A:362[B]:TRP:CD1	1:A:431:MET:HE1	1.97	0.98
1:A:694:LYS:HE3	1:A:708:GLU:OE1	1.65	0.96
1:A:772:THR:HG22	1:A:774:LYS:H	1.30	0.94
1:B:418:HIS:HD2	1:B:455:ASN:HD21	0.97	0.93
1:B:472:HIS:HD2	1:B:538:ASN:H	0.96	0.90
1:B:418:HIS:CD2	1:B:455:ASN:HD21	1.88	0.90
1:B:472:HIS:CD2	1:B:538:ASN:H	1.89	0.90
1:A:74:PRO:HG3	1:A:132:ILE:HG12	1.51	0.89
1:A:556:VAL:HG13	1:A:563:ILE:HB	1.56	0.88
1:A:362[B]:TRP:HH2	1:A:446:GLN:OE1	1.57	0.87
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.57	0.87
1:A:742:GLN:HG3	1:A:793:ILE:O	1.75	0.85
3:A:1817[B]:N8E:H031	1:B:805:ARG:HD2	1.56	0.85
1:A:408:ASN:HB3	1:A:410:TRP:CD1	2.14	0.82
1:A:109:GLN:OE1	1:A:114:THR:HG22	1.79	0.82
1:A:470:ARG:NH1	1:A:538:ASN:OD1	2.13	0.81
1:A:308:ARG:NH1	1:A:337:GLU:OE1	2.14	0.81
1:B:446:GLN:NE2	1:B:491:TRP:HB2	1.96	0.81
1:B:418:HIS:HD2	1:B:455:ASN:ND2	1.79	0.79
1:B:472:HIS:HD2	1:B:538:ASN:N	1.77	0.79
1:B:540:THR:HG22	1:B:541:ASP:H	1.47	0.79
1:B:446:GLN:NE2	1:B:491:TRP:CB	2.46	0.78
1:B:493:LEU:HD12	1:B:493:LEU:H	1.50	0.76
1:B:646:GLU:O	1:B:662:ALA:O	2.02	0.76
1:B:772:THR:HG22	1:B:774:LYS:N	1.99	0.76
1:B:512:LYS:HE3	4:B:1818:PO4:O3	1.86	0.76
1:A:772:THR:HG22	1:A:774:LYS:N	2.01	0.74
1:A:722:LYS:HG3	1:A:723:GLY:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ASN:HB3	1:A:410:TRP:HD1	1.52	0.74
1:A:245:ARG:NH1	1:A:247:GLU:OE1	2.21	0.73
1:A:777:ALA:HB1	3:A:1817[B]:N8E:H191	1.70	0.73
1:A:53:GLN:OE1	1:A:57:SER:HB2	1.89	0.73
1:A:73:ARG:HG3	1:A:131:MET:HE3	1.70	0.71
1:A:443:ILE:HG13	1:A:510:ILE:HD13	1.71	0.71
1:B:201:ASP:O	1:B:203:ASP:N	2.24	0.71
1:B:418:HIS:HE1	4:B:1821:PO4:O1	1.73	0.71
1:A:809:PHE:HB3	3:A:1817[B]:N8E:H201	1.71	0.71
1:A:239:ASP:CG	1:A:292:ARG:HH22	1.98	0.71
1:B:50:ILE:HG12	1:B:61:GLU:HG2	1.71	0.70
1:A:239:ASP:OD2	1:A:292:ARG:NH2	2.23	0.70
1:B:347:THR:HB	1:B:401:ASN:HB2	1.73	0.70
1:A:778:SER:O	3:A:1817[B]:N8E:H192	1.92	0.70
1:B:195:ILE:HD11	1:B:248:VAL:HG11	1.72	0.69
1:A:443:ILE:HG13	1:A:510:ILE:CD1	2.22	0.69
1:A:214:ILE:HG12	1:A:264:ALA:HB3	1.75	0.69
1:B:666:ILE:HB	1:B:699:ASP:OD2	1.93	0.67
1:A:699:ASP:N	1:A:699:ASP:OD1	2.27	0.67
1:B:764:ASP:HB3	1:B:782:ASN:HA	1.76	0.67
1:A:53:GLN:OE1	1:A:57:SER:CB	2.43	0.66
1:B:542:ASP:O	1:B:577:TYR:HA	1.97	0.65
1:B:156:THR:O	1:B:157:ARG:HB2	1.97	0.64
1:A:271:LYS:HD3	1:A:310:ARG:NH2	2.12	0.64
1:A:580:ASN:CB	1:A:582:THR:H	2.10	0.64
1:A:362[B]:TRP:CG	1:A:431:MET:HE1	2.33	0.64
1:A:646:GLU:O	1:A:647:ASP:CB	2.45	0.64
1:B:694:LYS:HE3	1:B:708:GLU:OE1	1.98	0.64
1:A:667:LYS:O	1:A:699:ASP:OD1	2.17	0.63
1:A:109:GLN:OE1	1:A:114:THR:CG2	2.45	0.63
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.35	0.62
1:B:436:ALA:HB1	1:B:437:PRO:HD2	1.81	0.62
1:B:446:GLN:NE2	1:B:491:TRP:HB3	2.13	0.62
1:A:580:ASN:HB3	1:A:582:THR:H	1.65	0.62
1:B:324:HIS:CE1	1:B:383:ASN:HB3	2.35	0.62
1:A:656:ASN:HB3	1:A:659:ILE:HD12	1.82	0.61
1:B:772:THR:CG2	1:B:774:LYS:H	2.09	0.61
1:B:95:ILE:HG12	1:B:113:ILE:CD1	2.32	0.60
1:B:446:GLN:HE21	1:B:491:TRP:HB2	1.65	0.60
1:A:371:SER:OG	1:A:436:ALA:HA	2.02	0.60
1:B:388:TRP:CZ2	1:B:513:PRO:HD3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.37	0.59
1:B:774:LYS:HB3	1:B:814:ASP:O	2.02	0.59
1:A:362[B]:TRP:CH2	1:A:446:GLN:OE1	2.48	0.59
1:A:401:ASN:ND2	1:A:415:GLN:HG2	2.16	0.59
1:A:410:TRP:CD2	1:A:463:GLY:HA3	2.37	0.59
1:A:721:PHE:O	1:A:726:ASP:HA	2.02	0.59
1:A:174:ARG:HB2	1:A:244:ASP:O	2.03	0.58
1:B:601:ARG:NH1	1:B:605:ASN:O	2.36	0.58
1:A:392:GLU:HG3	1:A:424:HIS:HB3	1.86	0.58
1:B:797:THR:HG22	1:B:797:THR:O	2.01	0.58
1:A:391:TRP:HB2	1:A:427:LEU:HD21	1.84	0.58
1:B:371:SER:OG	1:B:436:ALA:HA	2.03	0.58
1:A:362[B]:TRP:CH2	1:A:446:GLN:CD	2.81	0.58
1:A:775:LEU:HD23	1:A:775:LEU:C	2.28	0.58
1:A:97:GLU:O	1:A:100:ARG:HB2	2.04	0.58
1:A:362[B]:TRP:HH2	1:A:446:GLN:CD	2.11	0.58
1:B:95:ILE:HG12	1:B:113:ILE:HD13	1.85	0.58
1:B:394:TYR:OH	1:B:451:GLU:HG3	2.03	0.58
1:A:417:ASP:HB2	1:A:456:SER:HB2	1.85	0.58
1:A:556:VAL:CG1	1:A:563:ILE:HB	2.32	0.58
1:A:447:LYS:HB3	1:A:490:TYR:HB2	1.86	0.57
1:A:199:ALA:HA	1:A:205:ASN:HD22	1.70	0.57
1:A:291:TYR:OH	1:B:772:THR:HG21	2.04	0.57
1:B:614:GLN:CD	1:B:614:GLN:N	2.63	0.57
1:A:151:THR:O	1:A:152:ILE:HD13	2.05	0.56
1:A:446:GLN:OE1	1:A:448:TYR:OH	2.17	0.56
1:A:580:ASN:HB2	1:A:583:TYR:H	1.70	0.56
1:B:92:ASN:O	1:B:96:THR:HB	2.06	0.55
1:B:380:ARG:HA	1:B:801:TYR:CE2	2.41	0.55
