



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:19 pm BST

PDB ID : 2W78
Title : Structures of *P. aeruginosa* FpvA bound to heterologous pyoverdines: FpvA-Pvd(ATCC13535)-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 : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

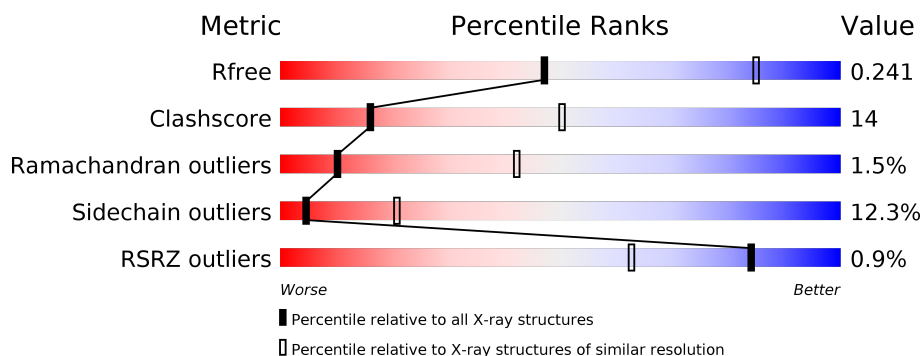
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	<div> <div style="width: 66%;"></div> <div style="width: 28%;"></div> <div style="width: 5%;"></div> </div>
1	B	772	<div> <div style="width: 2%;"></div> <div style="width: 64%;"></div> <div style="width: 29%;"></div> <div style="width: 5%;"></div> </div>
2	C	7	<div> <div style="width: 29%;"></div> <div style="width: 57%;"></div> <div style="width: 14%;"></div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12313 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.

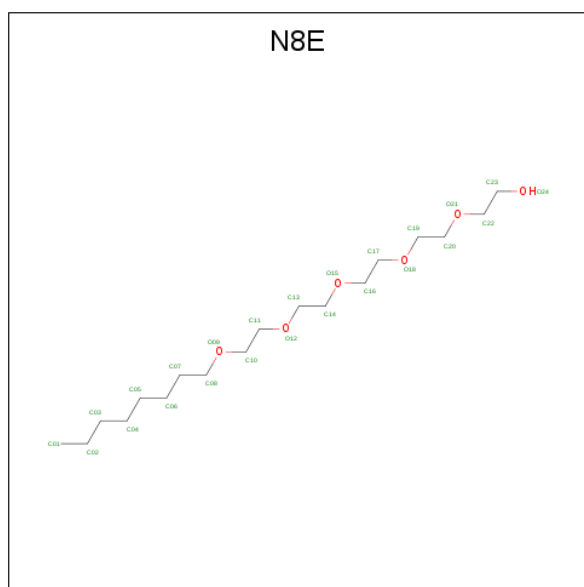
- Molecule 1 is a protein called FERRIPYOVERDINE RECEPTOR.

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 SER-LYS-GLY-FHO-LYS-FH7-SER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			56	32	11	13			

- Molecule 3 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (three-letter code: N8E) (formula: $C_{18}H_{38}O_6$).



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

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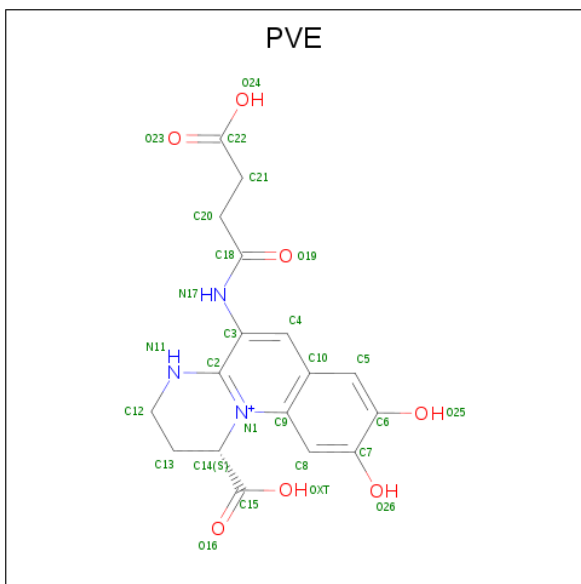
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			48	36	12		

- Molecule 4 is PHOSPHATE ION (three-letter code: 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-CARBOXYPROANOYL)AMINO]-8,9-DIHYDROXY-1,2,3,4-TETRAHYDROPYRIMIDO[1,2-A]QUINOLIN-11-IUM (three-letter code: PVE) (formula: C₁₇H₁₈N₃O₇).



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

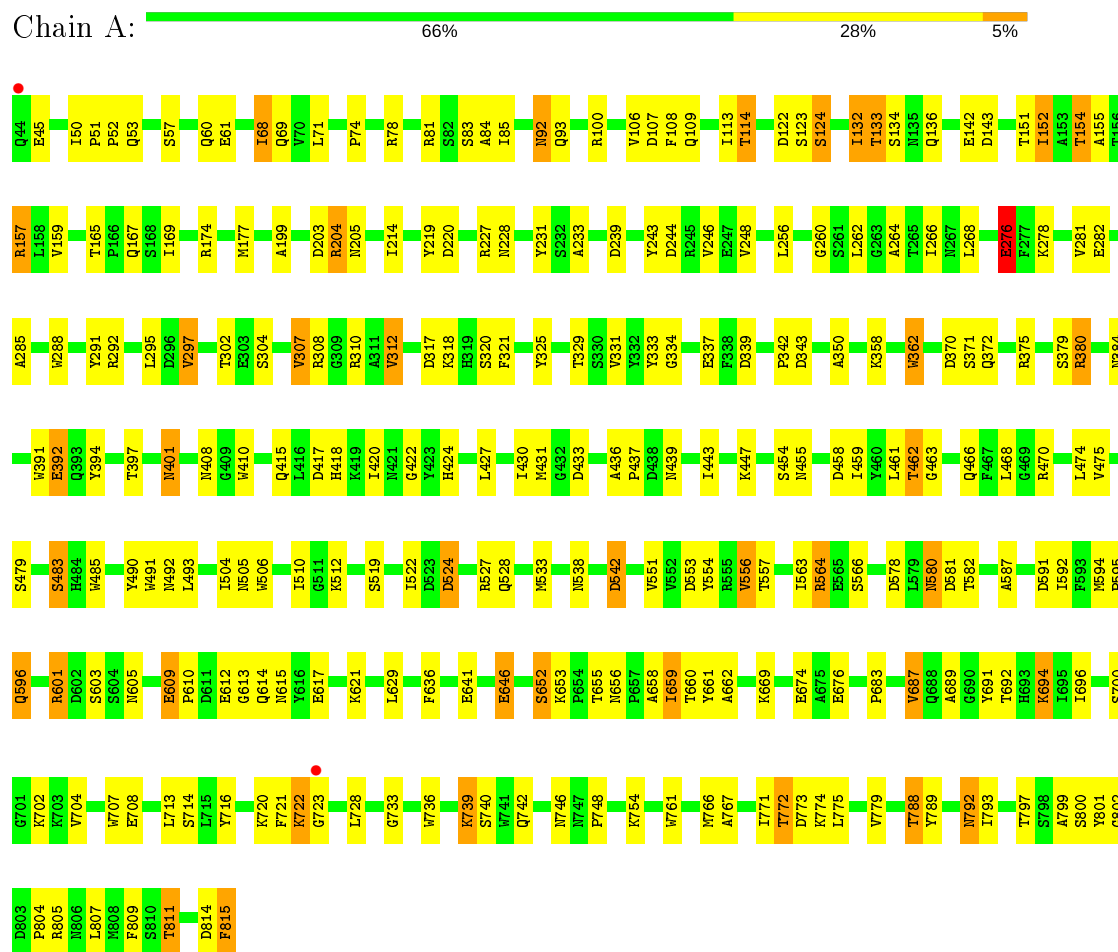
- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

