



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:11 AM GMT

PDB ID : 2W76
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

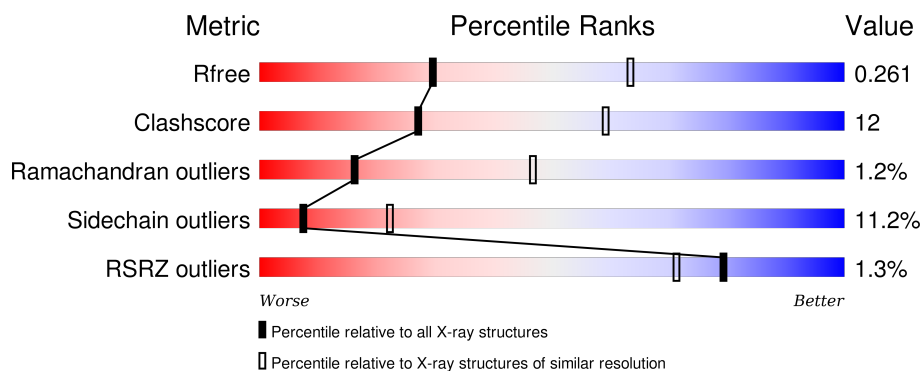
1 Overall quality at a glance

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>69%</div> <div>25%</div> <div>5%</div> </div>
1	B	772	<div> <div>66%</div> <div>28%</div> </div>
2	C	7	<div> <div>14%</div> <div>57%</div> <div>29%</div> </div>

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	-	-	-
3	N8E	A	1816	-	-	-	X
3	N8E	A	1817[A]	-	-	-	X
4	PO4	A	1823	-	-	-	X
4	PO4	B	1816	-	-	-	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			

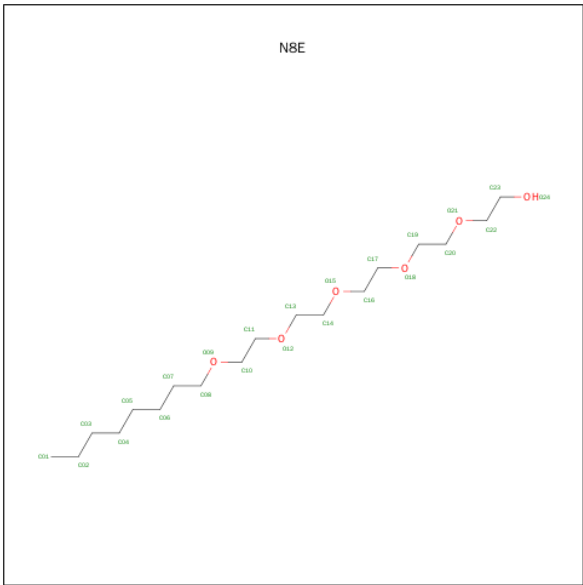
- Molecule 2 is a protein called PYOVERDIN R.

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:

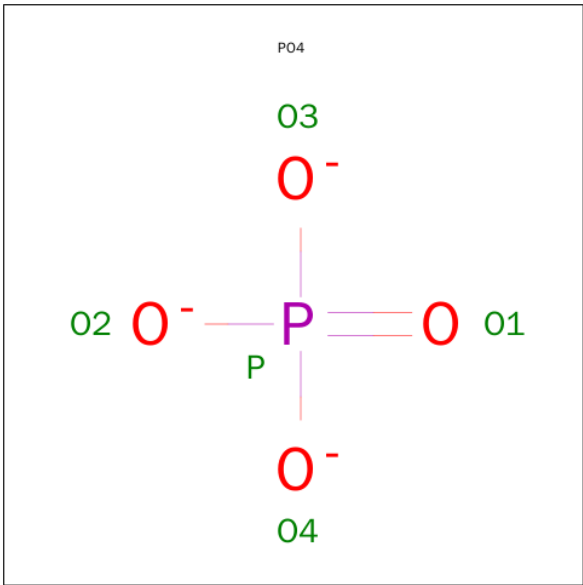
Chain	Residue	Modelled	Actual	Comment	Reference
C	8	FHO	FH7	CONFLICT	NOR NOR0020

- Molecule 3 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (three-letter code: 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 (three-letter code: PO4) (formula: O₄P).