1:A:772:THR:CG2	1:B:291:TYR:OH	2.43	0.55
3:A:1817[B]:N8E:H031	1:B:805:ARG:HH11	1.72	0.55
1:A:443:ILE:CG1	1:A:510:ILE:CD1	2.85	0.55
1:B:792:ASN:O	1:B:793:ILE:HG13	2.07	0.55
1:B:431:MET:SD	2:C:11:FH7:HB2C	2.45	0.55
1:B:174:ARG:HA	1:B:177:MET:HE2	1.89	0.55
1:A:554:TYR:CD2	1:A:595:PRO:HG2	2.42	0.55
1:A:280:HIS:NE2	4:A:1823:PO4:O4	2.39	0.54
1:A:739:LYS:H	1:A:739:LYS:HD2	1.73	0.54
1:A:286:GLY:O	1:A:287:SER:C	2.51	0.53
1:A:775:LEU:HD23	1:A:776:SER:N	2.23	0.53
1:B:792:ASN:HB3	1:B:800:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:SER:OG	1:A:483:SER:HB3	2.07	0.53
1:A:646:GLU:O	1:A:647:ASP:HB3	2.08	0.53
1:B:681:LEU:HD22	1:B:687:VAL:HG22	1.89	0.53
1:A:646:GLU:O	1:A:662:ALA:O	2.27	0.53
1:A:722:LYS:HG3	1:A:723:GLY:N	2.23	0.53
1:B:380:ARG:HD3	1:B:788:THR:HB	1.90	0.53
1:B:447:LYS:HE2	1:B:515:TRP:CD1	2.43	0.53
1:A:133:THR:HG21	1:A:159:VAL:HG21	1.90	0.53
1:A:674:GLU:HG3	1:A:692:THR:OG1	2.07	0.53
1:A:715:LEU:C	1:A:715:LEU:HD23	2.34	0.53
1:A:174:ARG:CZ	1:A:177:MET:HE3	2.38	0.53
1:B:341:ASN:HB2	1:B:342:PRO:CD	2.39	0.53
1:B:417:ASP:O	1:B:455:ASN:HA	2.09	0.53
1:A:262:LEU:HD21	1:A:613:GLY:HA3	1.91	0.52
1:A:98:LEU:C	1:A:98:LEU:HD23	2.34	0.52
1:A:491:TRP:CE2	1:A:519:SER:HB3	2.44	0.52
1:B:694:LYS:HD2	1:B:694:LYS:C	2.34	0.52
1:B:689:ALA:HA	1:B:714:SER:O	2.09	0.52
1:B:275:HIS:O	1:B:300:PRO:HD3	2.09	0.52
1:B:201:ASP:O	1:B:202:THR:C	2.53	0.52
1:A:542:ASP:HB3	1:A:578:ASP:HB2	1.92	0.51
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.46	0.51
1:A:52:PRO:HG3	1:A:84:ALA:HB2	1.92	0.51
1:A:775:LEU:HD21	1:A:811:THR:HG22	1.93	0.51
1:B:77:VAL:O	1:B:79:ASN:N	2.43	0.51
1:A:218:GLN:HG2	1:A:223:PRO:HA	1.92	0.51
1:A:769:TYR:OH	3:A:1817[B]:N8E:H041	2.11	0.51
1:B:156:THR:O	1:B:157:ARG:CB	2.58	0.51
1:A:419:LYS:HG2	1:A:420:ILE:N	2.24	0.51
1:B:137:LEU:HD21	1:B:413:LYS:HZ1	1.76	0.51
1:A:341:ASN:HB2	1:A:342:PRO:CD	2.37	0.50
1:B:199:ALA:HA	1:B:205:ASN:ND2	2.25	0.50
1:B:540:THR:HG22	1:B:541:ASP:N	2.23	0.50
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.47	0.50
1:B:52:PRO:HD3	1:B:84:ALA:HB2	1.93	0.50
1:A:50:ILE:HD12	1:A:85:ILE:HD11	1.94	0.49
1:A:389:SER:HB2	1:A:428:GLY:H	1.77	0.49
1:A:772:THR:CG2	1:A:774:LYS:H	2.13	0.49
1:B:445:ALA:O	1:B:446:GLN:HG3	2.13	0.49
1:B:448:TYR:CZ	2:C:6:FHO:HD2C	2.48	0.49
1:A:691:TYR:C	1:A:691:TYR:CD2	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLN:HG2	1:B:276:GLU:HA	1.93	0.49
1:B:201:ASP:C	1:B:203:ASP:H	2.20	0.49
1:A:132:ILE:HD11	1:A:464:PRO:HD3	1.94	0.49
1:A:380:ARG:HA	1:A:801:TYR:CD2	2.48	0.49
1:B:586:TYR:CE1	1:B:619:GLY:HA3	2.48	0.49
1:A:152:ILE:HG22	1:A:154:THR:H	1.77	0.49
1:B:329:THR:HA	1:B:354:ASP:O	2.13	0.49
1:B:308:ARG:NH2	1:B:339:ASP:OD2	2.46	0.49
1:B:445:ALA:O	1:B:446:GLN:CG	2.61	0.48
1:B:152:ILE:HD12	1:B:169:ILE:HG12	1.94	0.48
1:A:182:LEU:HD21	1:A:191:HIS:CD2	2.48	0.48
1:B:77:VAL:O	1:B:78:ARG:C	2.57	0.48
1:B:698:ASP:HB3	1:B:700:SER:H	1.78	0.48
1:A:636:PHE:CD1	1:A:636:PHE:C	2.91	0.48
1:B:771:ILE:H	1:B:771:ILE:HG13	1.50	0.48
1:A:344:THR:HA	1:A:403:GLU:O	2.13	0.47
1:B:527:ARG:HD2	1:B:527:ARG:C	2.38	0.47
1:A:410:TRP:CE2	1:A:463:GLY:HA3	2.49	0.47
1:A:653:LYS:O	1:A:653:LYS:HG3	2.13	0.47
1:A:536:ARG:HD2	1:A:546:PHE:CZ	2.50	0.47
1:A:53:GLN:OE1	1:A:57:SER:HB3	2.14	0.47
1:B:646:GLU:HG3	1:B:651:ASN:HD22	1.78	0.47
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.49	0.47
1:B:470:ARG:NH1	1:B:540:THR:O	2.45	0.47
1:B:436:ALA:HB1	1:B:437:PRO:CD	2.44	0.47
1:B:691:TYR:CD1	1:B:691:TYR:C	2.93	0.47
1:B:231:TYR:CZ	2:C:6:FHO:HG1C	2.50	0.47
1:B:721:PHE:HB2	1:B:725:LEU:O	2.15	0.47
1:A:177:MET:HA	1:A:182:LEU:HD12	1.97	0.47
1:A:736:TRP:HB2	1:A:761:TRP:CE3	2.50	0.47
1:B:142:GLU:HG3	4:B:1820:PO4:O1	2.15	0.47
1:B:493:LEU:HD12	1:B:493:LEU:N	2.25	0.47
1:A:321:PHE:CE2	1:A:322:MET:HG3	2.50	0.46
1:B:426:PRO:HB3	1:B:447:LYS:HG3	1.97	0.46
1:B:594:MET:SD	1:B:595:PRO:HD2	2.55	0.46
1:B:653:LYS:HA	1:B:654:PRO:HD2	1.68	0.46
1:A:73:ARG:CG	1:A:131:MET:HE3	2.42	0.46
1:A:99:LEU:O	1:A:102:THR:HG23	2.16	0.46
1:B:410:TRP:CD2	1:B:463:GLY:HA3	2.51	0.46
1:A:436:ALA:HB1	1:A:437:PRO:CD	2.45	0.46
1:B:154:THR:O	1:B:256:LEU:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ILE:O	1:A:669:LYS:HA	2.15	0.46
1:A:694:LYS:HD2	1:A:694:LYS:O	2.15	0.46
1:B:410:TRP:CG	1:B:463:GLY:HA3	2.51	0.46