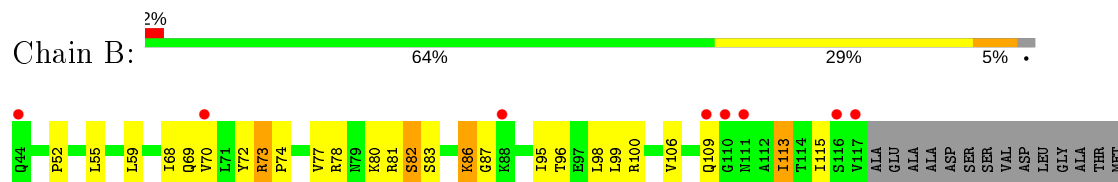
3 Residue-property plots

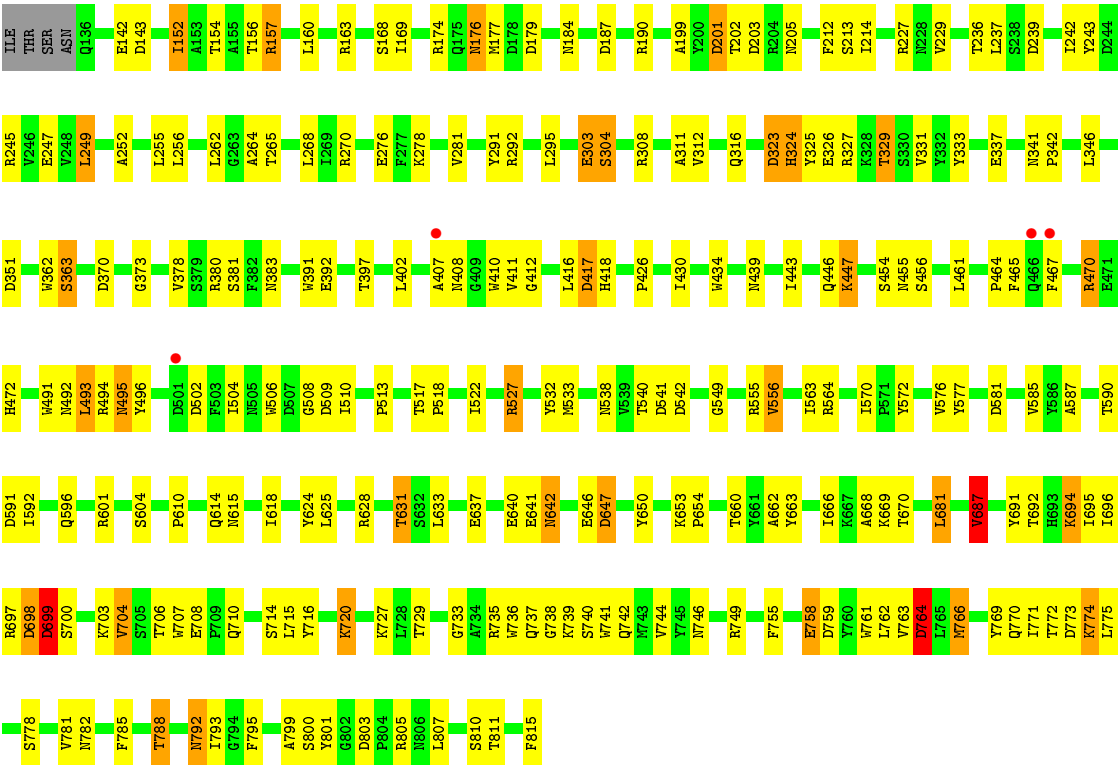
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

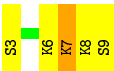
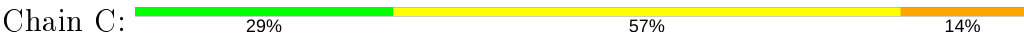


• Molecule 1: FERRIPYOVERDINE RECEPTOR





● Molecule 2: SER-LYS-GLY-FHO-LYS-FH7-SER



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.56Å 130.94Å 139.37Å 90.00° 130.43° 90.00°	Depositor
Resolution (Å)	97.59 – 3.00 54.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (97.59-3.00) 96.8 (54.72-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.242 0.191 , 0.241	Depositor DCC
R_{free} test set	2583 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 73.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12313	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FHO, PO4, N8E, PVE, FE, 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	0.98	3/6266 (0.0%)	1.01	8/8514 (0.1%)
1	B	0.83	2/6145 (0.0%)	0.89	6/8347 (0.1%)
2	C	0.88	0/31	0.96	0/34
All	All	0.91	5/12442 (0.0%)	0.95	14/16895 (0.1%)