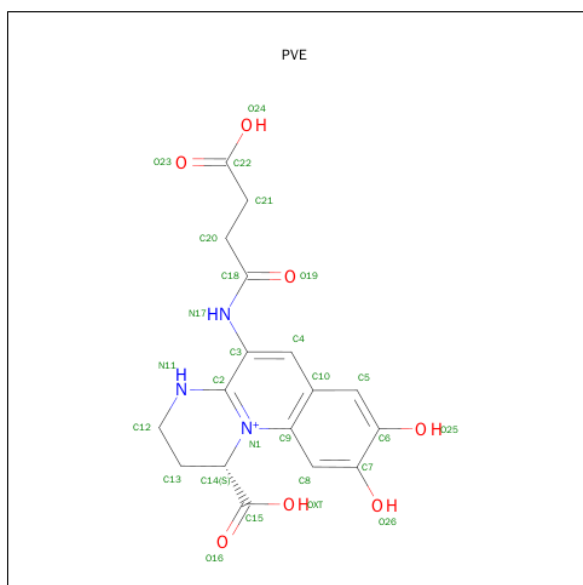
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		

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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-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		

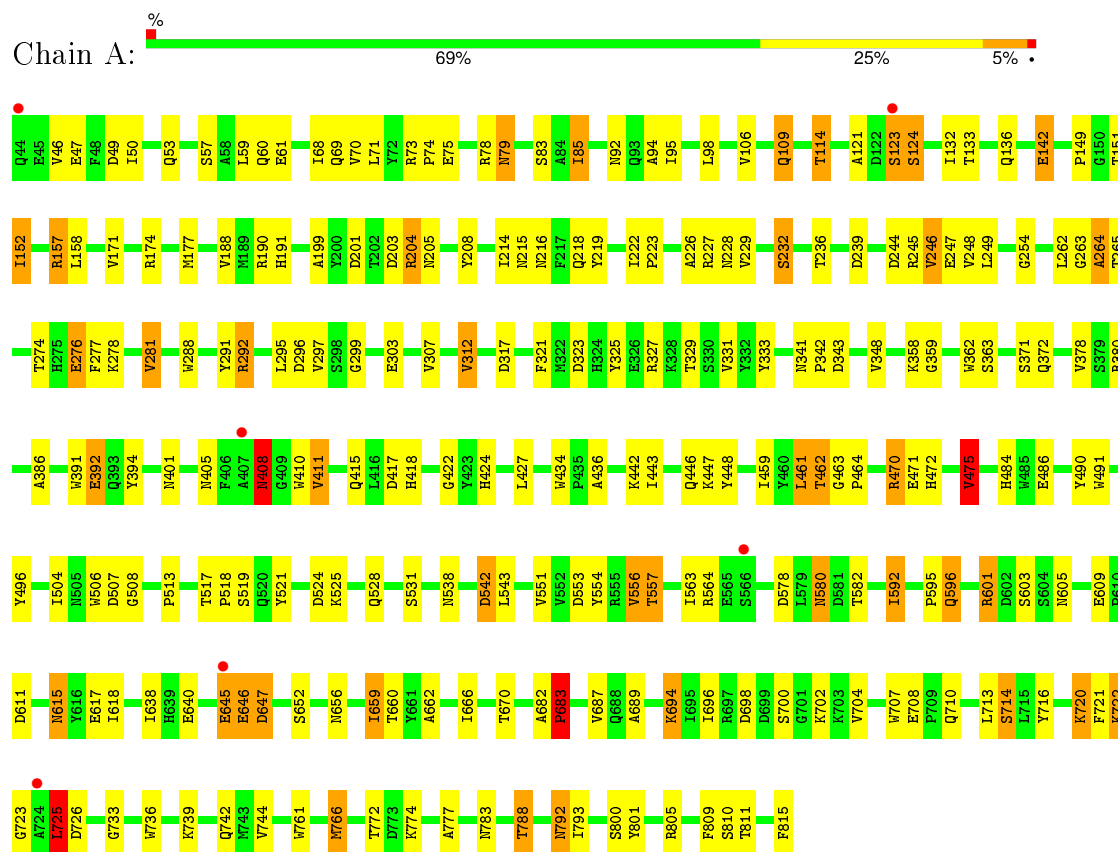
- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