1:B:721:PHE:CE2	1:B:728:LEU:HD23	2.51	0.46
1:B:506:TRP:CZ2	1:B:508:GLY:HA2	2.51	0.46
1:A:615:ASN:HD21	1:A:617:GLU:HB2	1.81	0.46
1:B:201:ASP:C	1:B:203:ASP:N	2.73	0.45
1:B:772:THR:HG22	1:B:775:LEU:H	1.80	0.45
1:A:596:GLN:NE2	1:A:609:GLU:O	2.49	0.45
1:B:459:ILE:HG12	1:B:478:THR:HG22	1.98	0.45
2:C:8:DSN:C	2:C:10:ORN:H	2.30	0.45
1:B:371:SER:HG	1:B:436:ALA:HA	1.81	0.45
1:A:402:LEU:O	1:A:413:LYS:HA	2.17	0.45
1:A:560:ASN:HB3	1:A:598:SER:OG	2.17	0.45
1:B:476:VAL:HG12	1:B:533:MET:HG3	1.98	0.45
1:B:489:SER:O	1:B:519:SER:N	2.48	0.45
1:B:790:TYR:CG	1:B:793:ILE:HD11	2.52	0.44
1:A:343:ASP:HB2	1:A:405:ASN:HB2	1.99	0.44
1:A:698:ASP:OD1	1:A:698:ASP:C	2.61	0.44
1:B:277:PHE:HA	1:B:298:SER:O	2.17	0.44
1:B:772:THR:CG2	1:B:773:ASP:N	2.81	0.44
1:B:489:SER:HB2	1:B:520:GLN:HB3	1.99	0.44
1:A:196:THR:HG21	1:A:709:PRO:HD3	1.98	0.44
1:A:203:ASP:OD1	1:A:325:TYR:OH	2.33	0.44
1:A:179:ASP:OD1	1:A:768:ARG:NH1	2.37	0.44
1:A:766:MET:SD	1:A:766:MET:C	3.01	0.44
1:B:239:ASP:OD2	1:B:292:ARG:NH2	2.51	0.44
1:B:792:ASN:HD22	1:B:800:SER:CB	2.31	0.44
1:A:322:MET:HE3	1:A:365:SER:HB3	2.00	0.43
1:B:462:THR:HA	1:B:474:LEU:O	2.18	0.43
1:A:580:ASN:HB2	1:A:582:THR:H	1.82	0.43
1:A:687:VAL:O	1:A:687:VAL:HG23	2.18	0.43
1:B:762:LEU:HD23	1:B:762:LEU:HA	1.85	0.43
1:A:736:TRP:HB2	1:A:761:TRP:CD2	2.53	0.43
1:B:215:ASN:HB3	1:B:261:SER:HB3	2.00	0.43
1:A:392:GLU:CG	1:A:424:HIS:HB3	2.47	0.43
1:A:656:ASN:OD1	1:A:658:ALA:HB3	2.18	0.43
1:B:446:GLN:HE21	1:B:491:TRP:CB	2.27	0.43
1:A:307:VAL:HA	1:A:337:GLU:O	2.18	0.43
1:A:602:ASP:O	1:A:603:SER:C	2.61	0.43
1:A:694:LYS:C	1:A:694:LYS:CD	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ILE:HG13	1:B:443:ILE:CD1	2.49	0.43
1:A:792:ASN:O	1:A:799:ALA:HA	2.18	0.43
1:B:168:SER:CB	1:B:210:ARG:HH22	2.31	0.43
1:A:789:TYR:CZ	1:A:802:GLY:HA3	2.54	0.43
1:B:418:HIS:CD2	1:B:455:ASN:ND2	2.66	0.43
1:A:553:ASP:OD1	1:A:564:ARG:NH2	2.52	0.42
1:A:638:ILE:HB	1:A:670:THR:HB	2.00	0.42
1:B:792:ASN:C	1:B:793:ILE:HG13	2.44	0.42
1:B:464:PRO:HA	1:B:472:HIS:O	2.19	0.42
1:B:47:GLU:OE1	1:B:88:LYS:HB2	2.19	0.42
1:A:273:PRO:HB3	1:A:309:GLY:C	2.44	0.42
1:A:640:GLU:CD	1:A:643:ARG:HB2	2.44	0.42
1:B:694:LYS:NZ	1:B:709:PRO:O	2.51	0.42
1:A:380:ARG:HD3	1:A:788:THR:HB	2.01	0.42
1:A:506:TRP:CZ2	1:A:508:GLY:HA2	2.55	0.42
1:B:394:TYR:CZ	1:B:422:GLY:HA3	2.55	0.42
1:B:737:GLN:O	1:B:759:ASP:HA	2.19	0.42
1:A:380:ARG:HA	1:A:801:TYR:CE2	2.55	0.42
1:A:435:PRO:HD3	1:A:503:PHE:CD1	2.55	0.42
1:B:706:THR:HB	1:B:741:TRP:CE2	2.55	0.42
1:B:180:PHE:HA	1:B:780:ASN:HD21	1.85	0.42
1:B:276:GLU:H	1:B:276:GLU:CD	2.27	0.42
1:A:435:PRO:HD3	1:A:503:PHE:CE1	2.55	0.41
1:B:137:LEU:HD21	1:B:413:LYS:NZ	2.34	0.41
1:B:341:ASN:HB2	1:B:342:PRO:HD2	2.02	0.41
1:B:373:GLY:HA3	1:B:749:ARG:HG3	2.01	0.41
1:B:430:ILE:CG1	1:B:443:ILE:CD1	2.98	0.41
1:B:593:PHE:CD2	1:B:593:PHE:C	2.98	0.41
1:B:646:GLU:HG3	1:B:651:ASN:ND2	2.36	0.41
1:B:792:ASN:HD22	1:B:800:SER:HB2	1.85	0.41
1:A:192:THR:HA	1:A:193:PRO:HD2	1.92	0.41
1:B:148:THR:OG1	1:B:149:PRO:HD2	2.20	0.41
1:A:407:ALA:O	1:A:409:GLY:N	2.52	0.41
1:A:436:ALA:HB1	1:A:437:PRO:HD2	2.02	0.41
1:A:395:THR:HA	1:A:420:ILE:O	2.21	0.41
1:B:74:PRO:HG3	1:B:303:GLU:CG	2.50	0.41
1:B:640:GLU:CD	1:B:643:ARG:HB2	2.46	0.41
1:A:330:SER:O	1:A:353:GLN:HA	2.21	0.41
1:B:410:TRP:HH2	1:B:474:LEU:HD23	1.86	0.41
1:A:308:ARG:NH2	1:A:339:ASP:OD1	2.54	0.41
1:A:547:LEU:HD23	1:A:547:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:SER:HA	1:A:730:VAL:O	2.21	0.41
1:B:62:PHE:CZ	1:B:95:ILE:HB	2.56	0.41
1:B:169:ILE:HD12	1:B:248:VAL:O	2.21	0.41
1:B:88:LYS:O	1:B:89:LEU:HD23	2.20	0.40
1:B:207:TYR:HB2	1:B:214:ILE:HB	2.04	0.40
1:A:62:PHE:CZ	1:A:95:ILE:HB	2.56	0.40
1:A:294:GLU:OE2	4:A:1823:PO4:O4	2.38	0.40
1:A:674:GLU:HA	1:A:691:TYR:O	2.22	0.40
1:B:636:PHE:CD1	1:B:636:PHE:C	2.99	0.40
1:B:645:GLU:HG3	1:B:646:GLU:H	1.86	0.40
1:A:55:LEU:HD23	1:A:77:VAL:HG12	2.03	0.40
1:A:229:VAL:HA	1:A:232:SER:HB3	2.03	0.40
1:A:407:ALA:C	1:A:409:GLY:H	2.30	0.40
1:B:506:TRP:CE2	1:B:508:GLY:HA2	2.56	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	771/772 (100%)	718 (93%)	40 (5%)	13 (2%)	7	26
1	B	750/772 (97%)	707 (94%)	38 (5%)	5 (1%)	18	48
2	C	4/10 (40%)	4 (100%)	0	0	100	100
All	All	1525/1554 (98%)	1429 (94%)	78 (5%)	18 (1%)	10	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	408	ASN
1	A	646	GLU