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	0
All	All	1	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	GLU	CG-CD	6.81	1.62	1.51
1	A	276	GLU	CG-CD	5.82	1.60	1.51
1	A	362	TRP	CE3-CZ3	5.77	1.48	1.38
1	B	758	GLU	CG-CD	5.47	1.60	1.51
1	B	326	GLU	CG-CD	5.03	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	VAL	CB-CA-C	-8.02	96.15	111.40
1	A	362	TRP	CA-CB-CG	6.19	125.46	113.70
1	B	764	ASP	CB-CG-OD1	-6.19	112.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	580	ASN	CB-CA-C	-5.86	98.69	110.40
1	B	687	VAL	CB-CA-C	-5.78	100.42	111.40
1	A	317	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	581	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	474	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	713	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	380	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	B	681	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	98	LEU	CA-CB-CG	5.11	127.04	115.30
1	B	312	VAL	CB-CA-C	-5.07	101.77	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	SER	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	698	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6114	0	5788	168	0
1	B	5994	0	5675	179	0
2	C	56	0	53	4	0
3	A	72	0	114	13	0
4	A	30	0	0	3	0
4	B	20	0	0	0	0
5	C	26	0	14	1	0
6	C	1	0	0	0	0
All	All	12313	0	11644	347	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 14.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:HH11	1:B:73:ARG:HG2	1.06	1.11
3:A:1817[B]:N8E:H031	1:B:805:ARG:HD2	1.10	1.06
1:A:772:THR:HG22	1:A:774:LYS:H	1.17	1.05
1:A:53:GLN:OE1	1:A:57:SER:HB3	1.58	1.03
1:B:772:THR:HG22	1:B:774:LYS:H	1.21	1.02
3:A:1817[B]:N8E:H031	1:B:805:ARG:CD	2.00	0.91
1:A:772:THR:HG21	1:B:291:TYR:OH	1.72	0.89
1:A:454:SER:OG	1:A:483:SER:HB3	1.76	0.86
1:A:700:SER:OG	1:A:702:LYS:HG2	1.77	0.84
1:B:772:THR:HG22	1:B:774:LYS:N	1.92	0.83
1:B:73:ARG:NH1	1:B:73:ARG:HG2	1.83	0.83
2:C:6:FHO:O	2:C:7:LYS:HB3	1.78	0.83
3:A:1817[B]:N8E:C03	1:B:805:ARG:HD2	2.03	0.82
1:B:169:ILE:HD13	1:B:249:LEU:HD22	1.61	0.81
1:B:540:THR:HG22	1:B:541:ASP:H	1.45	0.80
1:A:443:ILE:HG13	1:A:510:ILE:HD13	1.62	0.79
1:B:418:HIS:CD2	1:B:455:ASN:HD21	2.02	0.77
1:B:341:ASN:HB2	1:B:342:PRO:CD	2.15	0.76
1:B:744:VAL:HG21	1:B:755:PHE:CE1	2.21	0.76
1:A:133:THR:HG21	1:A:159:VAL:HG21	1.66	0.75
1:B:742:GLN:HG3	1:B:793:ILE:O	1.88	0.74
1:B:214:ILE:HD13	1:B:264:ALA:HB3	1.70	0.74
1:B:418:HIS:HD2	1:B:455:ASN:HD21	1.33	0.73
1:A:807:LEU:HD11	3:A:1817[A]:N8E:H041	1.69	0.73
1:A:739:LYS:HD2	1:A:739:LYS:H	1.53	0.72
1:B:744:VAL:CG2	1:B:755:PHE:CE1	2.73	0.72
1:B:764:ASP:HB3	1:B:782:ASN:HA	1.71	0.72
1:A:439:ASN:ND2	1:A:504:ILE:HD12	2.04	0.72
1:B:738:GLY:HA2	1:B:759:ASP:HB3	1.72	0.71
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.25	0.71
1:B:176:ASN:C	1:B:176:ASN:HD22	1.95	0.71
1:B:744:VAL:CG2	1:B:755:PHE:HE1	2.03	0.70
1:A:805:ARG:HD2	3:A:1817[A]:N8E:H032	1.71	0.70
1:B:527:ARG:HH21	1:B:555:ARG:HD3	1.57	0.70
1:B:698:ASP:HB3	1:B:700:SER:H	1.57	0.70
1:B:735:ARG:NH2	1:B:737:GLN:OE1	2.26	0.68
1:A:742:GLN:HG3	1:A:793:ILE:O	1.94	0.68
1:A:556:VAL:HG13	1:A:563:ILE:HB	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:LYS:HE3	1:B:708:GLU:OE1	1.94	0.67
1:A:92:ASN:N	1:A:92:ASN:OD1	2.26	0.67
1:A:443:ILE:HG13	1:A:510:ILE:CD1	2.25	0.66
1:A:231:TYR:OH	1:A:524:ASP:HB3	1.95	0.66
1:A:239:ASP:OD2	1:A:292:ARG:NH2	2.29	0.65
1:A:109:GLN:OE1	1:A:114:THR:CG2	2.44	0.64
1:A:807:LEU:HD21	3:A:1817[A]:N8E:H061	1.79	0.64
1:A:308:ARG:NH1	1:A:337:GLU:OE1	2.30	0.64
1:A:443:ILE:CG1	1:A:510:ILE:CD1	2.75	0.64
1:A:809:PHE:CD1	1:B:771:ILE:HG12	2.33	0.64
1:A:50:ILE:HD12	1:A:85:ILE:HD11	1.80	0.63
1:A:772:THR:HG22	1:A:774:LYS:N	2.01	0.63
1:A:268:LEU:N	1:A:268:LEU:HD12	2.12	0.63
1:A:199:ALA:HA	1:A:205:ASN:HD22	1.63	0.63
1:A:580:ASN:HB2	1:A:582:THR:H	1.64	0.63
1:A:262:LEU:HD11	1:A:613:GLY:HA3	1.79	0.63
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.34	0.63
1:B:792:ASN:HB3	1:B:800:SER:HB2	1.80	0.62
1:B:341:ASN:HB2	1:B:342:PRO:HD3	1.81	0.62
1:B:694:LYS:HD2	1:B:694:LYS:C	2.20	0.62
1:B:772:THR:CG2	1:B:774:LYS:H	2.05	0.62
1:B:556:VAL:HG13	1:B:563:ILE:HB	1.81	0.62
1:B:73:ARG:HG3	1:B:304:SER:HB2	1.83	0.61
1:B:694:LYS:HD2	1:B:694:LYS:O	2.00	0.61
1:B:736:TRP:HB2	1:B:761:TRP:CE3	2.35	0.61
1:B:152:ILE:HD12	1:B:169:ILE:HG12	1.83	0.61
1:A:109:GLN:OE1	1:A:114:THR:HG22	2.01	0.61
3:A:1817[B]:N8E:H052	1:B:805:ARG:HD3	1.83	0.61
3:A:1817[A]:N8E:H222	1:B:811:THR:OG1	2.01	0.61
1:B:614:GLN:NE2	1:B:641:GLU:OE2	2.32	0.60
1:A:439:ASN:HD21	1:A:504:ILE:HD12	1.66	0.60
1:B:255:LEU:HD22	1:B:572:TYR:CD2	2.37	0.60
1:B:418:HIS:HD2	1:B:455:ASN:ND2	1.99	0.60
1:B:380:ARG:HD3	1:B:788:THR:HB	1.83	0.60
1:B:446:GLN:NE2	2:C:8:FH7:O	2.35	0.59
1:B:540:THR:HG22	1:B:541:ASP:N	2.16	0.59
1:A:410:TRP:CD2	1:A:463:GLY:HA3	2.37	0.59
1:B:470:ARG:NH1	1:B:538:ASN:OD1	2.35	0.59
1:A:542:ASP:HB3	1:A:578:ASP:HB2	1.83	0.59
1:B:157:ARG:HD2	1:B:256:LEU:HD13	1.84	0.59
1:B:772:THR:CG2	1:B:773:ASP:N	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ILE:HD11	1:B:115:ILE:HD11	1.83	0.59
1:A:646:GLU:HG3	1:A:661:TYR:OH	2.04	0.58
2:C:6:FHO:O	2:C:7:LYS:CB	2.50	0.58
1:A:596:GLN:NE2	1:A:609:GLU:O	2.37	0.58
1:A:408:ASN:CB	1:A:410:TRP:HD1	2.16	0.58
1:B:380:ARG:HA	1:B:801:TYR:CE2	2.39	0.58
1:B:744:VAL:HG21	1:B:755:PHE:HE1	1.61	0.58
1:A:392:GLU:CG	1:A:424:HIS:HB3	2.33	0.58
1:A:371:SER:OG	1:A:436:ALA:HA	2.04	0.58
1:B:698:ASP:HB3	1:B:700:SER:N	2.19	0.57
1:A:408:ASN:HB3	1:A:410:TRP:HD1	1.70	0.57
1:A:436:ALA:HB1	1:A:437:PRO:CD	2.34	0.57
1:A:736:TRP:HB2	1:A:761:TRP:CE3	2.40	0.57
1:A:133:THR:HG21	1:A:159:VAL:CG2	2.35	0.57
1:B:410:TRP:CD1	1:B:464:PRO:HD2	2.40	0.57
1:B:362:TRP:CZ2	2:C:8:FH7:HD1C	2.40	0.56
1:B:532:TYR:HA	1:B:549:GLY:O	2.05	0.56
1:A:609:GLU:HG3	1:A:610:PRO:HD2	1.88	0.56
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.40	0.56
1:A:157:ARG:HB3	1:A:475:VAL:HG11	1.86	0.56
1:A:219:TYR:N	1:A:219:TYR:CD1	2.74	0.55
1:B:86:LYS:HG3	1:B:87:GLY:N	2.21	0.55
1:B:696:ILE:HG23	1:B:704:VAL:HG12	1.88	0.55
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.41	0.55
1:A:527:ARG:HH12	1:A:564:ARG:NH2	2.05	0.55
1:B:625:LEU:O	1:B:628:ARG:HB2	2.07	0.55
1:A:805:ARG:HH11	3:A:1817[A]:N8E:H032	1.72	0.55
1:A:443:ILE:HG12	1:A:510:ILE:CD1	2.37	0.55
1:A:609:GLU:HG3	1:A:610:PRO:CD	2.37	0.55
1:A:74:PRO:HG3	1:A:132:ILE:HG12	1.88	0.55
1:B:792:ASN:O	1:B:799:ALA:HA	2.07	0.55
1:B:270:ARG:NH1	1:B:351:ASP:OD2	2.40	0.54
1:B:323:ASP:HB2	1:B:381:SER:O	2.07	0.54
1:A:392:GLU:HG2	1:A:424:HIS:HB3	1.88	0.54
1:B:55:LEU:HB2	1:B:80:LYS:HB2	1.89	0.54
1:B:706:THR:OG1	1:B:741:TRP:O	2.23	0.54
1:A:384:ASN:HB2	1:A:430:ILE:HB	1.89	0.54
1:A:746:ASN:OD1	1:A:748:PRO:HD2	2.07	0.54
1:B:646:GLU:O	1:B:663:TYR:HA	2.08	0.54
1:A:470:ARG:NH1	1:A:538:ASN:OD1	2.41	0.53
1:B:694:LYS:NZ	1:B:708:GLU:O	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD21	1:A:613:GLY:HA3	1.91	0.53
1:B:542:ASP:O	1:B:577:TYR:HA	2.08	0.53
1:B:276:GLU:N	1:B:276:GLU:OE1	2.32	0.53
1:A:51:PRO:O	1:A:53:GLN:HG2	2.09	0.53
1:B:55:LEU:HD23	1:B:77:VAL:HB	1.91	0.53
1:A:302:THR:HG23	1:A:307:VAL:HG22	1.90	0.53
1:A:52:PRO:HD3	1:A:84:ALA:HB2	1.90	0.53
1:B:55:LEU:HD11	1:B:99:LEU:HD23	1.89	0.53
1:B:184:ASN:O	1:B:187:ASP:HB2	2.10	0.52
1:B:276:GLU:H	1:B:276:GLU:CD	2.10	0.52
1:B:472:HIS:HD2	1:B:538:ASN:H	1.57	0.52
1:A:174:ARG:HB2	1:A:244:ASP:O	2.09	0.52
1:B:646:GLU:O	1:B:647:ASP:HB3	2.09	0.52
1:B:69:GLN:HG2	1:B:276:GLU:HA	1.91	0.52
1:A:700:SER:HG	1:A:702:LYS:HG2	1.73	0.52
1:B:570:ILE:HG23	1:B:591:ASP:HB3	1.91	0.52
1:A:282:GLU:HG3	1:A:811:THR:O	2.10	0.52
1:B:646:GLU:O	1:B:662:ALA:O	2.27	0.52
1:B:74:PRO:HG3	1:B:303:GLU:HG2	1.91	0.52
1:A:580:ASN:CB	1:A:582:THR:H	2.22	0.51
1:A:109:GLN:OE1	1:A:114:THR:HG21	2.08	0.51
1:B:95:ILE:HG12	1:B:106:VAL:HG11	1.92	0.51
1:A:774:LYS:HD2	1:A:814:ASP:O	2.11	0.51
1:B:370:ASP:HA	1:B:434:TRP:O	2.11	0.51
1:B:591:ASP:OD1	1:B:614:GLN:HG3	2.11	0.51
1:B:637:GLU:HA	1:B:670:THR:O	2.10	0.51
4:A:1820:PO4:O1	4:A:1823:PO4:O2	2.29	0.51
1:B:74:PRO:O	1:B:78:ARG:HB3	2.10	0.51
1:B:262:LEU:HD23	1:B:592:ILE:HG22	1.91	0.51
1:B:772:THR:HG22	1:B:773:ASP:N	2.25	0.51
1:A:659:ILE:H	1:A:659:ILE:HD12	1.76	0.51
1:B:494:ARG:O	1:B:495:ASN:C	2.49	0.51
1:B:646:GLU:O	1:B:647:ASP:CB	2.59	0.51
1:A:288:TRP:CZ2	1:A:321:PHE:HB3	2.45	0.50
1:A:155:ALA:HB1	1:A:167:GLN:OE1	2.11	0.50
1:B:113:ILE:O	1:B:113:ILE:HG13	2.10	0.50
1:A:722:LYS:HE2	1:A:723:GLY:H	1.76	0.50
1:B:666:ILE:HG22	1:B:699:ASP:OD2	2.12	0.50
1:A:792:ASN:HB3	1:A:800:SER:HB2	1.92	0.50
1:B:74:PRO:HG3	1:B:303:GLU:CG	2.42	0.50