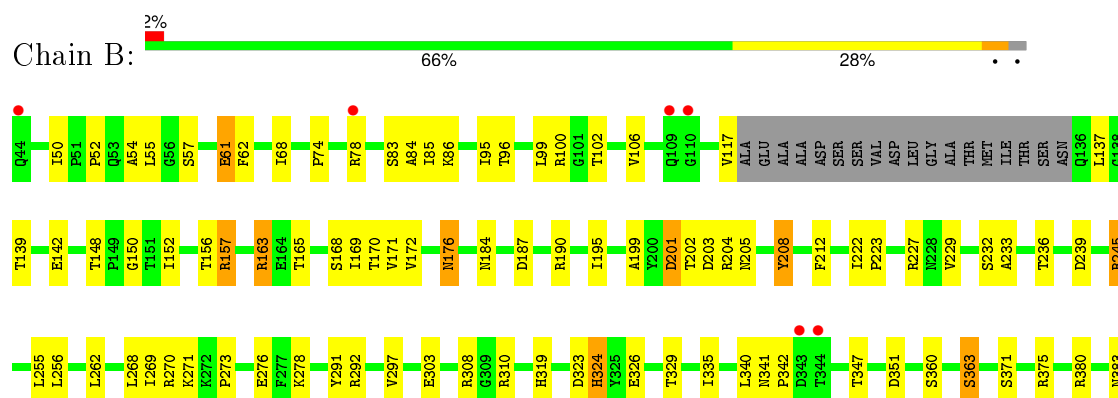
3 Residue-property plots [i](#)

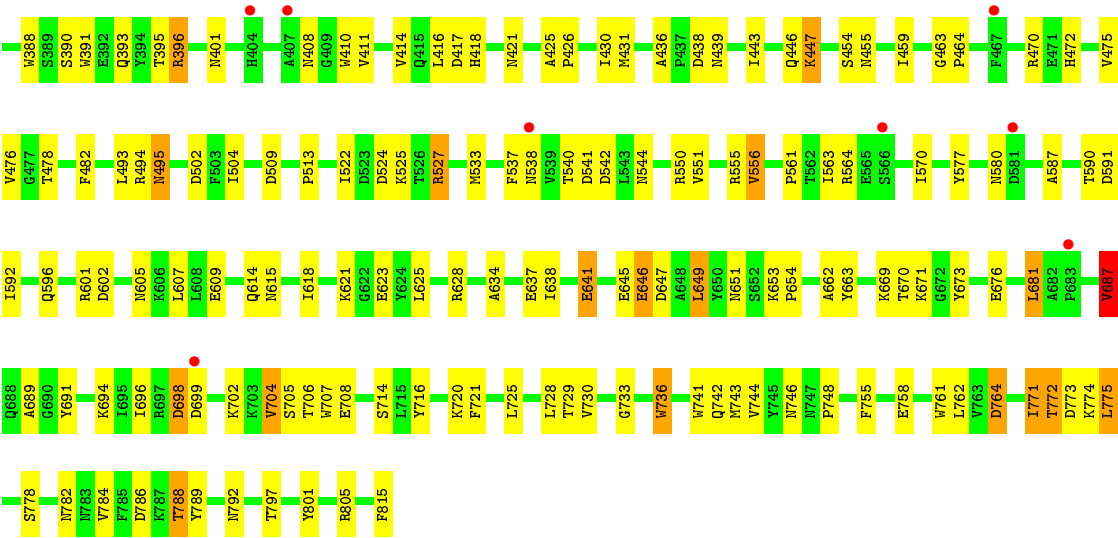
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

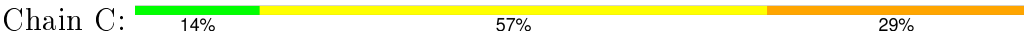


• Molecule 1: FERRIPYOVERDINE RECEPTOR





● 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 33.44 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.1 (97.13-2.80) 89.1 (33.44-2.80)	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 (5.32%)	DCC
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.3	EDS
Estimated twinning fraction	0.001 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 57915 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: DSN, FHO, DAB, PO4, DGN, N8E, PVE, FE