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Mol	Chain	Res	Type
1	A	653	LYS
1	A	699	ASP
1	B	202	THR
1	B	408	ASN
1	A	182	LEU
1	A	324	HIS
1	A	651	ASN
1	B	78	ARG
1	B	495	ASN
1	A	287	SER
1	A	603	SER
1	A	647	ASP
1	A	220	ASP
1	B	786	ASP
1	A	683	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	651/650 (100%)	565 (87%)	86 (13%)	4	13
1	B	637/650 (98%)	561 (88%)	76 (12%)	5	16
2	C	3/3 (100%)	3 (100%)	0	100	100
All	All	1291/1303 (99%)	1129 (88%)	162 (12%)	4	15

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	60	GLN
1	A	61	GLU
1	A	68	ILE
1	A	71	LEU
1	A	81	ARG
1	A	97	GLU

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Mol	Chain	Res	Type
1	A	100	ARG
1	A	109	GLN
1	A	114	THR
1	A	115	ILE
1	A	131	MET
1	A	132	ILE
1	A	133	THR
1	A	143	ASP
1	A	148	THR
1	A	152	ILE
1	A	157	ARG
1	A	204	ARG
1	A	246	VAL
1	A	248	VAL
1	A	250	LYS
1	A	257	THR
1	A	272	LYS
1	A	295	LEU
1	A	297	VAL
1	A	304	SER
1	A	307	VAL
1	A	312	VAL
1	A	318	LYS
1	A	326	GLU
1	A	329	THR
1	A	331	VAL
1	A	343	ASP
1	A	344	THR
1	A	372	GLN
1	A	379	SER
1	A	392	GLU
1	A	401	ASN
1	A	408	ASN
1	A	417	ASP
1	A	431	MET
1	A	458	ASP
1	A	459	ILE
1	A	461	LEU
1	A	470	ARG
1	A	475	VAL
1	A	499	THR
1	A	524	ASP