1:A:174:ARG:CZ	1:A:177:MET:CE	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:VAL:HG22	1:B:755:PHE:CE1	2.45	0.50
1:A:71:LEU:HD22	1:A:133:THR:OG1	2.12	0.49
1:B:418:HIS:CD2	1:B:455:ASN:ND2	2.76	0.49
1:A:380:ARG:HA	1:A:801:TYR:CD2	2.47	0.49
1:A:50:ILE:CD1	1:A:85:ILE:HD11	2.43	0.49
1:A:260:GLY:HA2	1:A:594:MET:HE2	1.93	0.49
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.95	0.49
1:B:624:TYR:HE1	1:B:631:THR:HG1	1.60	0.49
1:B:727:LYS:HG3	1:B:770:GLN:HB3	1.94	0.49
1:A:458:ASP:OD2	1:A:479:SER:HB3	2.12	0.49
1:B:373:GLY:HA3	1:B:749:ARG:HG3	1.95	0.49
1:B:325:TYR:OH	1:B:327:ARG:HD3	2.12	0.49
1:A:591:ASP:CG	1:A:592:ILE:N	2.65	0.49
1:A:68:ILE:HG21	1:A:113:ILE:HG23	1.95	0.49
1:A:334:GLY:HA3	3:A:1816:N8E:H082	1.95	0.48
1:A:408:ASN:CB	1:A:410:TRP:CD1	2.96	0.48
1:B:316:GLN:HB3	1:B:329:THR:HG23	1.95	0.48
1:A:174:ARG:CZ	1:A:177:MET:HE2	2.43	0.48
1:A:505:ASN:O	1:A:506:TRP:C	2.50	0.48
1:B:426:PRO:HA	1:B:447:LYS:HG2	1.95	0.48
1:A:401:ASN:ND2	1:A:415:GLN:HG2	2.28	0.48
1:A:789:TYR:N	1:A:789:TYR:CD1	2.81	0.48
1:A:203:ASP:OD1	1:A:325:TYR:OH	2.31	0.48
1:B:239:ASP:CG	1:B:292:ARG:HH22	2.16	0.48
1:A:601:ARG:HD3	1:A:605:ASN:OD1	2.12	0.48
1:A:797:THR:HG22	1:A:797:THR:O	2.13	0.48
1:B:308:ARG:NH1	1:B:337:GLU:OE1	2.46	0.48
1:A:53:GLN:O	1:A:81:ARG:HB3	2.13	0.48
1:B:59:LEU:HD22	1:B:70:VAL:HG11	1.95	0.48
1:A:646:GLU:O	1:A:662:ALA:O	2.32	0.48
1:A:165:THR:O	1:A:621:LYS:NZ	2.47	0.47
1:B:268:LEU:N	1:B:268:LEU:HD12	2.29	0.47
1:B:715:LEU:O	1:B:733:GLY:HA2	2.15	0.47
1:A:669:LYS:O	1:A:696:ILE:HA	2.14	0.47
1:B:696:ILE:HG12	1:B:704:VAL:HG12	1.95	0.47
1:A:60:GLN:NE2	1:A:134:SER:HA	2.30	0.47
1:A:475:VAL:O	1:A:533:MET:HA	2.14	0.47
1:B:214:ILE:CD1	1:B:264:ALA:HB3	2.42	0.47
1:B:157:ARG:HD2	1:B:256:LEU:CD1	2.44	0.47
1:B:346:LEU:HB2	1:B:402:LEU:HD13	1.97	0.47
1:B:252:ALA:O	1:B:590:THR:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:LYS:HG2	1:B:729:THR:HG23	1.97	0.47
1:A:587:ALA:HA	1:A:617:GLU:O	2.14	0.47
1:B:654:PRO:HG3	1:B:660:THR:HG23	1.97	0.47
1:B:746:ASN:C	1:B:746:ASN:OD1	2.53	0.47
1:A:154:THR:O	1:A:256:LEU:HD12	2.15	0.47
1:A:694:LYS:HZ2	1:A:708:GLU:HB3	1.79	0.47
1:B:311:ALA:HA	1:B:333:TYR:O	2.14	0.47
1:B:262:LEU:CD2	1:B:592:ILE:HG22	2.45	0.47
1:B:744:VAL:HG22	1:B:755:PHE:CD1	2.50	0.47
1:A:239:ASP:CG	1:A:292:ARG:HH22	2.17	0.47
1:B:496:TYR:CD1	1:B:513:PRO:HB3	2.50	0.46
1:A:792:ASN:O	1:A:799:ALA:HA	2.15	0.46
1:B:281:VAL:HG22	1:B:295:LEU:HD13	1.96	0.46
1:B:72:TYR:O	1:B:304:SER:HA	2.15	0.46
1:B:691:TYR:C	1:B:691:TYR:CD1	2.89	0.46
1:B:695:ILE:HG12	1:B:710:GLN:HG2	1.98	0.46
1:A:106:VAL:HG11	1:A:108:PHE:CZ	2.51	0.46
1:B:443:ILE:HG12	1:B:510:ILE:HD12	1.98	0.46
1:A:689:ALA:HA	1:A:714:SER:O	2.15	0.46
1:A:789:TYR:CZ	1:A:802:GLY:HA3	2.51	0.46
1:B:99:LEU:CD1	1:B:106:VAL:HG22	2.45	0.46
1:B:199:ALA:HA	1:B:205:ASN:HD22	1.79	0.46
1:B:212:PHE:CD1	1:B:262:LEU:HB2	2.51	0.46
1:B:446:GLN:HG2	1:B:491:TRP:HB3	1.97	0.46
1:B:640:GLU:HB3	1:B:668:ALA:HB3	1.97	0.46
1:B:236:THR:HG23	1:B:237:LEU:HG	1.98	0.46
1:B:641:GLU:O	1:B:642:ASN:HB2	2.16	0.46
1:B:681:LEU:HD13	1:B:687:VAL:CG2	2.46	0.45
1:A:204:ARG:HG3	1:A:391:TRP:CH2	2.52	0.45
1:B:762:LEU:HD23	1:B:762:LEU:HA	1.82	0.45
1:A:219:TYR:O	1:A:220:ASP:C	2.55	0.45
1:A:276:GLU:OE2	1:A:278:LYS:HD3	2.16	0.45
1:A:142:GLU:O	1:A:143:ASP:HB2	2.17	0.45
1:A:350:ALA:HA	1:A:397:THR:O	2.17	0.45
1:A:408:ASN:HB2	1:A:410:TRP:CD1	2.52	0.45
1:A:392:GLU:HG3	1:A:424:HIS:HB3	1.97	0.45
1:B:694:LYS:CD	1:B:694:LYS:C	2.83	0.45
1:A:285:ALA:O	1:B:771:ILE:HG21	2.17	0.45
1:A:370:ASP:OD1	1:A:370:ASP:C	2.55	0.45
1:A:554:TYR:CD2	1:A:595:PRO:HG2	2.52	0.45
1:A:656:ASN:ND2	1:A:658:ALA:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:THR:O	1:A:152:ILE:HD13	2.17	0.45
1:A:420:ILE:HD11	4:A:1821:PO4:O1	2.16	0.45
1:A:447:LYS:HB3	1:A:490:TYR:HB2	1.98	0.45
1:B:163:ARG:HH22	1:B:581:ASP:C	2.20	0.45
1:A:107:ASP:HB3	1:A:114:THR:HG23	1.99	0.45
1:A:542:ASP:CB	1:A:578:ASP:HB2	2.47	0.45
1:B:439:ASN:ND2	1:B:502:ASP:HA	2.32	0.44
1:B:74:PRO:CG	1:B:303:GLU:HG2	2.47	0.44
1:B:99:LEU:HD12	1:B:106:VAL:HG22	1.99	0.44
1:B:391:TRP:O	1:B:391:TRP:CD1	2.71	0.44
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.52	0.44
1:A:694:LYS:O	1:A:694:LYS:HG3	2.16	0.44
1:A:767:ALA:HB3	1:A:779:VAL:HG12	1.98	0.44
1:B:99:LEU:HD11	1:B:115:ILE:HD12	2.00	0.44
1:A:320:SER:OG	1:A:321:PHE:N	2.50	0.44
1:B:506:TRP:CZ2	1:B:508:GLY:HA2	2.52	0.44
1:B:807:LEU:HD12	1:B:807:LEU:N	2.32	0.44
3:A:1817[A]:N8E:H042	1:B:769:TYR:OH	2.17	0.44
1:B:653:LYS:HA	1:B:654:PRO:HD2	1.51	0.44
1:A:443:ILE:HD13	1:A:443:ILE:N	2.32	0.44
1:A:391:TRP:C	1:A:391:TRP:CD1	2.90	0.44
1:A:504:ILE:HG22	1:A:505:ASN:ND2	2.33	0.44
1:A:707:TRP:CH2	1:A:793:ILE:HG13	2.53	0.44
1:A:443:ILE:CG1	1:A:510:ILE:HD13	2.35	0.43
1:B:324:HIS:CE1	1:B:383:ASN:HB3	2.53	0.43
1:A:410:TRP:CE2	1:A:463:GLY:HA3	2.54	0.43
1:A:614:GLN:CD	1:A:614:GLN:N	2.71	0.43
1:B:412:GLY:HA3	1:B:461:LEU:HD23	1.99	0.43
1:A:123:SER:O	1:A:124:SER:HB3	2.17	0.43
1:A:721:PHE:CD2	1:A:728:LEU:HD23	2.54	0.43
1:A:380:ARG:HA	1:A:801:TYR:CE2	2.54	0.43
1:B:707:TRP:O	1:B:740:SER:HB2	2.18	0.43
1:B:95:ILE:HG12	1:B:113:ILE:HD13	2.00	0.43
1:B:492:ASN:C	1:B:493:LEU:HG	2.38	0.43
1:B:472:HIS:HD2	1:B:538:ASN:N	2.16	0.43
1:B:430:ILE:HG12	1:B:443:ILE:HD13	2.01	0.43
1:B:472:HIS:CD2	1:B:538:ASN:H	2.36	0.43
1:A:391:TRP:HB2	1:A:427:LEU:HD21	2.00	0.43
1:A:674:GLU:HG3	1:A:692:THR:OG1	2.18	0.43
1:B:142:GLU:HB2	1:B:174:ARG:HG2	2.01	0.43
1:B:506:TRP:CE2	1:B:508:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:HG12	1:A:264:ALA:HB3	2.00	0.42
1:A:243:TYR:CE1	1:A:268:LEU:HB3	2.54	0.42
1:A:50:ILE:HA	1:A:51:PRO:HD2	1.77	0.42
1:A:60:GLN:HE22	1:A:134:SER:HA	1.83	0.42
1:A:380:ARG:HD3	1:A:788:THR:HB	2.01	0.42
1:A:408:ASN:HB2	1:A:410:TRP:H	1.84	0.42
1:A:605:ASN:HB2	1:A:659:ILE:HG13	2.01	0.42
1:A:612:GLU:HB3	1:A:641:GLU:OE2	2.20	0.42
1:A:281:VAL:HG23	1:A:815:PHE:CZ	2.54	0.42
1:B:417:ASP:O	1:B:455:ASN:HA	2.20	0.42
1:B:696:ILE:CG2	1:B:704:VAL:HG12	2.49	0.42
1:A:512:LYS:HD2	4:A:1818:PO4:O1	2.20	0.42
1:B:363:SER:HA	1:B:795:PHE:CE2	2.55	0.42
3:A:1817[B]:N8E:H031	1:B:805:ARG:HH11	1.85	0.42
1:B:243:TYR:CD1	1:B:268:LEU:HB3	2.55	0.42
1:A:308:ARG:NH2	1:A:339:ASP:OD2	2.52	0.42
1:A:408:ASN:HB2	1:A:410:TRP:HB2	2.01	0.42
1:A:491:TRP:CE2	1:A:519:SER:HB3	2.54	0.42
1:A:69:GLN:O	1:A:113:ILE:N	2.37	0.42
1:B:152:ILE:HG22	1:B:247:GLU:OE2	2.20	0.42
1:B:669:LYS:O	1:B:696:ILE:HA	2.20	0.42
1:B:681:LEU:HD13	1:B:687:VAL:HG21	2.02	0.42
1:B:697:ARG:NH2	1:B:703:LYS:HE3	2.35	0.42
1:B:706:THR:HB	1:B:741:TRP:CE2	2.55	0.42
1:A:297:VAL:O	1:A:310:ARG:HA	2.20	0.42
1:A:527:ARG:NH1	1:A:564:ARG:HH21	2.18	0.42
1:A:700:SER:OG	1:A:702:LYS:CG	2.60	0.41
1:A:68:ILE:CG2	1:A:113:ILE:HG23	2.50	0.41
1:A:418:HIS:HA	1:A:455:ASN:HD22	1.84	0.41
1:A:804:PRO:O	1:A:805:ARG:C	2.59	0.41
1:B:587:ALA:HB2	1:B:618:ILE:HG13	2.02	0.41
1:B:736:TRP:HB2	1:B:761:TRP:CZ3	2.54	0.41
1:B:179:ASP:O	1:B:766:MET:HG3	2.20	0.41
1:A:312:VAL:HG13	1:A:333:TYR:HD2	1.86	0.41
1:B:86:LYS:HG3	1:B:87:GLY:H	1.83	0.41
1:B:176:ASN:ND2	1:B:176:ASN:C	2.67	0.41
1:B:691:TYR:CD1	1:B:692:THR:N	2.89	0.41
1:A:805:ARG:CD	3:A:1817[A]:N8E:H032	2.46	0.41
1:A:418:HIS:HA	1:A:455:ASN:ND2	2.35	0.41
1:B:142:GLU:O	1:B:143:ASP:HB2	2.21	0.41
1:B:781:VAL:HG22	1:B:807:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ASN:ND2	1:A:519:SER:OG	2.54	0.41
1:A:674:GLU:HA	1:A:691:TYR:O	2.21	0.41
1:B:201:ASP:O	1:B:203:ASP:N	2.54	0.41
1:B:81:ARG:HG2	1:B:82:SER:O	2.20	0.41
1:A:527:ARG:HH12	1:A:564:ARG:HH21	1.67	0.41
1:A:636:PHE:C	1:A:636:PHE:CD1	2.94	0.41
1:B:715:LEU:C	1:B:715:LEU:HD23	2.40	0.41
1:A:485:TRP:CE2	1:A:522:ILE:HG21	2.56	0.41
1:B:156:THR:O	1:B:157:ARG:HB2	2.21	0.41
1:A:152:ILE:HD13	1:A:152:ILE:HA	1.64	0.41
1:A:136:GLN:HE22	1:A:462:THR:HG21	1.85	0.41
5:C:1:PVE:H8	5:C:1:PVE:H14	1.79	0.41
1:A:281:VAL:HG22	1:A:295:LEU:HD13	2.03	0.40
1:A:591:ASP:CG	1:A:592:ILE:H	2.22	0.40
1:B:650:TYR:CD2	1:B:650:TYR:C	2.95	0.40
1:A:199:ALA:O	1:A:792:ASN:HB2	2.21	0.40
1:B:341:ASN:CB	1:B:342:PRO:CD	2.88	0.40
1:B:363:SER:HA	1:B:795:PHE:HE2	1.86	0.40
1:B:95:ILE:HD11	1:B:115:ILE:CD1	2.48	0.40
1:A:214:ILE:HG21	1:A:266:ILE:CD1	2.52	0.40
1:A:291:TYR:OH	1:B:772:THR:HG21	2.21	0.40
1:B:763:VAL:HG21	1:B:785:PHE:HE2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	770/772 (100%)	700 (91%)	59 (8%)	11 (1%)	11	43
1	B	750/772 (97%)	681 (91%)	58 (8%)	11 (2%)	10	42
2	C	3/7 (43%)	2 (67%)	0	1 (33%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1523/1551 (98%)	1383 (91%)	117 (8%)	23 (2%)	10	42

