



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:24 AM UTC

PDB ID : 2W76 / pdb_00002w76
Title : Structures of *P. aeruginosa* FpvA bound to heterologous pyoverdines: FpvA-Pvd(Pa6)-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 : 2.80 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

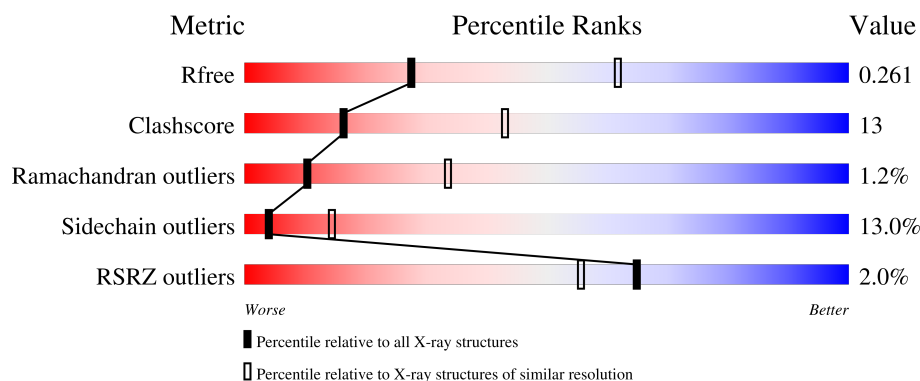
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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% 67% 26% 7%
1	B	772	2% 63% 29% 5% ..
2	C	7	14% 29% 57%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DSN	C	3	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12314 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			

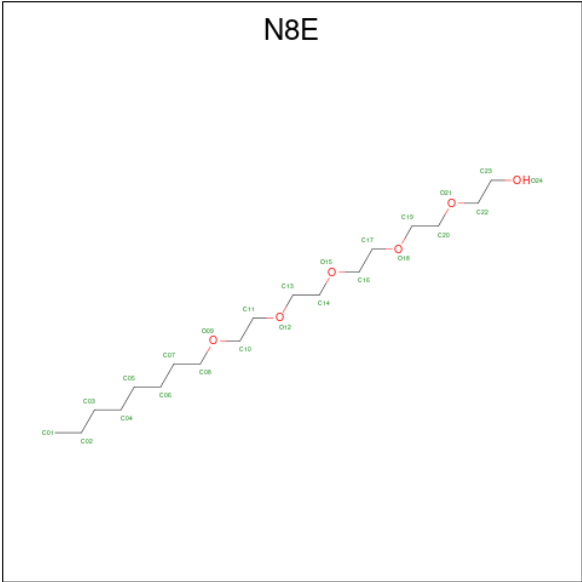
- Molecule 2 is a protein called PYOVERDIN R.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			57	31	12	14			

There is a discrepancy between the modelled and reference sequences:

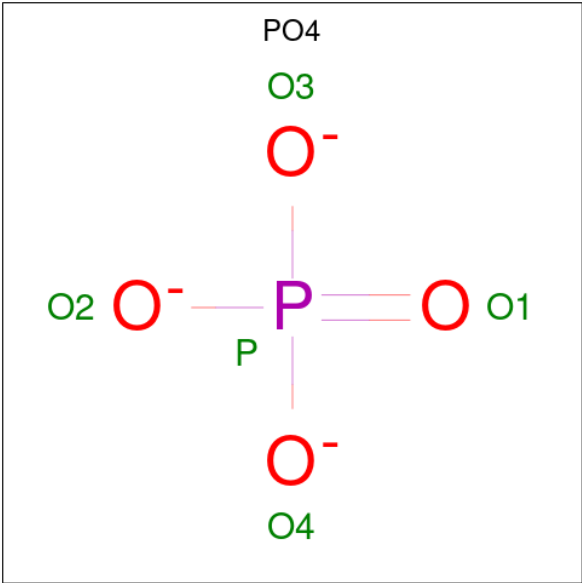
Chain	Residue	Modelled	Actual	Comment	Reference
C	8	FHO	FH7	conflict	NOR NOR0020

- 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		
3	A	1	Total	C	O	0	1
			48	36	12		

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



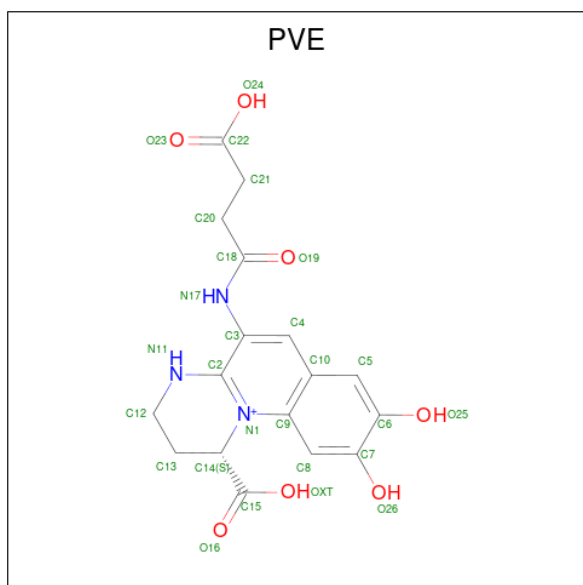
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		

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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	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: C₁₇H₁₈N₃O₇).



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

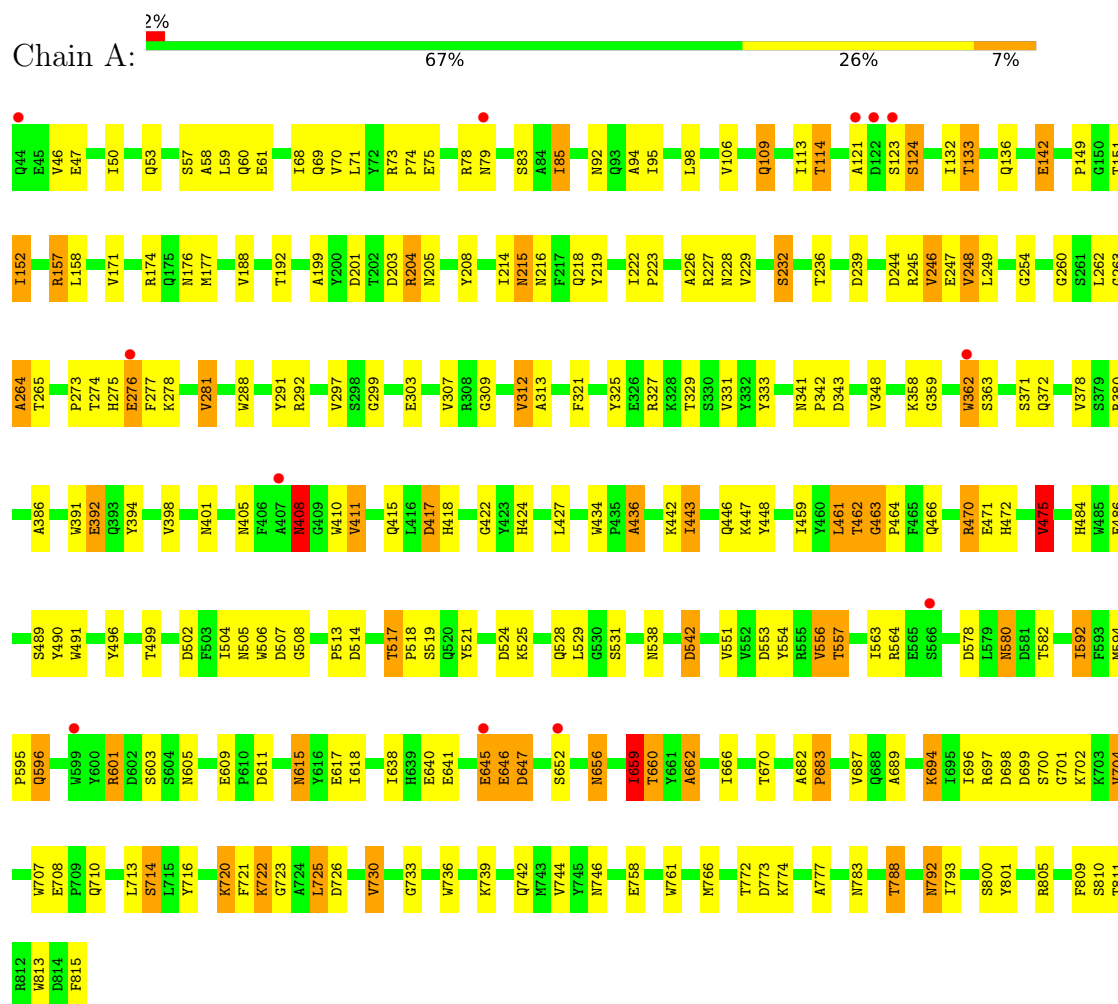
- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