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Mol	Chain	Res	Type
1	A	527	ARG
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	603	SER
1	A	609	GLU
1	A	615	ASN
1	A	618	ILE
1	A	628	ARG
1	A	646	GLU
1	A	653	LYS
1	A	655	THR
1	A	659	ILE
1	A	660	THR
1	A	676	GLU
1	A	683	PRO
1	A	694	LYS
1	A	698	ASP
1	A	699	ASP
1	A	704	VAL
1	A	705	SER
1	A	720	LYS
1	A	730	VAL
1	A	739	LYS
1	A	744	VAL
1	A	758	GLU
1	A	766	MET
1	A	772	THR
1	A	788	THR
1	A	792	ASN
1	A	810	SER
1	A	811	THR
1	A	815	PHE
1	B	68	ILE
1	B	78	ARG
1	B	83	SER
1	B	96	THR
1	B	105	SER

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Mol	Chain	Res	Type
1	B	106	VAL
1	B	109	GLN
1	B	113	ILE
1	B	114	THR
1	B	139	THR
1	B	152	ILE
1	B	154	THR
1	B	157	ARG
1	B	168	SER
1	B	169	ILE
1	B	177	MET
1	B	201	ASP
1	B	236	THR
1	B	238	SER
1	B	249	LEU
1	B	265	THR
1	B	303	GLU
1	B	329	THR
1	B	331	VAL
1	B	360	SER
1	B	396	ARG
1	B	411	VAL
1	B	413	LYS
1	B	416	LEU
1	B	417	ASP
1	B	440	SER
1	B	447	LYS
1	B	454	SER
1	B	459	ILE
1	B	481	SER
1	B	493	LEU
1	B	495	ASN
1	B	512	LYS
1	B	533	MET
1	B	539	VAL
1	B	551	VAL
1	B	556	VAL
1	B	557	THR
1	B	559	LEU
1	B	564	ARG
1	B	566	SER
1	B	576	VAL

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Mol	Chain	Res	Type
1	B	585	VAL
1	B	596	GLN
1	B	598	SER
1	B	618	ILE
1	B	646	GLU
1	B	649	LEU
1	B	660	THR
1	B	671	LYS
1	B	676	GLU
1	B	678	SER
1	B	681	LEU
1	B	687	VAL
1	B	688	GLN
1	B	694	LYS
1	B	699	ASP
1	B	704	VAL
1	B	720	LYS
1	B	730	VAL
1	B	744	VAL
1	B	759	ASP
1	B	764	ASP
1	B	772	THR
1	B	774	LYS
1	B	781	VAL
1	B	788	THR
1	B	792	ASN
1	B	810	SER
1	B	811	THR
1	B	815	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	176	ASN
1	A	183	ASN
1	A	191	HIS
1	A	205	ASN
1	A	372	GLN
1	A	374	ASN
1	A	408	ASN
1	A	439	ASN

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Mol	Chain	Res	Type
1	A	455	ASN
1	A	505	ASN
1	A	596	GLN
1	A	615	ASN
1	A	710	GLN
1	A	737	GLN
1	B	60	GLN
1	B	109	GLN
1	B	136	GLN
1	B	176	ASN
1	B	183	ASN
1	B	191	HIS
1	B	205	ASN
1	B	401	ASN
1	B	415	GLN
1	B	418	HIS
1	B	455	ASN
1	B	466	GLN
1	B	472	HIS
1	B	528	GLN
1	B	642	ASN
1	B	742	GLN
1	B	780	ASN
1	B	792	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	ORN	C	10	2	6,7,8	0.52	0	2,7,9	0.65	0
2	FHO	C	6	2,6	9,10,11	4.10	2 (22%)	4,11,13	3.57	2 (50%)
2	FH7	C	11	2,6	9,10,11	4.68	2 (22%)	4,11,13	2.24	3 (75%)

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	ORN	C	10	2	-	2/5/6/8	-
2	FHO	C	6	2,6	-	5/7/10/12	-
2	FH7	C	11	2,6	-	0/7/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	FH7	OZ-NE	-13.26	1.23	1.39
2	C	6	FHO	OZ-NE	-11.34	1.26	1.39
2	C	6	FHO	CZ-NE	-4.51	1.27	1.34
2	C	11	FH7	CZ-NE	-4.48	1.27	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	FHO	OZ-NE-CD	6.08	127.88	113.81
2	C	6	FHO	CG-CD-NE	3.00	117.25	111.12
2	C	11	FH7	CG-CD-NE	2.42	116.06	111.12
2	C	11	FH7	OZ-NE-CD	2.40	119.36	113.81
2	C	11	FH7	OH-CZ-NE	-2.35	119.47	125.49

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6	FHO	N-CA-CB-CG
2	C	6	FHO	C-CA-CB-CG
2	C	6	FHO	CG-CD-NE-OZ
2	C	6	FHO	CG-CD-NE-CZ
2	C	10	ORN	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
2	C	10	ORN	NE-CD-CG-CB
2	C	6	FHO	CA-CB-CG-CD