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	124	SER
1	A	646	GLU
1	B	324	HIS
1	B	408	ASN
2	C	7	LYS
1	A	227	ARG
1	A	228	ASN
1	A	773	ASP
1	B	407	ALA
1	B	518	PRO
1	B	699	ASP
1	A	652	SER
1	B	363	SER
1	B	642	ASN
1	A	233	ALA
1	A	433	ASP
1	A	683	PRO
1	B	610	PRO
1	B	647	ASP
1	B	52	PRO
1	B	202	THR
1	A	342	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	650/650 (100%)	571 (88%)	79 (12%)	5	21
1	B	637/650 (98%)	559 (88%)	78 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	4/4 (100%)	2 (50%)	2 (50%)	0	0
All	All	1291/1304 (99%)	1132 (88%)	159 (12%)	4	21

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	68	ILE
1	A	78	ARG
1	A	83	SER
1	A	92	ASN
1	A	93	GLN
1	A	100	ARG
1	A	114	THR
1	A	132	ILE
1	A	133	THR
1	A	152	ILE
1	A	154	THR
1	A	157	ARG
1	A	169	ILE
1	A	204	ARG
1	A	246	VAL
1	A	248	VAL
1	A	276	GLU
1	A	297	VAL
1	A	304	SER
1	A	307	VAL
1	A	312	VAL
1	A	318	LYS
1	A	329	THR
1	A	331	VAL
1	A	343	ASP
1	A	358	LYS
1	A	362	TRP
1	A	372	GLN
1	A	375	ARG
1	A	379	SER
1	A	392	GLU
1	A	401	ASN
1	A	417	ASP
1	A	431	MET
1	A	459	ILE