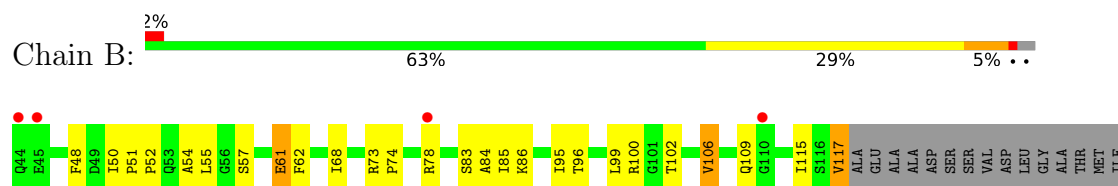
3 Residue-property plots

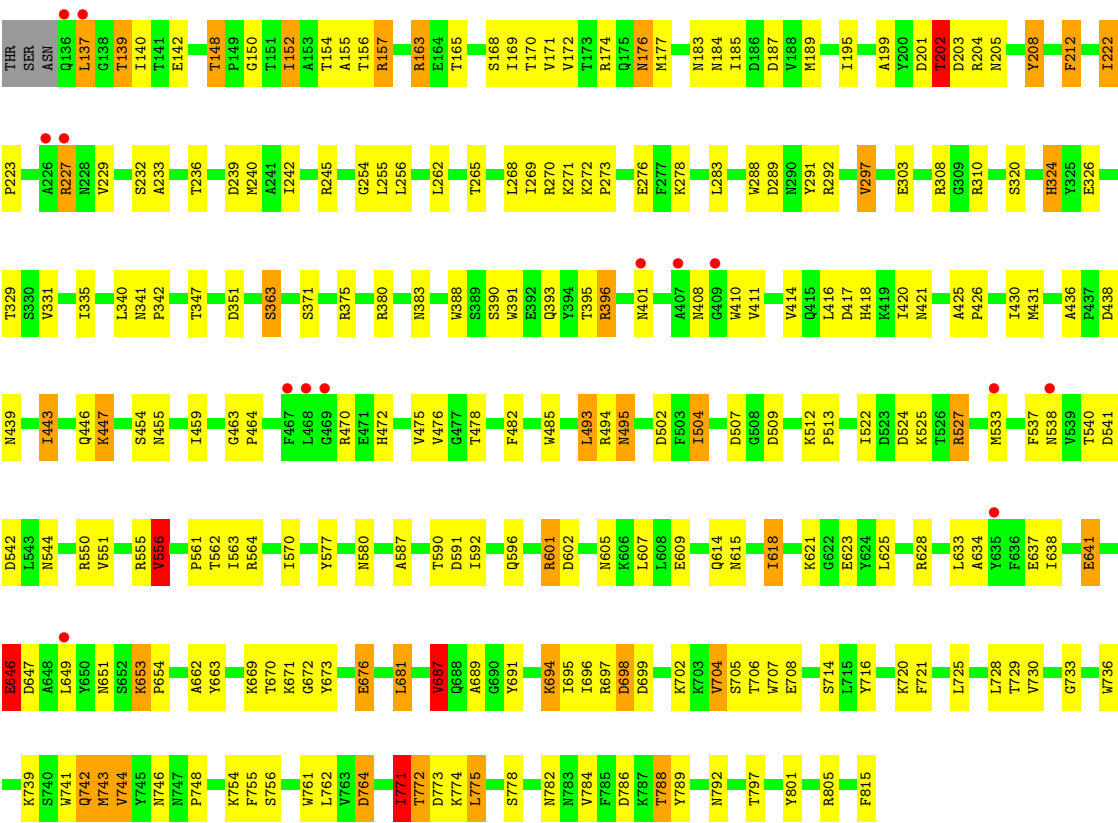
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





● Molecule 2: PYOVERDIN R



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.42Å 129.93Å 140.88Å 90.00° 130.77° 90.00°	Depositor
Resolution (Å)	97.13 – 2.80 97.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.1 (97.13-2.80) 89.1 (97.13-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.265 0.213 , 0.261	Depositor DCC
R_{free} test set	2923 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12314	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.14	2/6266 (0.0%)	1.28	31/8514 (0.4%)
1	B	1.04	3/6145 (0.0%)	1.19	34/8347 (0.4%)
2	C	0.86	0/12	1.11	0/11
All	All	1.09	5/12423 (0.0%)	1.24	65/16872 (0.4%)

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	1
2	C	1	2
All	All	1	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148	THR	CA-CB	5.61	1.61	1.53
1	B	202	THR	C-O	-5.58	1.17	1.24
1	A	662	ALA	CA-C	-5.24	1.46	1.52
1	A	398	VAL	CA-CB	-5.23	1.48	1.54
1	B	556	VAL	CA-CB	5.16	1.61	1.54

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	GLY	CA-C-N	9.46	130.97	120.66
1	A	463	GLY	C-N-CA	9.46	130.97	120.66
1	A	687	VAL	CB-CA-C	-8.10	96.62	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	653	LYS	CA-C-N	7.88	127.94	119.90
1	B	653	LYS	C-N-CA	7.88	127.94	119.90
1	A	113	ILE	CA-C-N	-7.82	112.20	123.00
1	A	113	ILE	C-N-CA	-7.82	112.20	123.00
1	B	687	VAL	CB-CA-C	-7.65	98.92	110.55
1	A	281	VAL	N-CA-C	-7.18	97.16	108.86
1	A	362	TRP	N-CA-C	-6.79	101.17	111.56
1	A	704	VAL	N-CA-CB	-6.72	104.68	112.34
1	B	764	ASP	N-CA-C	6.57	119.70	109.52
1	B	73	ARG	N-CA-C	-6.44	101.67	109.72
1	A	517	THR	CA-C-N	-6.42	112.90	119.83
1	A	517	THR	C-N-CA	-6.42	112.90	119.83
1	A	475	VAL	CB-CA-C	-6.10	101.42	110.33
1	B	507	ASP	N-CA-C	-6.09	103.57	113.19
1	A	106	VAL	CB-CA-C	-6.06	101.59	110.62
1	B	676	GLU	N-CA-C	6.06	118.39	109.24
1	A	660	THR	N-CA-C	-5.99	107.21	114.75
1	B	283	LEU	CA-C-N	-5.97	118.06	122.18
1	B	283	LEU	C-N-CA	-5.97	118.06	122.18
1	B	320	SER	N-CA-C	5.94	116.93	108.74
1	B	154	THR	CA-C-N	5.88	128.42	120.65
1	B	154	THR	C-N-CA	5.88	128.42	120.65
1	A	730	VAL	CB-CA-C	5.86	119.84	110.82
1	B	646	GLU	N-CA-C	5.83	117.72	111.36
1	B	222	ILE	CA-C-N	5.80	125.99	119.90
1	B	222	ILE	C-N-CA	5.80	125.99	119.90
1	B	148	THR	CA-C-N	-5.70	112.72	119.84
1	B	148	THR	C-N-CA	-5.70	112.72	119.84
1	A	656	ASN	N-CA-C	-5.67	101.36	109.24
1	A	61	GLU	N-CA-C	-5.65	105.12	111.28
1	A	436	ALA	N-CA-C	-5.64	103.55	110.31
1	B	272	LYS	CA-C-N	-5.57	114.86	120.21
1	B	272	LYS	C-N-CA	-5.57	114.86	120.21
1	A	507	ASP	N-CA-CB	-5.56	103.64	110.98
1	B	212	PHE	N-CA-C	5.49	118.34	109.40
1	B	297	VAL	CB-CA-C	-5.44	102.51	110.62
1	B	756	SER	N-CA-C	5.40	118.29	109.59
1	A	659	ILE	CB-CA-C	-5.40	104.36	111.70
1	B	672	GLY	N-CA-C	5.39	119.39	110.55
1	B	771	ILE	CB-CA-C	-5.39	102.46	111.29
1	A	313	ALA	N-CA-C	-5.31	100.03	109.06
1	B	137	LEU	N-CA-C	-5.29	106.59	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	493	LEU	N-CA-C	5.27	117.83	109.24
1	A	58	ALA	N-CA-C	-5.26	105.72	111.82
1	B	48	PHE	N-CA-C	5.25	118.12	109.72
1	A	275	HIS	N-CA-C	5.23	117.89	111.82
1	A	502	ASP	N-CA-C	5.22	117.91	107.62
1	A	208	TYR	CA-CB-CG	5.21	123.28	113.90
1	B	183	ASN	N-CA-C	5.17	119.68	112.90
1	B	51	PRO	O-C-N	5.17	123.58	121.15
1	A	529	LEU	CA-C-N	-5.14	117.65	121.61
1	A	529	LEU	C-N-CA	-5.14	117.65	121.61
1	A	660	THR	CB-CA-C	5.13	115.77	109.16
1	B	106	VAL	CB-CA-C	-5.12	104.64	110.73
1	A	176	ASN	N-CA-C	-5.11	105.72	111.28
1	B	227	ARG	N-CA-C	5.10	119.19	112.92
1	A	514	ASP	CB-CA-C	5.09	118.44	110.19
1	A	417	ASP	N-CA-C	5.06	117.69	109.24
1	B	744	VAL	N-CA-C	5.05	115.75	108.48
1	B	155	ALA	N-CA-C	5.04	116.47	110.97
1	B	208	TYR	CA-CB-CG	5.03	122.95	113.90
1	A	248	VAL	CB-CA-C	5.02	117.52	110.99

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	DSN	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	698	ASP	Peptide
2	C	4	DAB	Mainchain,Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6114	0	5788	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5994	0	5675	158	0
2	C	57	0	40	9	0
3	A	72	0	114	6	0
4	A	30	0	0	2	0
4	B	20	0	0	2	0
5	C	26	0	14	0	0
6	C	1	0	0	0	0
All	All	12314	0	11631	310	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 13.