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	10	ORN	1	0
2	C	6	FHO	2	0
2	C	11	FH7	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	1823	-	4,4,4	0.97	0	6,6,6	0.80	0
4	PO4	B	1819	-	4,4,4	0.91	0	6,6,6	0.85	0
4	PO4	B	1821	-	4,4,4	0.95	0	6,6,6	0.81	0
3	N8E	A	1817[A]	-	23,23,23	0.76	0	22,22,22	0.80	0
4	PO4	A	1819	-	4,4,4	0.96	0	6,6,6	1.61	2 (33%)
4	PO4	B	1818	-	4,4,4	0.74	0	6,6,6	1.41	1 (16%)
4	PO4	B	1820	-	4,4,4	0.88	0	6,6,6	0.53	0
4	PO4	A	1822	-	4,4,4	0.96	0	6,6,6	0.75	0
4	PO4	A	1820	-	4,4,4	1.07	0	6,6,6	1.22	0
3	N8E	A	1817[B]	-	23,23,23	0.78	0	22,22,22	0.75	1 (4%)
4	PO4	A	1821	-	4,4,4	1.07	0	6,6,6	0.74	0
3	N8E	A	1816	-	23,23,23	0.60	0	22,22,22	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	A	1818	-	4,4,4	0.81	0	6,6,6	1.62	2 (33%)
5	PVE	C	1	2,6	26,28,29	2.51	4 (15%)	30,40,42	1.65	6 (20%)

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
5	PVE	C	1	2,6	-	6/10/21/23	0/2/3/3
3	N8E	A	1817[A]	-	-	12/21/21/21	-
3	N8E	A	1817[B]	-	-	9/21/21/21	-
3	N8E	A	1816	-	-	7/21/21/21	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	PVE	C20-C18	-9.65	1.32	1.51
5	C	1	PVE	C8-C7	4.81	1.42	1.37
5	C	1	PVE	C5-C6	4.74	1.41	1.37
5	C	1	PVE	C4-C3	2.57	1.42	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	PVE	C15-C14-N1	-3.91	106.38	111.53
5	C	1	PVE	C13-C12-N11	-3.77	104.44	110.04
5	C	1	PVE	C21-C20-C18	-3.55	105.36	112.67
5	C	1	PVE	C3-C2-N11	-2.51	116.46	122.87
4	A	1818	PO4	O4-P-O3	2.49	115.65	107.91
4	A	1819	PO4	O3-P-O2	2.40	115.39	107.91
4	B	1818	PO4	O3-P-O2	2.28	115.00	107.91
3	A	1817[B]	N8E	O18-C19-C20	2.27	120.71	110.35
5	C	1	PVE	C5-C6-C7	2.24	121.30	119.87
4	A	1818	PO4	O3-P-O2	-2.19	101.09	107.91
4	A	1819	PO4	O2-P-O1	-2.17	103.29	110.95
5	C	1	PVE	O19-C18-N17	2.05	127.31	123.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 11 short contacts:

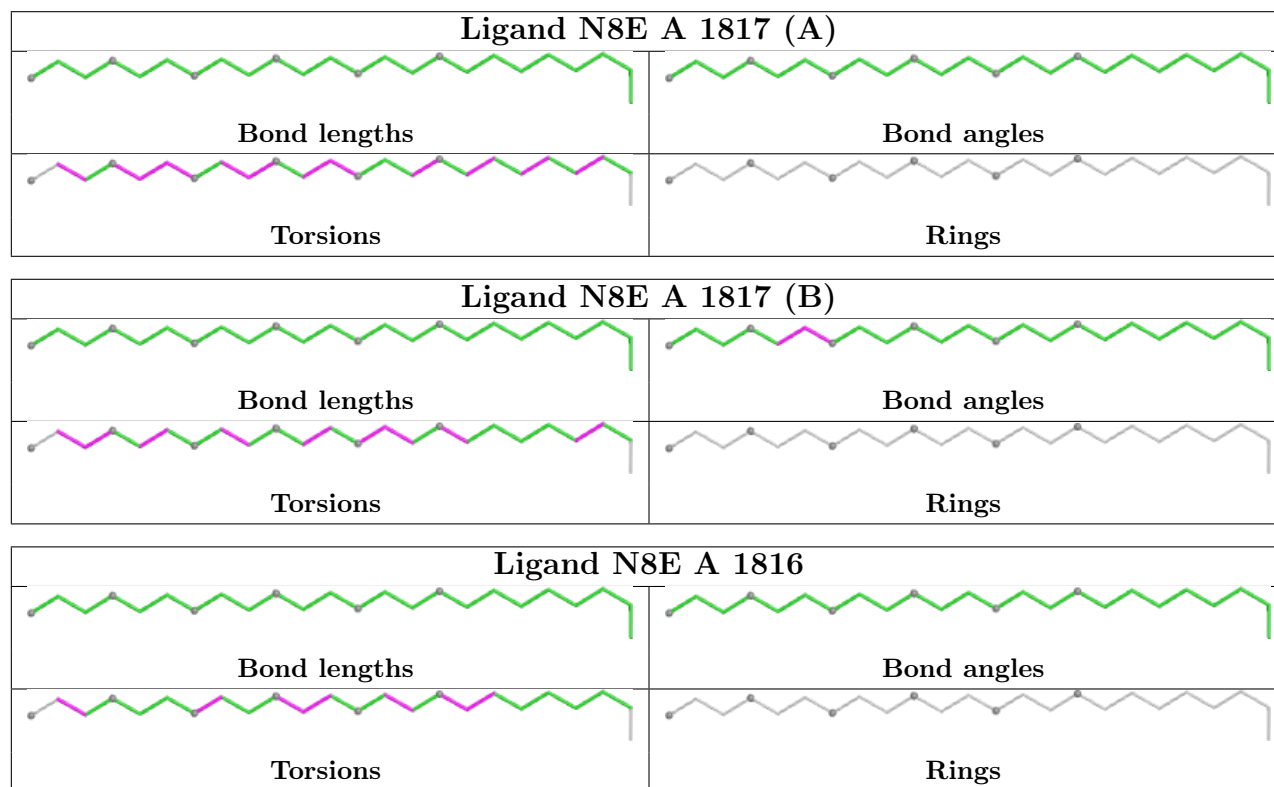
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1823	PO4	2	0
4	B	1821	PO4	1	0
4	B	1818	PO4	1	0
4	B	1820	PO4	1	0