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Mol	Chain	Res	Type
1	A	461	LEU
1	A	462	THR
1	A	466	GLN
1	A	468	LEU
1	A	483	SER
1	A	493	LEU
1	A	524	ASP
1	A	528	GLN
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	566	SER
1	A	596	GLN
1	A	601	ARG
1	A	603	SER
1	A	609	GLU
1	A	615	ASN
1	A	629	LEU
1	A	652	SER
1	A	653	LYS
1	A	655	THR
1	A	659	ILE
1	A	660	THR
1	A	676	GLU
1	A	687	VAL
1	A	694	LYS
1	A	704	VAL
1	A	720	LYS
1	A	722	LYS
1	A	739	LYS
1	A	740	SER
1	A	754	LYS
1	A	766	MET
1	A	771	ILE
1	A	772	THR
1	A	775	LEU
1	A	788	THR
1	A	792	ASN
1	A	811	THR

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Mol	Chain	Res	Type
1	A	815	PHE
1	B	68	ILE
1	B	73	ARG
1	B	82	SER
1	B	83	SER
1	B	86	LYS
1	B	96	THR
1	B	100	ARG
1	B	109	GLN
1	B	113	ILE
1	B	152	ILE
1	B	154	THR
1	B	157	ARG
1	B	160	LEU
1	B	168	SER
1	B	176	ASN
1	B	177	MET
1	B	201	ASP
1	B	213	SER
1	B	227	ARG
1	B	229	VAL
1	B	242	ILE
1	B	245	ARG
1	B	249	LEU
1	B	265	THR
1	B	278	LYS
1	B	303	GLU
1	B	304	SER
1	B	323	ASP
1	B	329	THR
1	B	331	VAL
1	B	378	VAL
1	B	392	GLU
1	B	397	THR
1	B	411	VAL
1	B	416	LEU
1	B	417	ASP
1	B	447	LYS
1	B	454	SER
1	B	456	SER
1	B	465	PHE
1	B	467	PHE

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Mol	Chain	Res	Type
1	B	470	ARG
1	B	493	LEU
1	B	495	ASN
1	B	504	ILE
1	B	509	ASP
1	B	517	THR
1	B	522	ILE
1	B	527	ARG
1	B	533	MET
1	B	556	VAL
1	B	564	ARG
1	B	576	VAL
1	B	585	VAL
1	B	596	GLN
1	B	601	ARG
1	B	604	SER
1	B	615	ASN
1	B	631	THR
1	B	633	LEU
1	B	687	VAL
1	B	694	LYS
1	B	699	ASP
1	B	704	VAL
1	B	714	SER
1	B	720	LYS
1	B	739	LYS
1	B	758	GLU
1	B	764	ASP
1	B	766	MET
1	B	774	LYS
1	B	775	LEU
1	B	778	SER
1	B	788	THR
1	B	792	ASN
1	B	803	ASP
1	B	810	SER
1	B	815	PHE
2	C	3	SER
2	C	9	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	136	GLN
1	A	183	ASN
1	A	205	ASN
1	A	218	GLN
1	A	372	GLN
1	A	401	ASN
1	A	455	ASN
1	A	484	HIS
1	A	492	ASN
1	A	505	ASN
1	A	596	GLN
1	B	176	ASN
1	B	205	ASN
1	B	408	ASN
1	B	418	HIS
1	B	455	ASN
1	B	472	HIS
1	B	596	GLN
1	B	615	ASN
1	B	688	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	6	2,6	8,10,11	1.77	1 (12%)	4,11,13	2.21	3 (75%)
2	FH7	C	8	2,6	8,10,11	2.29	1 (12%)	4,11,13	1.75	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FHO	C	6	2,6	-	2/7/10/12	-
2	FH7	C	8	2,6	-	5/7/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	8	FH7	CZ-NE	-6.30	1.25	1.34
2	C	6	FHO	CZ-NE	-4.63	1.27	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	FH7	OZ-NE-CD	3.41	122.05	113.67
2	C	6	FHO	OH-CZ-NE	-2.67	118.11	125.80
2	C	6	FHO	OZ-NE-CD	2.47	119.74	113.67
2	C	6	FHO	CG-CD-NE	2.04	115.26	111.07