All (310) 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	1.52	1.07
2:C:6:GLN:O	2:C:6:GLN:HG3	1.20	0.99
2:C:6:GLN:O	2:C:6:GLN:CG	2.11	0.98
1:B:446:GLN:HE22	2:C:6:GLN:HG2	1.31	0.95
1:A:742:GLN:HG3	1:A:793:ILE:O	1.67	0.94
1:B:446:GLN:NE2	2:C:6:GLN:HG2	1.86	0.91
1:B:694:LYS:HE3	1:B:708:GLU:OE1	1.77	0.84
1:B:772:THR:HG22	1:B:775:LEU:H	1.42	0.84
1:A:777:ALA:HB1	3:A:1817[B]:N8E:H191	1.60	0.81
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.17	0.80
1:A:556:VAL:HG13	1:A:563:ILE:HB	1.64	0.79
1:A:700:SER:OG	1:A:702:LYS:HG2	1.83	0.78
1:A:722:LYS:HG3	1:A:723:GLY:H	1.45	0.78
1:A:772:THR:HG22	1:A:774:LYS:H	1.46	0.78
1:A:792:ASN:HB3	1:A:800:SER:HB2	1.64	0.78
1:B:772:THR:HG22	1:B:774:LYS:H	1.50	0.77
2:C:4:DAB:HB2	2:C:5:FHO:HG1C	1.67	0.76
1:B:743:MET:HE1	1:B:754:LYS:HD2	1.65	0.76
1:A:254:GLY:CA	1:A:592:ILE:HG13	2.17	0.75
1:B:418:HIS:HD2	1:B:455:ASN:HD21	1.32	0.74
3:A:1817[B]:N8E:H031	1:B:805:ARG:HD2	1.70	0.74
1:B:772:THR:CG2	1:B:774:LYS:H	2.00	0.74
1:A:470:ARG:NH1	1:A:538:ASN:OD1	2.20	0.74
1:A:805:ARG:HD2	3:A:1817[A]:N8E:H031	1.70	0.73
1:A:777:ALA:HB1	3:A:1817[B]:N8E:C19	2.19	0.73
1:B:418:HIS:CD2	1:B:455:ASN:HD21	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASP:OD2	1:A:292:ARG:NH2	2.21	0.72
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.70	0.72
1:B:363:SER:OG	1:B:431:MET:HE1	1.89	0.72
1:B:363:SER:OG	1:B:431:MET:CE	2.38	0.72
1:B:764:ASP:HB3	1:B:782:ASN:HA	1.73	0.71
1:B:744:VAL:HG21	1:B:755:PHE:CE1	2.27	0.70
1:B:744:VAL:CG2	1:B:755:PHE:CE1	2.75	0.69
1:B:430:ILE:HG12	1:B:443:ILE:CD1	2.24	0.67
1:A:554:TYR:CD2	1:A:595:PRO:HG2	2.30	0.67
1:A:214:ILE:HG12	1:A:264:ALA:HB3	1.76	0.66
1:B:380:ARG:HD3	1:B:788:THR:HB	1.77	0.66
1:A:151:THR:O	1:A:152:ILE:HD13	1.96	0.66
1:A:615:ASN:HD21	1:A:617:GLU:HB2	1.61	0.66
1:B:540:THR:HG22	1:B:541:ASP:N	2.11	0.65
1:B:239:ASP:OD2	1:B:292:ARG:NH2	2.29	0.65
1:A:809:PHE:CD1	1:B:771:ILE:HG12	2.32	0.65
1:B:152:ILE:HD12	1:B:169:ILE:HG12	1.77	0.64
1:B:542:ASP:O	1:B:577:TYR:HA	1.96	0.64
1:A:254:GLY:HA2	1:A:592:ILE:HG13	1.79	0.64
1:B:696:ILE:HG23	1:B:704:VAL:HG12	1.79	0.64
1:B:341:ASN:HB2	1:B:342:PRO:CD	2.28	0.63
1:A:109:GLN:OE1	1:A:114:THR:CG2	2.46	0.63
1:B:270:ARG:NH1	1:B:351:ASP:OD2	2.32	0.62
1:A:136:GLN:HE22	1:A:462:THR:HG21	1.64	0.62
1:B:268:LEU:N	1:B:268:LEU:HD12	2.15	0.62
1:B:245:ARG:NH1	1:B:269:ILE:HG13	2.14	0.62
1:B:772:THR:HG22	1:B:775:LEU:N	2.11	0.62
1:B:772:THR:HG22	1:B:774:LYS:N	2.14	0.62
1:B:744:VAL:CG2	1:B:755:PHE:HE1	2.13	0.62
1:A:109:GLN:OE1	1:A:114:THR:HG22	1.99	0.61
1:A:721:PHE:O	1:A:726:ASP:HA	2.00	0.61
1:B:347:THR:HB	1:B:401:ASN:HB2	1.82	0.61
1:A:157:ARG:HB3	1:A:475:VAL:HG11	1.82	0.61
1:A:410:TRP:HE3	1:A:461:LEU:HD23	1.66	0.61
1:A:410:TRP:CD2	1:A:463:GLY:HA3	2.37	0.60
1:A:694:LYS:HE3	1:A:708:GLU:OE1	2.02	0.60
1:A:239:ASP:CG	1:A:292:ARG:HH22	2.09	0.60
1:A:410:TRP:CE2	1:A:463:GLY:HA3	2.36	0.60
1:B:681:LEU:HD13	1:B:687:VAL:HG22	1.84	0.60
1:A:325:TYR:OH	1:A:327:ARG:NH1	2.35	0.59
1:B:417:ASP:O	1:B:455:ASN:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ASN:OD1	1:B:504:ILE:HG13	2.02	0.59
1:B:646:GLU:O	1:B:662:ALA:O	2.20	0.59
1:A:447:LYS:HB3	1:A:490:TYR:HB2	1.84	0.58
1:A:670:THR:OG1	1:A:696:ILE:HD12	2.04	0.58
1:A:411:VAL:HG13	1:A:462:THR:HG22	1.85	0.58
1:A:199:ALA:HA	1:A:205:ASN:HD22	1.69	0.58
1:A:722:LYS:HG3	1:A:723:GLY:N	2.17	0.58
1:A:371:SER:OG	1:A:436:ALA:HA	2.03	0.57
1:A:525:LYS:HB2	1:A:557:THR:HG22	1.87	0.57
1:B:736:TRP:HB2	1:B:761:TRP:CE3	2.39	0.57
1:A:312:VAL:HG13	1:A:333:TYR:HB3	1.87	0.57
1:A:218:GLN:HG2	1:A:223:PRO:HA	1.86	0.57
1:B:363:SER:HB3	2:C:8:FHO:HZ	1.86	0.57
1:A:123:SER:O	1:A:124:SER:HB3	2.06	0.56
1:B:587:ALA:HB2	1:B:618:ILE:HG13	1.87	0.56
1:B:744:VAL:HG22	1:B:755:PHE:CD1	2.40	0.56
1:A:392:GLU:HG3	1:A:424:HIS:HB3	1.87	0.56
1:A:188:VAL:HG11	1:A:246:VAL:HG13	1.87	0.55
1:A:646:GLU:O	1:A:662:ALA:O	2.23	0.55
1:B:472:HIS:HD2	1:B:538:ASN:H	1.54	0.55
1:A:46:VAL:HG12	1:A:47:GLU:N	2.21	0.55
1:B:139:THR:OG1	1:B:150:GLY:HA3	2.07	0.55
1:B:707:TRP:HB2	1:B:742:GLN:HE21	1.72	0.55
1:A:53:GLN:OE1	1:A:57:SER:HB3	2.07	0.55
1:A:766:MET:SD	1:A:766:MET:C	2.90	0.54
1:B:199:ALA:HA	1:B:205:ASN:HD22	1.72	0.54
1:B:772:THR:HG23	1:B:773:ASP:N	2.22	0.54
1:A:694:LYS:C	1:A:694:LYS:CD	2.80	0.54
1:B:418:HIS:HD2	1:B:455:ASN:ND2	2.04	0.54
1:B:430:ILE:HG12	1:B:443:ILE:HD11	1.89	0.54
1:A:615:ASN:ND2	1:A:617:GLU:HB2	2.21	0.54
1:A:470:ARG:HD3	1:A:538:ASN:O	2.08	0.54
1:A:809:PHE:HB3	3:A:1817[B]:N8E:H231	1.89	0.54
1:A:343:ASP:HB2	1:A:405:ASN:HB2	1.89	0.53
1:A:174:ARG:CZ	1:A:177:MET:HE2	2.37	0.53
1:A:517:THR:O	1:A:518:PRO:C	2.48	0.53
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.43	0.53
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.44	0.53
1:B:375:ARG:NE	1:B:755:PHE:CE2	2.77	0.53
1:A:506:TRP:CZ2	1:A:508:GLY:HA2	2.44	0.53
1:A:447:LYS:NZ	4:A:1818:PO4:O3	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:THR:HG22	1:B:797:THR:O	2.10	0.52
1:B:637:GLU:HA	1:B:670:THR:O	2.09	0.52
2:C:4:DAB:O	2:C:7:DGN:HG3	2.09	0.52
1:B:74:PRO:HG3	1:B:303:GLU:CG	2.40	0.52
1:A:203:ASP:OD1	1:A:325:TYR:OH	2.27	0.52
1:A:611:ASP:OD1	1:A:640:GLU:OE2	2.28	0.52
1:B:165:THR:O	1:B:621:LYS:NZ	2.43	0.52
1:B:772:THR:CG2	1:B:773:ASP:N	2.72	0.52
1:A:580:ASN:HD22	1:A:582:THR:H	1.58	0.52
1:B:276:GLU:H	1:B:276:GLU:CD	2.18	0.52
1:B:646:GLU:HG3	1:B:651:ASN:HD22	1.73	0.52
1:A:174:ARG:CZ	1:A:177:MET:CE	2.88	0.52
1:B:174:ARG:CZ	1:B:177:MET:HE2	2.39	0.52
1:A:484:HIS:CE1	1:A:486:GLU:OE2	2.63	0.51
1:A:92:ASN:HA	1:A:95:ILE:HG22	1.92	0.51
1:B:728:LEU:HD12	1:B:729:THR:N	2.26	0.51
1:B:177:MET:HE3	1:B:240:MET:HB3	1.92	0.51
1:B:201:ASP:O	1:B:203:ASP:N	2.44	0.51
1:A:53:GLN:OE1	1:A:57:SER:CB	2.59	0.51
1:A:260:GLY:HA2	1:A:594:MET:HE2	1.92	0.51
1:A:694:LYS:HD2	1:A:694:LYS:O	2.10	0.51
1:A:262:LEU:HD23	1:A:592:ILE:HG22	1.92	0.51
1:A:656:ASN:HB3	1:A:659:ILE:HD12	1.92	0.51
1:A:380:ARG:HA	1:A:801:TYR:CD2	2.47	0.50
1:B:74:PRO:HG3	1:B:303:GLU:HG2	1.93	0.50
1:B:570:ILE:HG23	1:B:591:ASP:HB3	1.92	0.50
1:B:494:ARG:O	1:B:495:ASN:C	2.53	0.50
1:A:391:TRP:HB2	1:A:427:LEU:HD21	1.92	0.50
1:A:725:LEU:HD23	1:A:725:LEU:H	1.75	0.50
1:B:156:THR:O	1:B:157:ARG:HB2	2.10	0.50
1:B:52:PRO:HD3	1:B:84:ALA:HB2	1.93	0.50
1:A:276:GLU:OE2	1:A:278:LYS:HD3	2.12	0.49
1:A:228:ASN:O	1:A:232:SER:HB2	2.12	0.49
1:B:184:ASN:O	1:B:187:ASP:HB2	2.12	0.49
1:B:363:SER:OG	1:B:431:MET:HE2	2.11	0.49
1:A:69:GLN:HE21	1:A:133:THR:CG2	2.25	0.49
1:B:239:ASP:CG	1:B:292:ARG:HH22	2.21	0.49
1:A:542:ASP:HB3	1:A:578:ASP:HB2	1.94	0.49
1:A:249:LEU:O	1:A:264:ALA:HA	2.13	0.49
1:B:418:HIS:HE1	4:B:1819:PO4:O1	1.95	0.49
1:B:50:ILE:HG12	1:B:61:GLU:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:LYS:O	1:B:556:VAL:HA	2.13	0.48
1:B:590:THR:OG1	1:B:615:ASN:HB3	2.13	0.48
1:B:744:VAL:CG2	1:B:755:PHE:CD1	2.96	0.48
1:A:204:ARG:NH1	1:A:229:VAL:HG12	2.28	0.48
1:B:537:PHE:O	1:B:544:ASN:HA	2.13	0.48
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.48	0.48
1:B:208:TYR:HA	1:B:212:PHE:O	2.14	0.48
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.94	0.48
1:B:653:LYS:HA	1:B:654:PRO:HD2	1.52	0.48
1:A:443:ILE:HD13	1:A:443:ILE:N	2.28	0.48
1:A:725:LEU:HD23	1:A:725:LEU:N	2.28	0.48