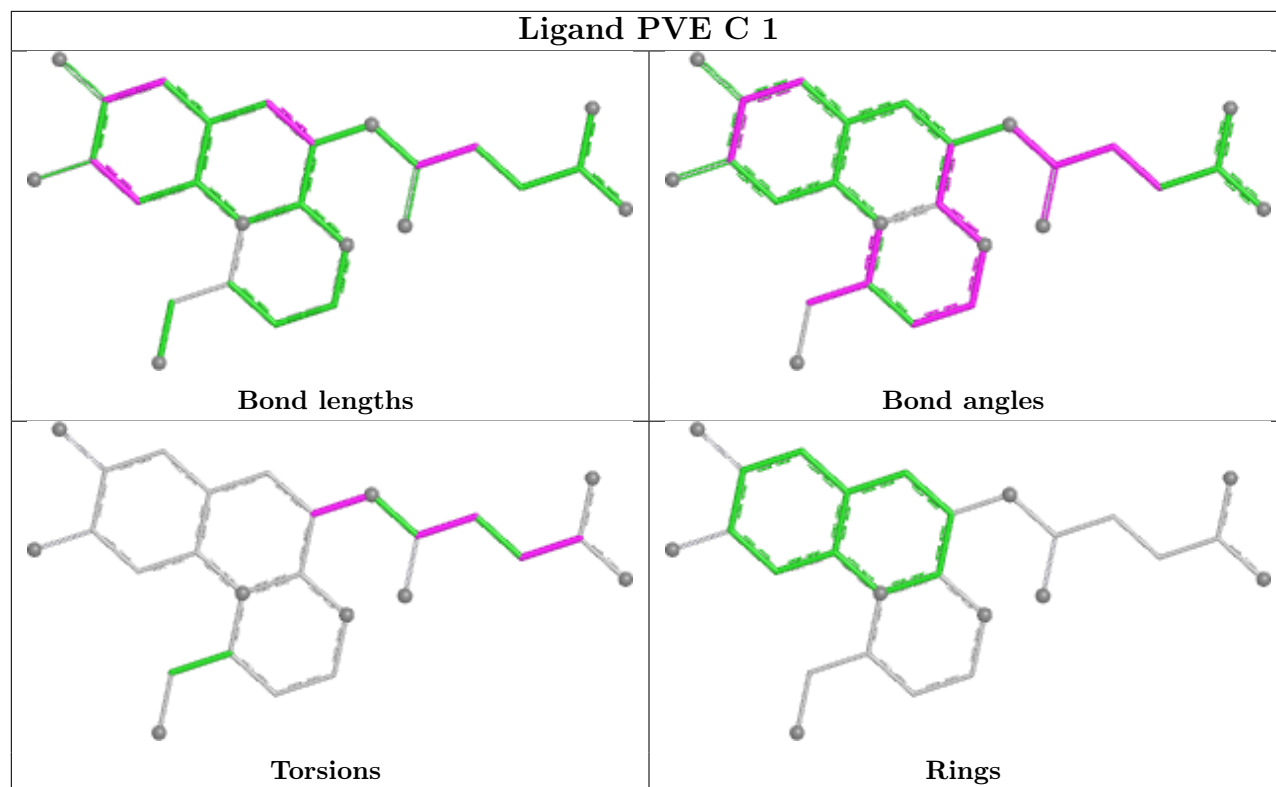
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1817[B]	N8E	6	0

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%)	-0.04	10 (1%) 75 67	3, 17, 26, 37	1 (0%)
1	B	754/772 (97%)	-0.03	16 (2%) 63 54	3, 15, 24, 62	0
2	C	5/10 (50%)	-0.17	0 100 100	6, 7, 9, 10	0
All	All	1531/1554 (98%)	-0.04	26 (1%) 69 61	3, 16, 26, 62	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	LEU	7.7
1	A	123	SER	6.4
1	B	87	GLY	3.3
1	A	747	ASN	3.2
1	A	362[A]	TRP	3.2
1	B	44	GLN	3.1
1	B	109	GLN	3.1
1	A	773	ASP	3.0
1	B	581	ASP	3.0
1	B	47	GLU	3.0
1	B	110	GLY	3.0
1	A	44	GLN	2.9
1	B	78	ARG	2.8
1	B	407	ALA	2.7
1	A	599	TRP	2.6
1	B	533	MET	2.6
1	B	405	ASN	2.5
1	A	758	GLU	2.3
1	B	473	GLU	2.3
1	B	49	ASP	2.1
1	B	88	LYS	2.1
1	A	122	ASP	2.1
1	A	407	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	75	GLU	2.1
1	A	303	GLU	2.0
1	B	542	ASP	2.0

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(Å ²)	Q<0.9
2	DSN	C	8	6/7	0.88	0.10	9,10,10,11	0
2	DSN	C	3	6/7	0.94	0.08	5,7,7,8	0
2	ORN	C	10	8/9	0.94	0.08	7,8,8,9	0
2	FHO	C	6	11/12	0.97	0.06	4,6,7,8	0
2	FH7	C	11	11/12	0.97	0.08	4,7,8,8	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(Å ²)	Q<0.9
3	N8E	A	1817[A]	24/24	0.70	0.34	2,4,10,12	24
3	N8E	A	1817[B]	24/24	0.70	0.34	2,2,8,11	24
3	N8E	A	1816	24/24	0.85	0.23	40,57,59,60	0
4	PO4	A	1821	5/5	0.88	0.19	54,54,55,55	0
4	PO4	A	1822	5/5	0.90	0.11	55,56,57,58	0
4	PO4	A	1823	5/5	0.93	0.18	46,46,48,49	0
4	PO4	B	1818	5/5	0.93	0.14	37,38,39,39	0
5	PVE	C	1	26/27	0.94	0.10	2,5,35,39	5
4	PO4	B	1820	5/5	0.95	0.10	40,40,42,42	0
4	PO4	A	1820	5/5	0.96	0.11	25,26,28,29	0