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	8	FH7	C-CA-CB-CG
2	C	8	FH7	NE-CD-CG-CB
2	C	8	FH7	CG-CD-NE-OZ
2	C	8	FH7	CG-CD-NE-CZ
2	C	8	FH7	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	FHO	2	0
2	C	8	FH7	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	A	1822	-	4,4,4	0.78	0	6,6,6	0.64	0
3	N8E	A	1817[B]	-	23,23,23	0.76	0	22,22,22	0.56	0
4	PO4	B	1817	-	4,4,4	0.42	0	6,6,6	0.88	0
3	N8E	A	1817[A]	-	23,23,23	0.76	0	22,22,22	0.71	0
4	PO4	A	1821	-	4,4,4	0.67	0	6,6,6	1.20	0
4	PO4	A	1823	-	4,4,4	1.00	0	6,6,6	0.52	0
4	PO4	B	1816	-	4,4,4	0.71	0	6,6,6	0.93	0
4	PO4	B	1819	-	4,4,4	1.00	0	6,6,6	0.59	0
4	PO4	A	1820	-	4,4,4	0.80	0	6,6,6	0.77	0
5	PVE	C	1	2,6	23,28,29	3.14	4 (17%)	25,40,42	3.34	6 (24%)
3	N8E	A	1816	-	23,23,23	0.61	0	22,22,22	0.43	0
4	PO4	B	1818	-	4,4,4	0.85	0	6,6,6	1.04	1 (16%)
4	PO4	A	1818	-	4,4,4	0.51	0	6,6,6	1.09	0
4	PO4	A	1819	-	4,4,4	1.10	0	6,6,6	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N8E	A	1817[A]	-	-	8/21/21/21	-
3	N8E	A	1816	-	-	11/21/21/21	-
3	N8E	A	1817[B]	-	-	12/21/21/21	-
5	PVE	C	1	2,6	-	4/8/21/23	0/2/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	PVE	C20-C18	-13.15	1.26	1.51
5	C	1	PVE	C9-N1	-4.00	1.35	1.39
5	C	1	PVE	C5-C6	3.77	1.41	1.37
5	C	1	PVE	C7-C6	-3.00	1.35	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	PVE	O19-C18-C20	-9.88	103.94	122.02
5	C	1	PVE	C20-C18-N17	9.22	130.84	114.59
5	C	1	PVE	C21-C20-C18	-7.83	94.72	112.72
5	C	1	PVE	O26-C7-C6	-2.34	112.22	118.45
5	C	1	PVE	O26-C7-C8	2.25	126.93	120.85
5	C	1	PVE	C4-C3-C2	-2.22	116.33	119.29
4	B	1818	PO4	O3-P-O2	2.03	114.47	107.97

There are no chirality outliers.

All (35) torsion outliers are listed below:

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

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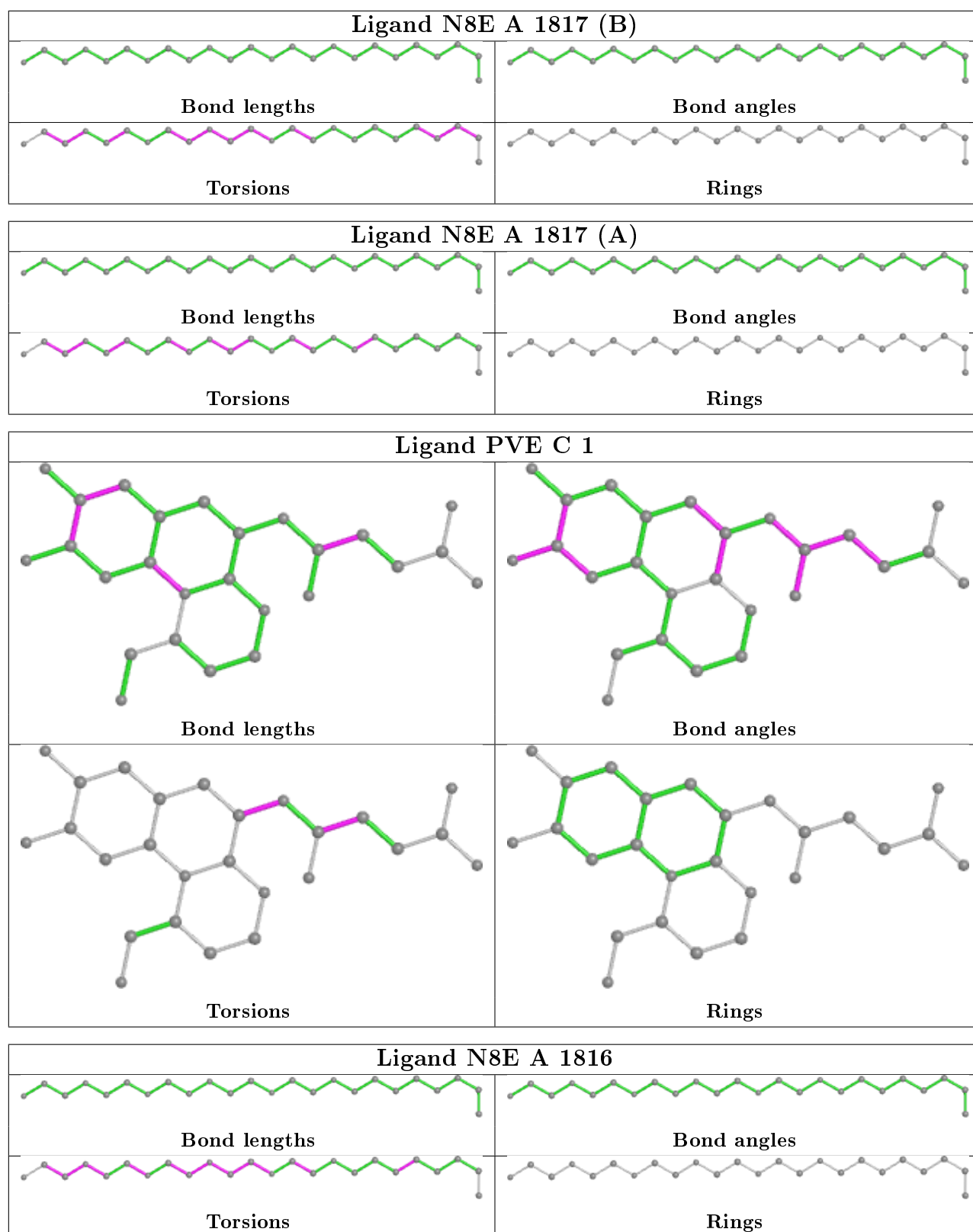
Mol	Chain	Res	Type	Atoms
3	A	1816	N8E	C17-C16-O15-C14
3	A	1817[A]	N8E	O09-C10-C11-O12
3	A	1816	N8E	C19-C20-O21-C22
3	A	1816	N8E	C23-C22-O21-C20
3	A	1816	N8E	C13-C14-O15-C16
3	A	1816	N8E	C14-C13-O12-C11
3	A	1817[B]	N8E	C17-C16-O15-C14
3	A	1817[A]	N8E	O21-C22-C23-O24
3	A	1817[A]	N8E	C13-C14-O15-C16
3	A	1817[B]	N8E	C01-C02-C03-C04
3	A	1817[B]	N8E	C13-C14-O15-C16
3	A	1817[A]	N8E	C06-C07-C08-O09
3	A	1817[B]	N8E	C02-C03-C04-C05
3	A	1816	N8E	O12-C13-C14-O15

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1817[B]	N8E	5	0
3	A	1817[A]	N8E	7	0
4	A	1821	PO4	1	0
4	A	1823	PO4	1	0
4	A	1820	PO4	1	0
5	C	1	PVE	1	0
3	A	1816	N8E	1	0
4	A	1818	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	772/772 (100%)	-0.45	2 (0%) 94 84	26, 41, 54, 68	0
1	B	754/772 (97%)	-0.23	12 (1%) 72 44	26, 46, 69, 86	0
2	C	5/7 (71%)	-0.69	0 100 100	55, 56, 63, 67	0
All	All	1531/1551 (98%)	-0.34	14 (0%) 84 63	26, 44, 63, 86	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	ALA	2.9
1	B	109	GLN	2.9
1	B	111	ASN	2.7
1	B	117	VAL	2.7
1	B	501	ASP	2.3
1	B	88	LYS	2.3
1	A	723	GLY	2.2
1	B	44	GLN	2.2
1	A	44	GLN	2.2
1	B	116	SER	2.1
1	B	70	VAL	2.1
1	B	466	GLN	2.1
1	B	467	PHE	2.0
1	B	110	GLY	2.0