1:A:222:ILE:HD11	1:A:415:GLN:NE2	2.29	0.48
1:B:691:TYR:CD1	1:B:691:TYR:C	2.92	0.48
1:B:744:VAL:HG22	1:B:755:PHE:CE1	2.49	0.48
1:B:185:ILE:N	1:B:240:MET:HE3	2.29	0.48
1:B:271:LYS:HD3	1:B:310:ARG:NH2	2.29	0.48
1:A:291:TYR:OH	1:B:772:THR:HG21	2.13	0.48
1:B:762:LEU:HD21	1:B:789:TYR:CE1	2.49	0.48
1:B:439:ASN:ND2	1:B:502:ASP:HA	2.29	0.48
1:B:638:ILE:O	1:B:669:LYS:HA	2.14	0.48
1:A:245:ARG:NH1	1:A:247:GLU:OE1	2.42	0.47
1:A:216:ASN:HB2	1:A:265:THR:HA	1.96	0.47
1:B:601:ARG:NH1	1:B:605:ASN:O	2.46	0.47
1:A:188:VAL:HG11	1:A:246:VAL:CG1	2.44	0.47
1:A:59:LEU:HD22	1:A:70:VAL:HG11	1.96	0.47
1:A:380:ARG:HD3	1:A:788:THR:HB	1.95	0.47
1:B:563:ILE:HG12	1:B:607:LEU:HD22	1.96	0.47
1:B:706:THR:OG1	1:B:741:TRP:O	2.31	0.47
1:A:277:PHE:CD2	1:A:277:PHE:C	2.92	0.47
1:B:646:GLU:HG3	1:B:651:ASN:ND2	2.30	0.47
1:B:470:ARG:NH2	1:B:541:ASP:OD1	2.47	0.47
1:B:743:MET:HE1	1:B:754:LYS:CD	2.40	0.47
1:A:204:ARG:HG3	1:A:391:TRP:CH2	2.50	0.47
1:B:276:GLU:N	1:B:276:GLU:OE1	2.47	0.47
1:B:371:SER:OG	1:B:436:ALA:HA	2.15	0.47
1:A:638:ILE:HB	1:A:670:THR:HB	1.97	0.46
1:A:408:ASN:HB3	1:A:410:TRP:H	1.80	0.46
1:A:446:GLN:OE1	1:A:448:TYR:OH	2.17	0.46
1:A:73:ARG:HA	1:A:74:PRO:HD2	1.82	0.46
1:B:540:THR:CG2	1:B:541:ASP:N	2.77	0.46
1:B:262:LEU:HD23	1:B:592:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:GLN:OE1	1:B:641:GLU:OE2	2.33	0.46
1:B:721:PHE:HB2	1:B:725:LEU:O	2.16	0.46
1:B:176:ASN:C	1:B:176:ASN:HD22	2.24	0.46
1:A:75:GLU:HB2	1:A:78:ARG:NH2	2.31	0.46
1:A:199:ALA:O	1:A:792:ASN:HB2	2.15	0.46
1:A:694:LYS:NZ	1:A:708:GLU:O	2.49	0.46
1:B:646:GLU:O	1:B:647:ASP:HB3	2.16	0.46
1:B:204:ARG:HD3	1:B:391:TRP:CH2	2.50	0.46
1:B:233:ALA:CB	1:B:421:ASN:HB3	2.46	0.46
1:B:614:GLN:NE2	1:B:641:GLU:OE2	2.47	0.46
1:A:694:LYS:HZ1	1:A:708:GLU:HB3	1.81	0.45
1:B:694:LYS:HE3	1:B:708:GLU:CD	2.39	0.45
1:A:689:ALA:HA	1:A:714:SER:O	2.16	0.45
1:B:54:ALA:O	1:B:55:LEU:C	2.58	0.45
1:B:669:LYS:O	1:B:696:ILE:HA	2.16	0.45
1:B:446:GLN:HE22	2:C:6:GLN:CG	2.15	0.45
1:A:464:PRO:HA	1:A:472:HIS:O	2.17	0.45
1:B:324:HIS:CE1	1:B:383:ASN:HB3	2.51	0.45
1:A:98:LEU:C	1:A:98:LEU:HD23	2.42	0.45
1:B:390:SER:O	1:B:425:ALA:HA	2.17	0.45
1:B:634:ALA:O	1:B:673:TYR:HA	2.16	0.45
1:A:158:LEU:HD21	1:A:475:VAL:HG22	1.98	0.45
1:B:438:ASP:OD1	1:B:438:ASP:N	2.50	0.45
1:A:362:TRP:HE3	1:A:363:SER:HB3	1.82	0.45
1:B:527:ARG:HH21	1:B:555:ARG:HD3	1.82	0.45
1:B:689:ALA:HA	1:B:714:SER:O	2.16	0.45
1:B:410:TRP:CD1	1:B:464:PRO:HD2	2.52	0.45
1:A:699:ASP:C	1:A:701:GLY:H	2.24	0.44
1:B:540:THR:HG22	1:B:541:ASP:H	1.80	0.44
1:A:505:ASN:O	1:A:506:TRP:C	2.60	0.44
1:B:410:TRP:CD2	1:B:463:GLY:HA3	2.52	0.44
1:A:682:ALA:O	1:A:683:PRO:C	2.58	0.44
1:A:288:TRP:CZ2	1:A:321:PHE:HB3	2.51	0.44
1:A:805:ARG:HD2	3:A:1817[A]:N8E:C03	2.43	0.44
1:B:189:MET:HE2	1:B:189:MET:HA	1.99	0.44
1:B:681:LEU:HD13	1:B:687:VAL:CG2	2.46	0.44
1:A:215:ASN:O	1:A:226:ALA:HB3	2.18	0.44
1:A:142:GLU:HB2	1:A:174:ARG:HG2	2.00	0.44
1:A:188:VAL:O	1:A:192:THR:OG1	2.33	0.44
1:B:254:GLY:O	1:B:255:LEU:C	2.61	0.44
1:B:340:LEU:HD23	1:B:340:LEU:HA	1.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:ASP:OD1	1:A:698:ASP:C	2.60	0.44
1:B:50:ILE:HD12	1:B:85:ILE:HD11	2.00	0.44
1:A:46:VAL:CG1	1:A:47:GLU:N	2.81	0.44
1:B:62:PHE:CZ	1:B:95:ILE:HB	2.53	0.44
1:A:263:GLY:O	1:A:264:ALA:HB2	2.17	0.43
1:A:418:HIS:NE2	4:A:1821:PO4:O2	2.50	0.43
1:B:157:ARG:HD3	1:B:256:LEU:HD13	1.99	0.43
1:A:707:TRP:CH2	1:A:793:ILE:HG13	2.53	0.43
1:B:142:GLU:HG3	4:B:1818:PO4:O2	2.18	0.43
1:A:783:ASN:O	1:A:805:ARG:HG3	2.19	0.43
1:A:698:ASP:OD1	1:A:700:SER:N	2.52	0.43
1:B:401:ASN:HA	1:B:414:VAL:O	2.18	0.43
1:B:426:PRO:HB3	1:B:447:LYS:HG3	2.00	0.43
1:B:782:ASN:O	1:B:805:ARG:HA	2.17	0.43
1:A:273:PRO:HB3	1:A:309:GLY:C	2.44	0.43
1:B:388:TRP:CZ2	1:B:513:PRO:HD3	2.54	0.43
1:A:596:GLN:HE21	1:A:596:GLN:HB2	1.53	0.43
1:B:242:ILE:C	1:B:271:LYS:HG3	2.43	0.43
1:A:736:TRP:HB2	1:A:761:TRP:CE3	2.53	0.43
1:B:152:ILE:CD1	1:B:169:ILE:HG12	2.44	0.43
1:A:149:PRO:HB3	1:A:171:VAL:HG11	2.00	0.43
1:A:601:ARG:NH1	1:A:605:ASN:O	2.52	0.43
1:B:625:LEU:O	1:B:628:ARG:HD3	2.19	0.43
1:A:75:GLU:HB3	1:A:471:GLU:HG3	2.01	0.42
1:B:199:ALA:HA	1:B:205:ASN:ND2	2.34	0.42
1:A:716:TYR:HD1	1:A:733:GLY:HA3	1.76	0.42
1:B:485:TRP:CD1	1:B:485:TRP:C	2.95	0.42
1:A:50:ILE:HD12	1:A:85:ILE:HD11	2.01	0.42
1:A:496:TYR:CD1	1:A:513:PRO:HB3	2.54	0.42
1:B:273:PRO:HG3	1:B:335:ILE:HG23	2.01	0.42
1:A:262:LEU:CD2	1:A:592:ILE:HG22	2.50	0.42
1:B:201:ASP:O	1:B:202:THR:C	2.62	0.42
1:B:233:ALA:HB3	1:B:421:ASN:HB3	2.00	0.42
1:A:174:ARG:HB2	1:A:244:ASP:O	2.20	0.42
1:A:281:VAL:HG23	1:A:815:PHE:CZ	2.53	0.42
1:B:744:VAL:HG21	1:B:755:PHE:HE1	1.77	0.42
1:A:725:LEU:N	1:A:725:LEU:CD2	2.83	0.42
1:B:171:VAL:HG12	1:B:172:VAL:N	2.34	0.42
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.55	0.42
1:B:255:LEU:O	1:B:550:ARG:HD2	2.19	0.42
1:A:254:GLY:HA3	1:A:592:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TRP:CZ2	1:A:442:LYS:HB2	2.55	0.42
1:B:156:THR:O	1:B:157:ARG:CB	2.68	0.42
1:A:710:GLN:HE21	1:A:710:GLN:HB3	1.59	0.41
1:B:746:ASN:OD1	1:B:748:PRO:HD2	2.19	0.41
1:A:199:ALA:HA	1:A:205:ASN:ND2	2.35	0.41
1:B:273:PRO:HB2	1:B:308:ARG:HB3	2.01	0.41
1:A:646:GLU:O	1:A:647:ASP:CB	2.69	0.41
1:B:137:LEU:HB3	1:B:269:ILE:HD12	2.00	0.41
1:B:602:ASP:HA	1:B:663:TYR:O	2.21	0.41
1:A:359:GLY:HA2	1:A:386:ALA:O	2.20	0.41
1:A:720:LYS:HE3	1:A:726:ASP:O	2.21	0.41
1:B:163:ARG:NH1	1:B:623:GLU:HB3	2.35	0.41
1:A:746:ASN:OD1	1:A:746:ASN:C	2.64	0.41
1:A:201:ASP:HB3	1:A:362:TRP:O	2.21	0.41
1:A:219:TYR:CD1	1:A:219:TYR:N	2.88	0.41
1:B:170:THR:OG1	1:B:676:GLU:OE2	2.36	0.41
1:B:222:ILE:HA	1:B:223:PRO:HD2	1.88	0.41
1:B:268:LEU:HD12	1:B:268:LEU:H	1.86	0.41
2:C:3:DSN:C	2:C:7:DGN:OE1	2.69	0.41
1:B:482:PHE:CE2	1:B:527:ARG:HG3	2.56	0.41
1:A:521:TYR:CD1	1:A:521:TYR:N	2.89	0.40
1:B:391:TRP:CD1	1:B:393:GLN:HG2	2.56	0.40
1:B:396:ARG:HH11	1:B:396:ARG:HG2	1.86	0.40
1:A:244:ASP:O	1:A:245:ARG:HB3	2.21	0.40
1:A:274:THR:O	1:A:299:GLY:HA2	2.21	0.40
1:A:281:VAL:HG23	1:A:815:PHE:CE1	2.57	0.40
1:A:491:TRP:CE2	1:A:519:SER:HB3	2.56	0.40
1:A:645:GLU:HG3	1:A:666:ILE:HD11	2.02	0.40
1:A:694:LYS:C	1:A:694:LYS:HD2	2.46	0.40
1:B:99:LEU:O	1:B:102:THR:HG23	2.21	0.40
1:B:117:VAL:O	1:B:117:VAL:HG12	2.20	0.40
1:B:288:TRP:O	1:B:289:ASP:C	2.64	0.40
1:B:614:GLN:CD	1:B:614:GLN:N	2.79	0.40
1:B:764:ASP:HA	1:B:784:VAL:HG23	2.03	0.40
1:B:395:THR:O	1:B:396:ARG:HB3	2.21	0.40
1:A:772:THR:O	1:A:773:ASP:C	2.64	0.40
1:A:813:TRP:CD1	1:A:813:TRP:C	2.99	0.40
1:B:363:SER:HG	1:B:431:MET:CE	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	714 (93%)	46 (6%)	10 (1%)	9	31
1	B	750/772 (97%)	694 (92%)	48 (6%)	8 (1%)	11	36
2	C	1/7 (14%)	0	1 (100%)	0	100	100
All	All	1521/1551 (98%)	1408 (93%)	95 (6%)	18 (1%)	10	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	SER
1	A	227	ARG
1	A	646	GLU
1	B	408	ASN
1	A	603	SER
1	A	647	ASP
1	A	121	ALA
1	A	408	ASN
1	B	202	THR
1	B	786	ASP
1	A	739	LYS
1	B	363	SER
1	B	580	ASN
1	B	698	ASP
1	A	94	ALA
1	A	264	ALA
1	B	561	PRO
1	B	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%)	568 (87%)	82 (13%)	4	15
1	B	637/650 (98%)	552 (87%)	85 (13%)	4	14
2	C	1/1 (100%)	0	1 (100%)	0	0
All	All	1288/1301 (99%)	1120 (87%)	168 (13%)	4	14