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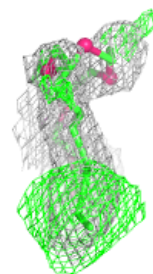
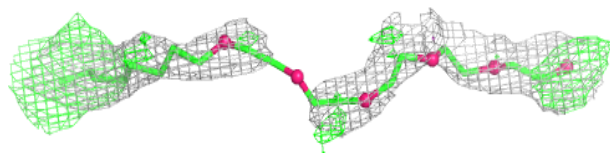
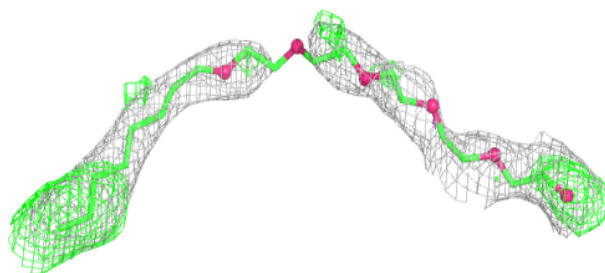
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	B	1821	5/5	0.97	0.06	41,43,43,44	0
4	PO4	B	1819	5/5	0.97	0.06	19,20,22,22	0
4	PO4	A	1819	5/5	0.98	0.07	16,17,18,22	0
4	PO4	A	1818	5/5	0.98	0.07	10,11,15,16	0
6	FE	C	2	1/1	1.00	0.03	2,2,2,2	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.

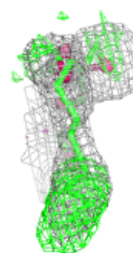
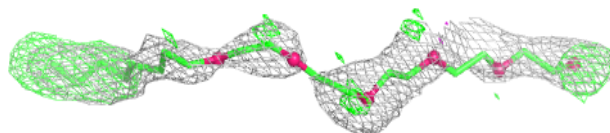
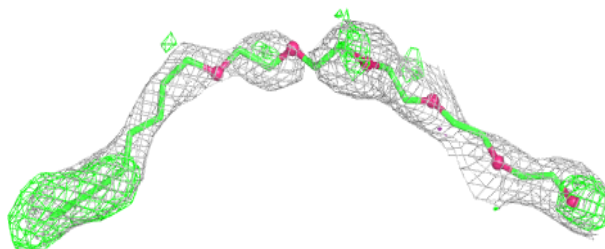
Electron density around N8E A 1817 (A):

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

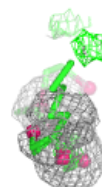
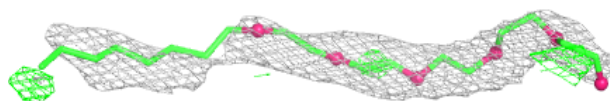
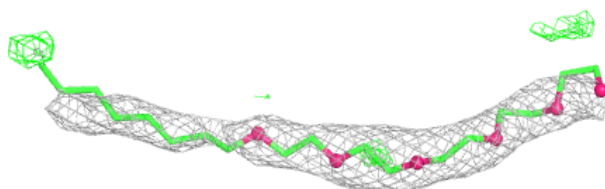


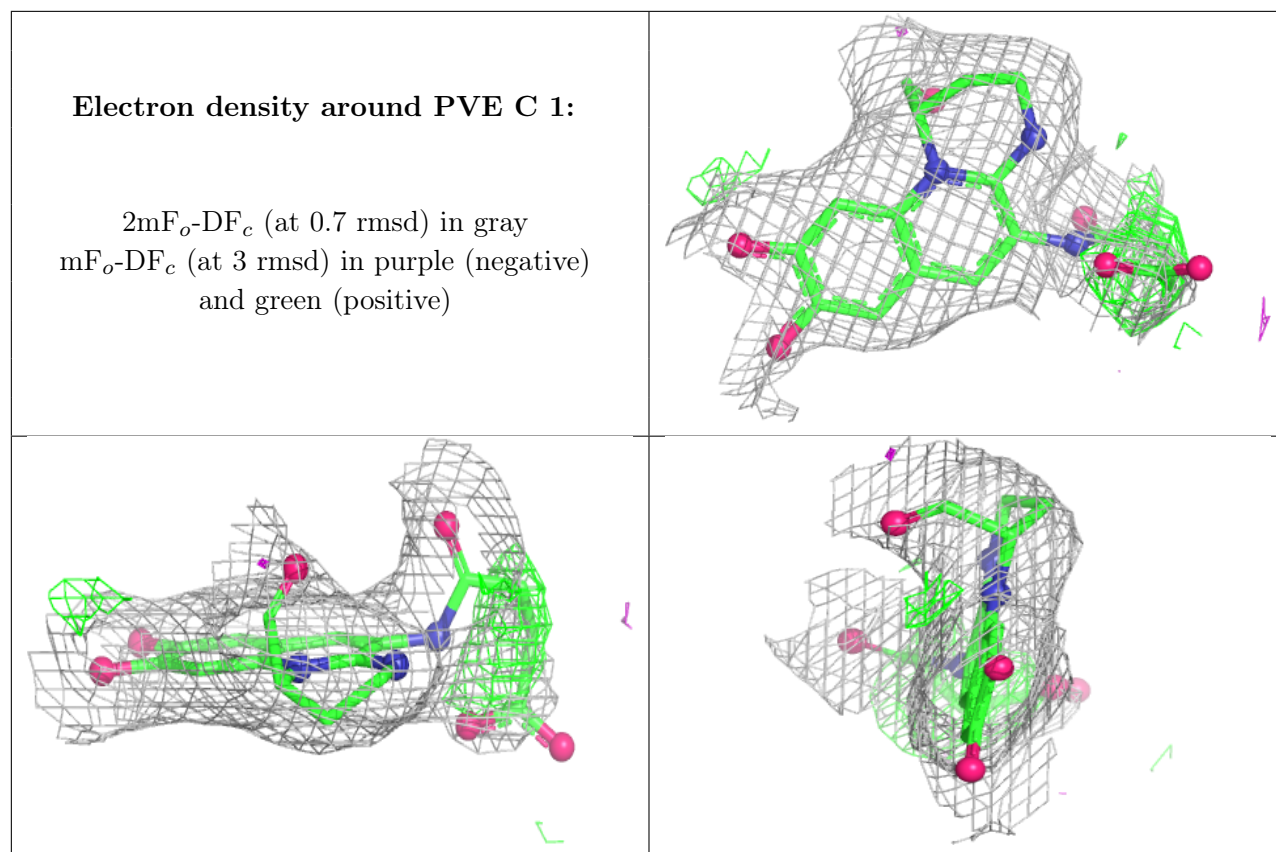
Electron density around N8E A 1817 (B):

$2mF_o-DF_c$ (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.