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

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(\AA^2)	Q<0.9
2	FHO	C	6	11/12	0.96	0.17	48,55,61,62	0
2	FH7	C	8	11/12	0.99	0.11	45,54,65,65	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

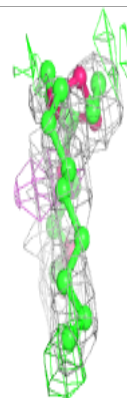
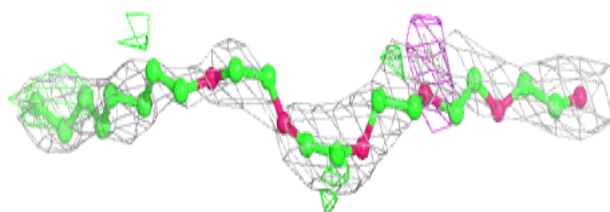
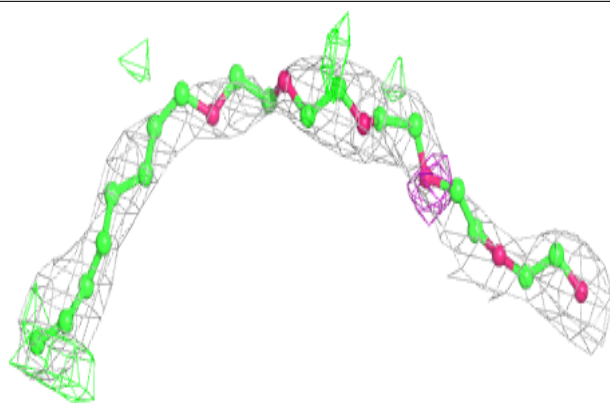
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	N8E	A	1817[B]	24/24	0.85	0.32	2,19,29,30	24
3	N8E	A	1817[A]	24/24	0.85	0.32	8,18,24,26	24
4	PO4	A	1822	5/5	0.86	0.25	115,115,116,116	0
4	PO4	B	1816	5/5	0.86	0.32	103,103,104,104	0
3	N8E	A	1816	24/24	0.89	0.38	60,72,83,85	0
4	PO4	A	1821	5/5	0.92	0.20	79,79,79,80	0
4	PO4	A	1823	5/5	0.95	0.16	89,89,90,91	0
4	PO4	B	1818	5/5	0.95	0.23	89,90,90,90	0
4	PO4	A	1820	5/5	0.95	0.16	76,76,77,78	0
4	PO4	B	1819	5/5	0.96	0.15	79,80,80,80	0
5	PVE	C	1	26/27	0.97	0.17	45,47,59,62	5
4	PO4	A	1818	5/5	0.97	0.13	48,48,49,50	0
4	PO4	B	1817	5/5	0.98	0.09	50,50,51,52	0
4	PO4	A	1819	5/5	0.98	0.11	46,46,47,48	0
6	FE	C	2	1/1	1.00	0.14	44,44,44,44	0

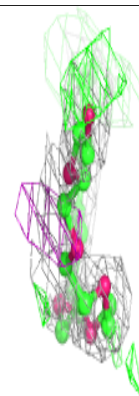
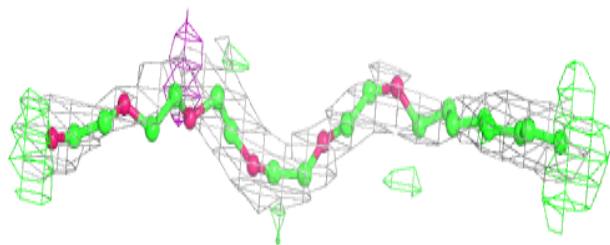
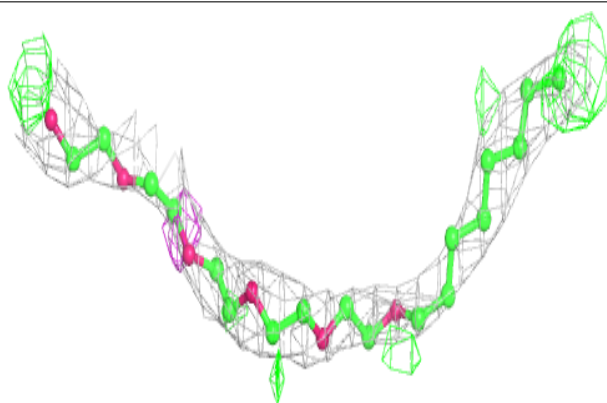
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around N8E A 1817 (B):

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

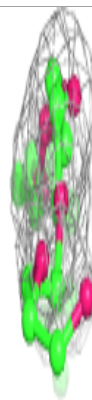
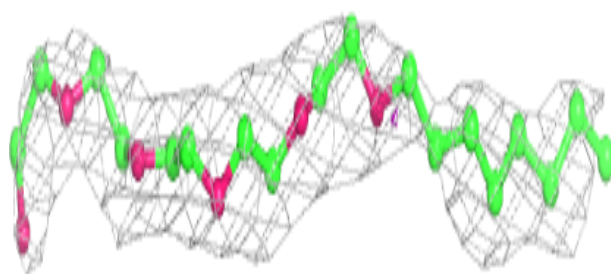
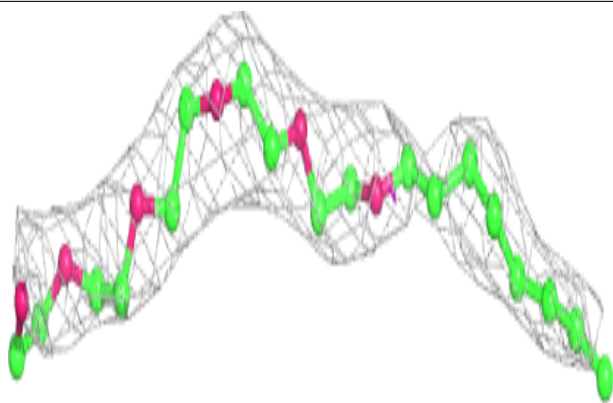
**Electron density around N8E A 1817 (A):**

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



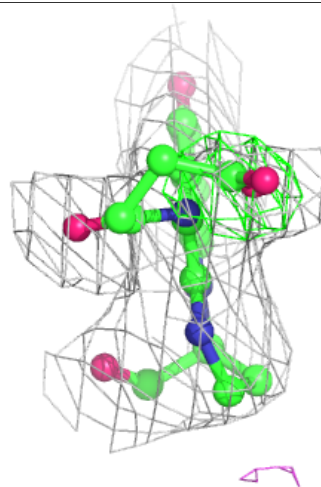
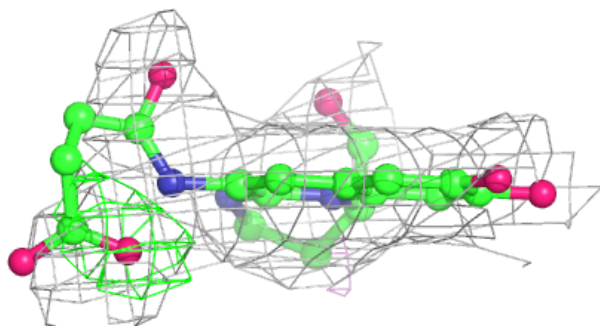
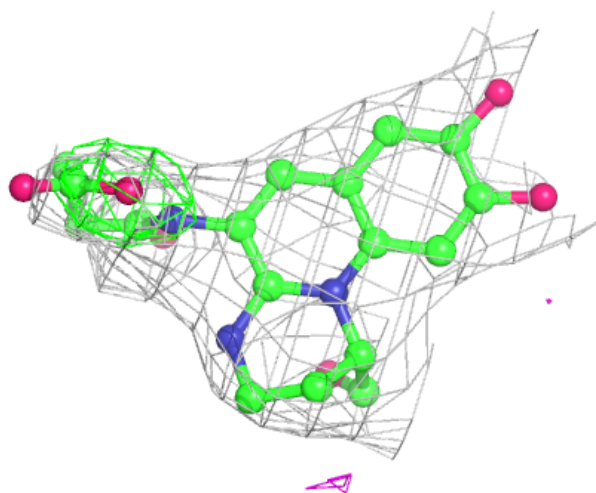
Electron density around N8E A 1816:

$2mF_o-DF_c$ (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.