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	68	ILE
1	A	71	LEU
1	A	79	ASN
1	A	83	SER
1	A	85	ILE
1	A	109	GLN
1	A	114	THR
1	A	132	ILE
1	A	133	THR
1	A	142	GLU
1	A	152	ILE
1	A	157	ARG
1	A	204	ARG
1	A	215	ASN
1	A	232	SER
1	A	236	THR
1	A	246	VAL
1	A	248	VAL
1	A	276	GLU
1	A	297	VAL
1	A	303	GLU
1	A	307	VAL
1	A	312	VAL
1	A	329	THR
1	A	331	VAL
1	A	348	VAL
1	A	358	LYS
1	A	372	GLN
1	A	378	VAL
1	A	392	GLU

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Mol	Chain	Res	Type
1	A	401	ASN
1	A	408	ASN
1	A	411	VAL
1	A	417	ASP
1	A	443	ILE
1	A	459	ILE
1	A	461	LEU
1	A	462	THR
1	A	466	GLN
1	A	470	ARG
1	A	475	VAL
1	A	489	SER
1	A	499	THR
1	A	504	ILE
1	A	524	ASP
1	A	528	GLN
1	A	531	SER
1	A	542	ASP
1	A	551	VAL
1	A	553	ASP
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	609	GLU
1	A	615	ASN
1	A	618	ILE
1	A	641	GLU
1	A	645	GLU
1	A	652	SER
1	A	659	ILE
1	A	660	THR
1	A	683	PRO
1	A	694	LYS
1	A	697	ARG
1	A	704	VAL
1	A	713	LEU
1	A	714	SER
1	A	720	LYS