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	0.97	2/6266 (0.0%)	1.02	18/8514 (0.2%)
1	B	0.87	3/6145 (0.0%)	0.92	6/8347 (0.1%)
2	C	0.85	0/12	1.05	0/11
All	All	0.92	5/12423 (0.0%)	0.97	24/16872 (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	2
All	All	1	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	GLU	CG-CD	6.77	1.62	1.51
1	B	758	GLU	CG-CD	5.92	1.60	1.51
1	A	79	ASN	CB-CG	5.22	1.63	1.51
1	B	736	TRP	CB-CG	5.21	1.59	1.50
1	B	645	GLU	CG-CD	5.09	1.59	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	VAL	CB-CA-C	-7.78	96.62	111.40
1	A	317	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	190	ARG	NE-CZ-NH2	-7.00	116.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	725	LEU	CA-CB-CG	6.95	131.27	115.30
1	B	190	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	687	VAL	CB-CA-C	-6.57	98.92	111.40
1	A	296	ASP	CB-CG-OD1	6.45	124.10	118.30
1	B	764	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	B	649	LEU	CB-CG-CD1	6.17	121.49	111.00
1	A	507	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	A	296	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	190	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	683	PRO	C-N-CA	-5.59	110.55	122.30
1	A	475	VAL	CB-CA-C	-5.25	101.42	111.40
1	A	49	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	208	TYR	CA-CB-CG	5.20	123.28	113.40
1	A	106	VAL	CB-CA-C	-5.16	101.59	111.40
1	A	292	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	281	VAL	N-CA-C	-5.13	97.16	111.00
1	A	295	LEU	CA-CB-CG	5.10	127.02	115.30
1	A	543	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	323	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	B	208	TYR	CA-CB-CG	5.03	122.95	113.40
1	B	323	ASP	CB-CG-OD1	-5.02	113.78	118.30