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Mol	Chain	Res	Type
1	A	722	LYS
1	A	725	LEU
1	A	730	VAL
1	A	744	VAL
1	A	758	GLU
1	A	788	THR
1	A	792	ASN
1	A	810	SER
1	A	811	THR
1	B	57	SER
1	B	61	GLU
1	B	68	ILE
1	B	78	ARG
1	B	83	SER
1	B	86	LYS
1	B	96	THR
1	B	100	ARG
1	B	106	VAL
1	B	109	GLN
1	B	115	ILE
1	B	117	VAL
1	B	139	THR
1	B	140	ILE
1	B	148	THR
1	B	152	ILE
1	B	157	ARG
1	B	163	ARG
1	B	168	SER
1	B	176	ASN
1	B	195	ILE
1	B	227	ARG
1	B	229	VAL
1	B	232	SER
1	B	236	THR
1	B	265	THR
1	B	278	LYS
1	B	297	VAL
1	B	326	GLU
1	B	329	THR
1	B	331	VAL
1	B	396	ARG
1	B	411	VAL

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Mol	Chain	Res	Type
1	B	416	LEU
1	B	420	ILE
1	B	443	ILE
1	B	447	LYS
1	B	454	SER
1	B	459	ILE
1	B	475	VAL
1	B	476	VAL
1	B	478	THR
1	B	493	LEU
1	B	495	ASN
1	B	504	ILE
1	B	509	ASP
1	B	512	LYS
1	B	522	ILE
1	B	524	ASP
1	B	527	ARG
1	B	533	MET
1	B	551	VAL
1	B	556	VAL
1	B	562	THR
1	B	564	ARG
1	B	596	GLN
1	B	601	ARG
1	B	609	GLU
1	B	618	ILE
1	B	633	LEU
1	B	641	GLU
1	B	646	GLU
1	B	649	LEU
1	B	671	LYS
1	B	681	LEU
1	B	687	VAL
1	B	694	LYS
1	B	695	ILE
1	B	697	ARG
1	B	699	ASP
1	B	702	LYS
1	B	704	VAL
1	B	705	SER
1	B	720	LYS
1	B	730	VAL

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Mol	Chain	Res	Type
1	B	739	LYS
1	B	742	GLN
1	B	743	MET
1	B	771	ILE
1	B	772	THR
1	B	775	LEU
1	B	778	SER
1	B	788	THR
1	B	792	ASN
1	B	815	PHE
2	C	6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	176	ASN
1	A	183	ASN
1	A	205	ASN
1	A	218	GLN
1	A	372	GLN
1	A	408	ASN
1	A	415	GLN
1	A	466	GLN
1	A	492	ASN
1	A	505	ASN
1	A	528	GLN
1	A	580	ASN
1	A	596	GLN
1	A	614	GLN
1	A	615	ASN
1	A	710	GLN
1	A	737	GLN
1	B	176	ASN
1	B	183	ASN
1	B	191	HIS
1	B	205	ASN
1	B	228	ASN
1	B	418	HIS
1	B	455	ASN
1	B	472	HIS
1	B	492	ASN

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Mol	Chain	Res	Type
1	B	520	GLN
1	B	544	ASN
1	B	596	GLN
1	B	614	GLN
1	B	615	ASN
1	B	642	ASN
1	B	710	GLN
1	B	742	GLN
1	B	747	ASN
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 ⓘ

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	FHO	C	8	6,2	9,10,11	5.37	2 (22%)	4,11,13	1.41	0
2	FHO	C	5	6,2	9,10,11	4.93	3 (33%)	4,11,13	2.02	1 (25%)
2	DAB	C	4	2	5,6,7	0.49	0	1,6,8	1.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FHO	C	8	6,2	-	3/7/10/12	-
2	FHO	C	5	6,2	-	2/7/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DSN	C	3	5,2	1/1/1/2	-	-
2	DAB	C	4	2	-	0/4/5/7	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	8	FHO	OZ-NE	-15.38	1.21	1.39
2	C	5	FHO	OZ-NE	-13.74	1.23	1.39
2	C	5	FHO	CZ-NE	-4.89	1.27	1.34
2	C	8	FHO	CZ-NE	-4.48	1.27	1.34
2	C	5	FHO	CA-N	2.21	1.54	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	FHO	OZ-NE-CD	3.70	122.37	113.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	DSN	CA

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	FHO	CG-CD-NE-OZ
2	C	5	FHO	CG-CD-NE-CZ
2	C	8	FHO	N-CA-CB-CG
2	C	8	FHO	CG-CD-NE-OZ
2	C	8	FHO	CA-CB-CG-CD

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	8	FHO	1	0
2	C	5	FHO	1	0
2	C	3	DSN	1	0
2	C	4	DAB	2	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
3	N8E	A	1817[A]	-	23,23,23	0.72	0	22,22,22	0.73	0
4	PO4	A	1819	-	4,4,4	1.19	0	6,6,6	0.99	0
4	PO4	B	1818	-	4,4,4	0.86	0	6,6,6	0.97	0
4	PO4	A	1823	-	4,4,4	1.17	0	6,6,6	1.19	1 (16%)
4	PO4	A	1818	-	4,4,4	0.73	0	6,6,6	1.58	2 (33%)
4	PO4	A	1822	-	4,4,4	1.08	0	6,6,6	0.54	0
4	PO4	A	1821	-	4,4,4	0.97	0	6,6,6	0.88	0
4	PO4	B	1816	-	4,4,4	0.61	0	6,6,6	1.16	1 (16%)
4	PO4	B	1817	-	4,4,4	0.68	0	6,6,6	0.86	0
3	N8E	A	1817[B]	-	23,23,23	0.86	0	22,22,22	0.97	1 (4%)
3	N8E	A	1816	-	23,23,23	0.55	0	22,22,22	0.41	0
4	PO4	B	1819	-	4,4,4	0.95	0	6,6,6	0.76	0
4	PO4	A	1820	-	4,4,4	1.30	0	6,6,6	0.99	0
5	PVE	C	1	6,2	26,28,29	1.86	5 (19%)	30,40,42	1.28	3 (10%)

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	1817[A]	-	-	11/21/21/21	-
3	N8E	A	1817[B]	-	-	14/21/21/21	-
3	N8E	A	1816	-	-	9/21/21/21	-
5	PVE	C	1	6,2	-	6/10/21/23	0/2/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	PVE	C20-C18	-5.34	1.40	1.51
5	C	1	PVE	C5-C6	5.02	1.42	1.37
5	C	1	PVE	C8-C7	3.44	1.40	1.37
5	C	1	PVE	C9-N1	-2.87	1.36	1.39
5	C	1	PVE	C4-C3	2.21	1.41	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	PVE	C21-C20-C18	-3.76	104.93	112.67
3	A	1817[B]	N8E	O18-C19-C20	3.05	124.27	110.35
5	C	1	PVE	C15-C14-N1	-2.79	107.86	111.53
4	A	1818	PO4	O4-P-O2	2.26	114.94	107.91
4	A	1818	PO4	O4-P-O1	-2.25	103.01	110.95
4	B	1816	PO4	O3-P-O1	-2.16	103.32	110.95
4	A	1823	PO4	O4-P-O2	-2.05	101.52	107.91
5	C	1	PVE	C3-C2-N11	-2.05	117.62	122.87

There are no chirality outliers.

All (40) torsion outliers are listed below:

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

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

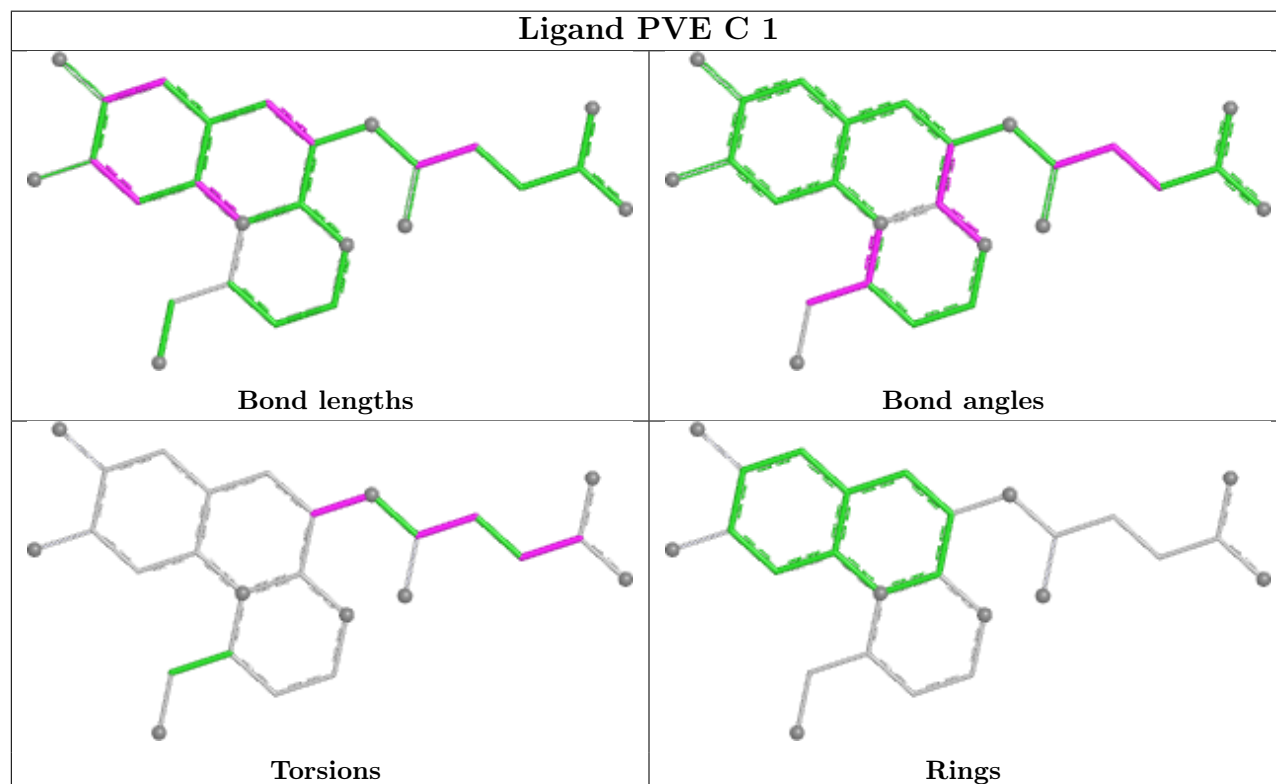
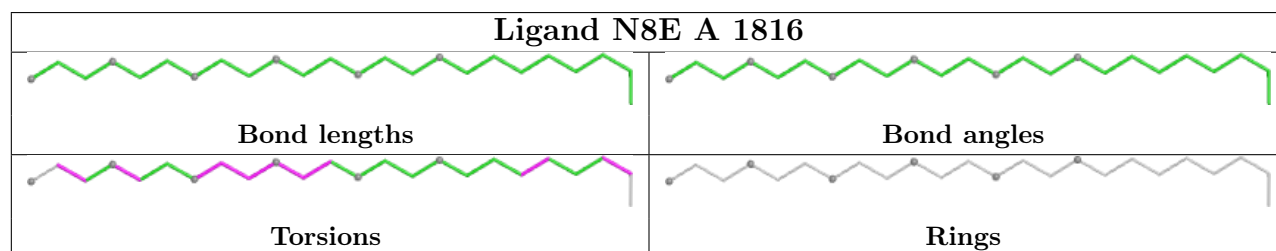
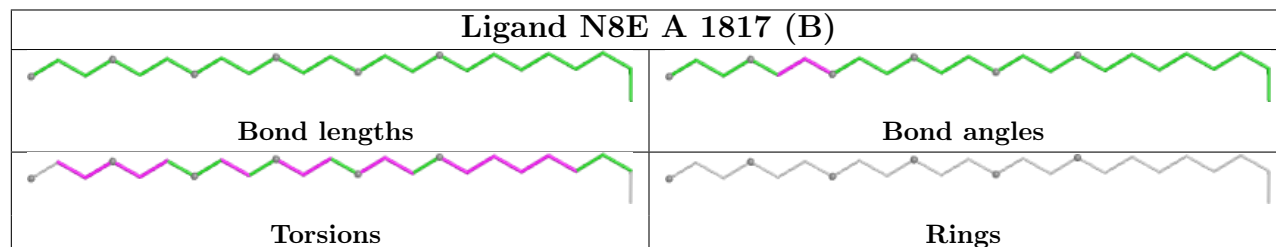
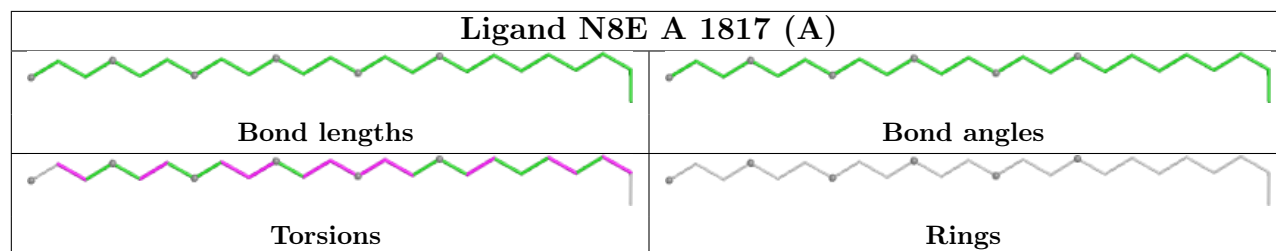
There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1817[A]	N8E	2	0
4	B	1818	PO4	1	0
4	A	1818	PO4	1	0
4	A	1821	PO4	1	0
3	A	1817[B]	N8E	4	0
4	B	1819	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	772/772 (100%)	-0.22	12 (1%) 70 61	12, 26, 41, 62	0
1	B	754/772 (97%)	0.05	18 (2%) 59 49	19, 34, 54, 65	0
2	C	2/7 (28%)	0.87	0 100 100	50, 50, 50, 56	0
All	All	1528/1551 (98%)	-0.09	30 (1%) 65 56	12, 29, 49, 65	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	ARG	4.9
1	B	110	GLY	4.5
1	B	407	ALA	3.7
1	A	79	ASN	3.3
1	A	407	ALA	3.1
1	B	44	GLN	3.1
1	A	44	GLN	2.8
1	A	276	GLU	2.8
1	A	123	SER	2.8
1	B	649	LEU	2.8
1	B	469	GLY	2.7
1	A	645	GLU	2.7
1	B	533	MET	2.6
1	A	566	SER	2.5
1	A	362	TRP	2.5
1	B	468	LEU	2.5
1	B	227	ARG	2.5
1	A	121	ALA	2.5
1	B	137	LEU	2.3
1	B	409	GLY	2.3
1	B	226	ALA	2.2
1	A	599	TRP	2.2
1	B	136	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	122	ASP	2.2
1	B	635	TYR	2.2
1	B	538	ASN	2.1
1	B	45	GLU	2.1
1	A	652	SER	2.0
1	B	401	ASN	2.0
1	B	467	PHE	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	DGN	C	7	9/10	0.79	0.17	49,53,54,54	0
2	DSN	C	3	5/7	0.80	0.14	57,57,58,58	0
2	DAB	C	4	7/8	0.87	0.14	56,57,58,58	0
2	FHO	C	5	11/12	0.93	0.11	47,50,55,56	0
2	FHO	C	8	11/12	0.93	0.10	41,44,50,52	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	0.84	0.20	2,6,16,17	24
3	N8E	A	1817[B]	24/24	0.84	0.20	2,7,12,13	24
5	PVE	C	1	26/27	0.88	0.12	44,48,60,63	5
3	N8E	A	1816	24/24	0.89	0.17	47,57,75,76	0
4	PO4	B	1816	5/5	0.90	0.18	58,58,58,59	0
4	PO4	A	1821	5/5	0.93	0.14	53,53,53,55	0