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

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	140	0
1	B	5994	0	5675	145	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	287	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (287) 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:HG3	2:C:6:GLN:O	1.20	1.01
2:C:6:GLN:CG	2:C:6:GLN:O	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: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
1:B:772:THR:CG2	1:B:774:LYS:H	2.00	0.74
3:A:1817[B]:N8E:H031	1:B:805:ARG:HD2	1.70	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
1:A:239:ASP:OD2	1:A:292:ARG:NH2	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.70	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:542:ASP:O	1:B:577:TYR:HA	1.96	0.64
1:B:152:ILE:HD12	1:B:169:ILE:HG12	1.77	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:363:SER:OG	1:B:431:MET:HE1	1.98	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:HD12	1:B:268:LEU:N	2.15	0.62
1:B:772:THR:HG22	1:B:775:LEU:N	2.11	0.62
1:B:245:ARG:NH1	1:B:269:ILE:HG13	2.14	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: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:B:417:ASP:O	1:B:455:ASN:HA	2.02	0.59
1:A:325:TYR:OH	1:A:327:ARG:NH1	2.35	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:363:SER:OG	1:B:431:MET:HE2	2.02	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:B:472:HIS:HD2	1:B:538:ASN:H	1.54	0.55
1:A:646:GLU:O	1:A:662:ALA:O	2.23	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:B:772:THR:HG23	1:B:773:ASP:N	2.22	0.54
1:B:199:ALA:HA	1:B:205:ASN:HD22	1.72	0.54
1:A:239:ASP:CG	1:A:292:ARG:HH22	2.09	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:809:PHE:HB3	3:A:1817[B]:N8E:H231	1.89	0.54
1:A:470:ARG:HD3	1:A:538:ASN:O	2.08	0.54
1:A:343:ASP:HB2	1:A:405:ASN:HB2	1.89	0.53
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.43	0.53
1:B:375:ARG:NE	1:B:755:PHE:CE2	2.77	0.53
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.44	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
1:B:797:THR:HG22	1:B:797:THR:O	2.10	0.52
2:C:4:DAB:O	2:C:7:DGN:HG3	2.09	0.52
1:B:637:GLU:HA	1:B:670:THR:O	2.09	0.52
1:B:74:PRO:HG3	1:B:303:GLU:CG	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ASP:OD1	1:A:640:GLU:OE2	2.28	0.52
1:B:772:THR:CG2	1:B:773:ASP:N	2.72	0.52
1:B:646:GLU:HG3	1:B:651:ASN:HD22	1.73	0.52
1:A:580:ASN:HD22	1:A:582:THR:H	1.58	0.52
1:A:174:ARG:CZ	1:A:177:MET:CE	2.88	0.52
1:A:484:HIS:CE1	1:A:486:GLU:OE2	2.63	0.51
1:B:728:LEU:HD12	1:B:729:THR:N	2.26	0.51
1:A:92:ASN:HA	1:A:95:ILE:HG22	1.92	0.51
1:B:201:ASP:O	1:B:203:ASP:N	2.44	0.51
1:A:694:LYS:O	1:A:694:LYS:HD2	2.10	0.51
1:A:53:GLN:OE1	1:A:57:SER:CB	2.59	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:B:74:PRO:HG3	1:B:303:GLU:HG2	1.93	0.50
1:A:380:ARG:HA	1:A:801:TYR:CD2	2.47	0.50
1:B:570:ILE:HG23	1:B:591:ASP:HB3	1.92	0.50
1:A:391:TRP:HB2	1:A:427:LEU:HD21	1.92	0.50
1:A:725:LEU:H	1:A:725:LEU:HD23	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:766:MET:C	1:A:766:MET:SD	2.90	0.50
1:A:694:LYS:C	1:A:694:LYS:CD	2.80	0.49
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:A:69:GLN:HE21	1:A:133:THR:CG2	2.25	0.49
1:A:542:ASP:HB3	1:A:578:ASP:HB2	1.94	0.49
1:B:418:HIS:HE1	4:B:1819:PO4:O1	1.95	0.49
1:A:249:LEU:O	1:A:264:ALA:HA	2.13	0.49
1:A:517:THR:O	1:A:518:PRO:C	2.48	0.49
1:B:744:VAL:CG2	1:B:755:PHE:CD1	2.96	0.48
1:B:50:ILE:HG12	1:B:61:GLU:HG2	1.94	0.48
1:B:590:THR:OG1	1:B:615:ASN:HB3	2.13	0.48
1:B:525:LYS:O	1:B:556:VAL:HA	2.13	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:725:LEU:N	1:A:725:LEU:HD23	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ILE:HD13	1:A:443:ILE:N	2.28	0.48
1:B:744:VAL:HG22	1:B:755:PHE:CE1	2.49	0.48
1:A:222:ILE:HD11	1:A:415:GLN:NE2	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:638:ILE:O	1:B:669:LYS:HA	2.14	0.48
1:B:439:ASN:ND2	1:B:502:ASP:HA	2.29	0.48
1:A:245:ARG:NH1	1:A:247:GLU:OE1	2.42	0.47
1:B:601:ARG:NH1	1:B:605:ASN:O	2.46	0.47