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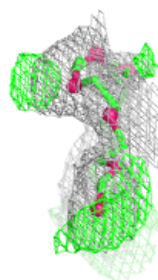
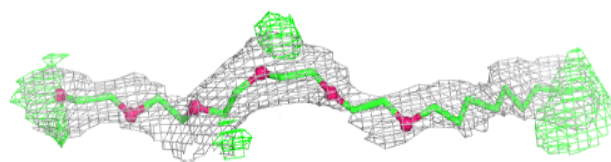
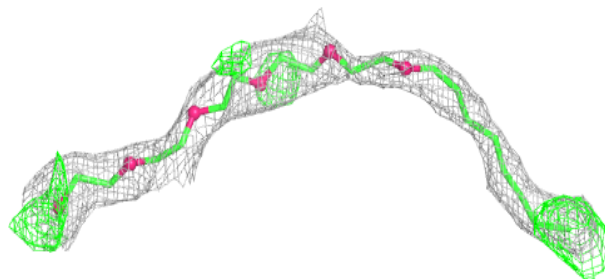
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	B	1819	5/5	0.94	0.14	46,46,50,51	0
4	PO4	B	1818	5/5	0.94	0.14	50,51,54,54	0
4	PO4	A	1823	5/5	0.95	0.13	54,55,55,56	0
4	PO4	B	1817	5/5	0.96	0.13	27,27,29,29	0
4	PO4	A	1822	5/5	0.96	0.12	57,59,60,61	0
4	PO4	A	1820	5/5	0.98	0.09	36,38,39,39	0
4	PO4	A	1818	5/5	0.98	0.12	33,34,34,34	0
4	PO4	A	1819	5/5	0.98	0.10	24,25,29,30	0
6	FE	C	2	1/1	1.00	0.07	44,44,44,44	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.

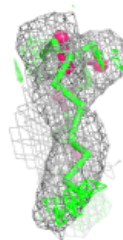
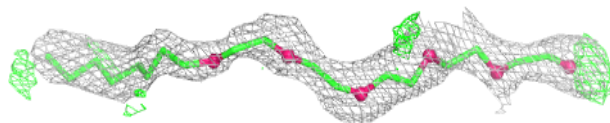
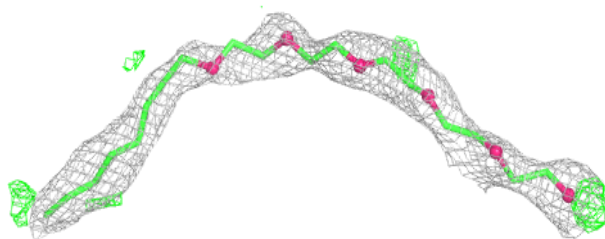
Electron density around N8E A 1817 (A):

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

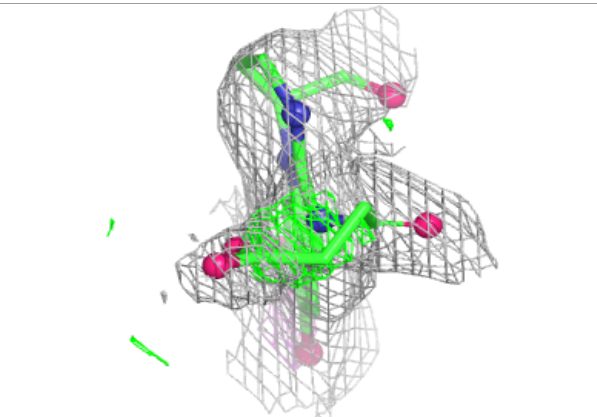
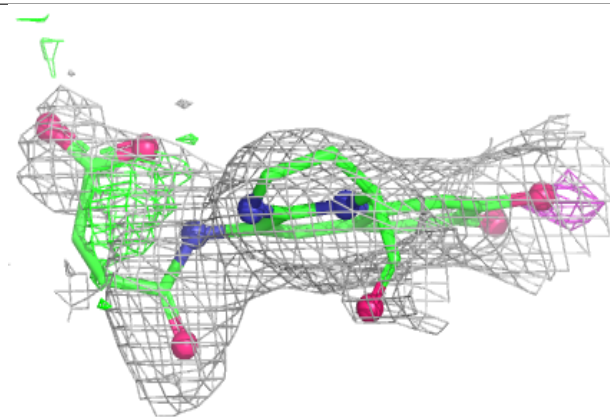
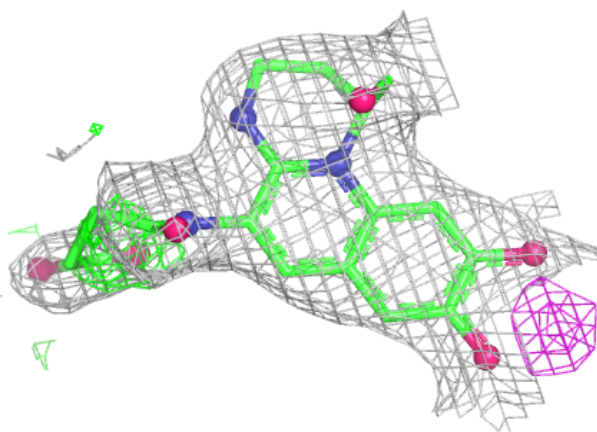


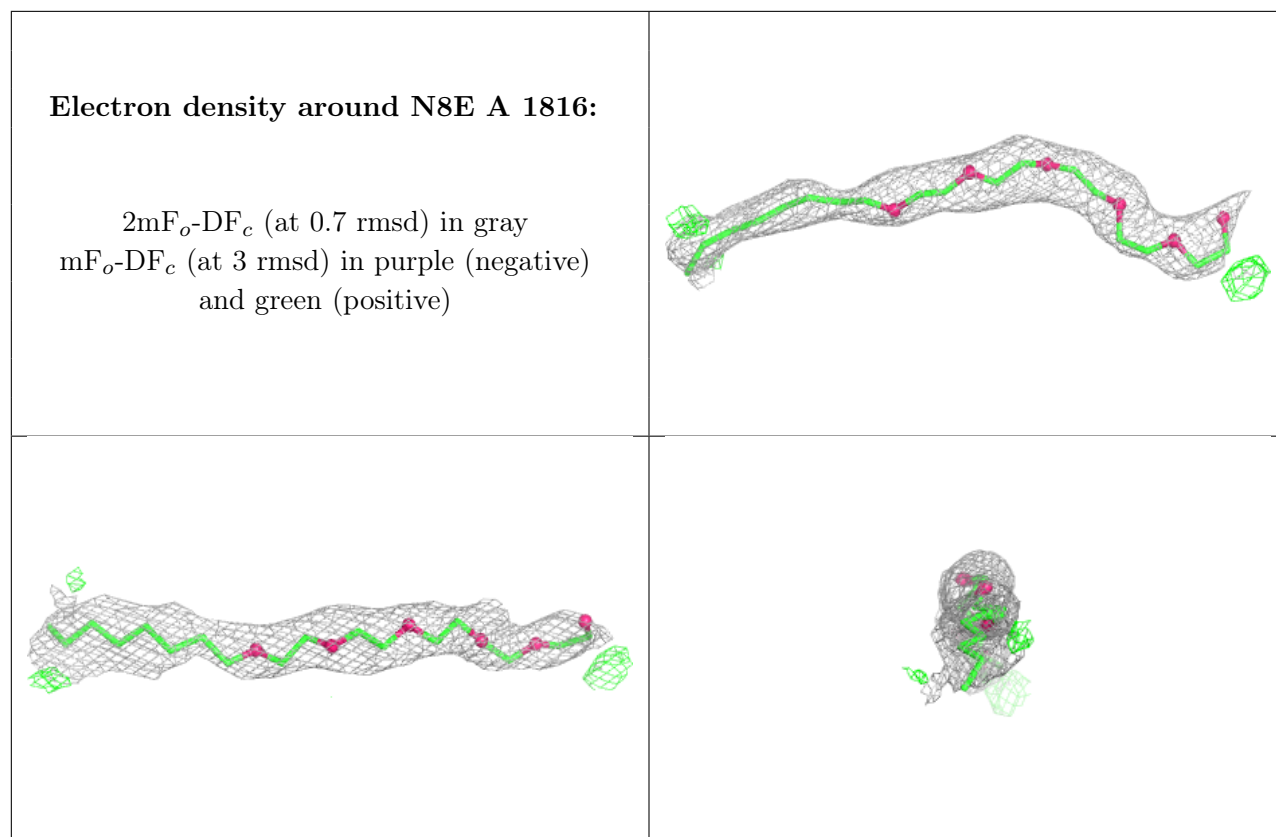
Electron density around N8E A 1817 (B):

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.