1:A:216:ASN:HB2	1:A:265:THR:HA	1.96	0.47
1:A:188:VAL:HG11	1:A:246:VAL:CG1	2.44	0.47
1:A:380:ARG:HD3	1:A:788:THR:HB	1.95	0.47
1:A:59:LEU:HD22	1:A:70:VAL:HG11	1.96	0.47
1:B:563:ILE:HG12	1:B:607:LEU:HD22	1.96	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:276:GLU:H	1:B:276:GLU:CD	2.18	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:B:494:ARG:O	1:B:495:ASN:C	2.53	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:B:165:THR:O	1:B:621:LYS:NZ	2.43	0.46
1:B:540:THR:CG2	1:B:541:ASP:N	2.77	0.46
1:A:73:ARG:HA	1:A:74:PRO:HD2	1.82	0.46
1:B:721:PHE:HB2	1:B:725:LEU:O	2.16	0.46
1:B:614:GLN:OE1	1:B:641:GLU:OE2	2.33	0.46
1:B:262:LEU:HD23	1:B:592:ILE:HG22	1.98	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:A:174:ARG:CZ	1:A:177:MET:HE2	2.45	0.46
1:A:75:GLU:HB2	1:A:78:ARG:NH2	2.31	0.46
1:A:363:SER:O	1:A:363:SER:OG	2.30	0.46
1:A:203:ASP:OD1	1:A:325:TYR:OH	2.27	0.46
1:B:614:GLN:NE2	1:B:641:GLU:OE2	2.47	0.46
1:B:233:ALA:CB	1:B:421:ASN:HB3	2.46	0.46
1:B:204:ARG:HD3	1:B:391:TRP:CH2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:LYS:O	1:B:696:ILE:HA	2.16	0.45
1:A:689:ALA:HA	1:A:714:SER:O	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:B:634:ALA:O	1:B:673:TYR:HA	2.16	0.45
1:B:390:SER:O	1:B:425:ALA:HA	2.17	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:689:ALA:HA	1:B:714:SER:O	2.16	0.45
1:B:527:ARG:HH21	1:B:555:ARG:HD3	1.82	0.45
1:B:410:TRP:CD1	1:B:464:PRO:HD2	2.52	0.45
1:B:540:THR:HG22	1:B:541:ASP:H	1.80	0.44
1:B:410:TRP:CD2	1:B:463:GLY:HA3	2.52	0.44
1:B:239:ASP:CG	1:B:292:ARG:HH22	2.21	0.44
1:A:805:ARG:HD2	3:A:1817[A]:N8E:C03	2.43	0.44
1:B:681:LEU:HD13	1:B:687:VAL:CG2	2.46	0.44
1:A:288:TRP:CZ2	1:A:321:PHE:HB3	2.51	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:B:340:LEU:HA	1:B:340:LEU:HD23	1.69	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:B:157:ARG:HD3	1:B:256:LEU:HD13	1.99	0.43
1:A:418:HIS:NE2	4:A:1821:PO4:O2	2.50	0.43
1:A:707:TRP:CH2	1:A:793:ILE:HG13	2.53	0.43
1:B:691:TYR:C	1:B:691:TYR:CD1	2.92	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:B:782:ASN:O	1:B:805:ARG:HA	2.17	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:388:TRP:CZ2	1:B:513:PRO:HD3	2.54	0.43
1:A:596:GLN:HB2	1:A:596:GLN:HE21	1.53	0.43
1:B:152:ILE:CD1	1:B:169:ILE:HG12	2.44	0.43
1:A:736:TRP:HB2	1:A:761:TRP:CE3	2.53	0.43
1:A:601:ARG:NH1	1:A:605:ASN:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PRO:HB3	1:A:171:VAL:HG11	2.00	0.43
1:B:625:LEU:O	1:B:628:ARG:HD3	2.19	0.43
1:B:199:ALA:HA	1:B:205:ASN:ND2	2.34	0.42
1:A:75:GLU:HB3	1:A:471:GLU:HG3	2.01	0.42
1:A:716:TYR:HD1	1:A:733:GLY:HA3	1.76	0.42
1:A:277:PHE:CD2	1:A:277:PHE:C	2.92	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:233:ALA:HB3	1:B:421:ASN:HB3	2.00	0.42
1:B:744:VAL:HG21	1:B:755:PHE:HE1	1.77	0.42
1:A:174:ARG:HB2	1:A:244:ASP:O	2.20	0.42
1:A:682:ALA:O	1:A:683:PRO:C	2.58	0.42
1:A:281:VAL:HG23	1:A:815:PHE:CZ	2.53	0.42
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.55	0.42
1:A:725:LEU:CD2	1:A:725:LEU:N	2.83	0.42
1:B:171:VAL:HG12	1:B:172:VAL:N	2.34	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
1:B:156:THR:O	1:B:157:ARG:CB	2.68	0.42
1:A:434:TRP:CZ2	1:A:442:LYS:HB2	2.55	0.42
1:A:710:GLN:HB3	1:A:710:GLN:HE21	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:B:137:LEU:HB3	1:B:269:ILE:HD12	2.00	0.41
1:A:646:GLU:O	1:A:647:ASP:CB	2.69	0.41
1:B:602:ASP:HA	1:B:663:TYR:O	2.21	0.41
1:A:720:LYS:HE3	1:A:726:ASP:O	2.21	0.41
1:A:359:GLY:HA2	1:A:386:ALA:O	2.20	0.41
1:B:54:ALA:O	1:B:55:LEU:C	2.58	0.41
1:B:176:ASN:C	1:B:176:ASN:HD22	2.24	0.41
1:B:163:ARG:NH1	1:B:623:GLU:HB3	2.35	0.41
1:B:694:LYS:HE3	1:B:708:GLU:CD	2.39	0.41
2:C:3:DSN:C	2:C:7:DGN:OE1	2.69	0.41
1:B:268:LEU:HD12	1:B:268:LEU:H	1.86	0.41
1:A:201:ASP:HB3	1:A:362:TRP:O	2.21	0.41
1:B:222:ILE:HA	1:B:223:PRO:HD2	1.88	0.41
1:A:219:TYR:N	1:A:219:TYR:CD1	2.88	0.41
1:B:170:THR:OG1	1:B:676:GLU:OE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:PHE:CE2	1:B:527:ARG:HG3	2.56	0.41
1:B:391:TRP:CD1	1:B:393:GLN:HG2	2.56	0.40
1:B:396:ARG:HG2	1:B:396:ARG:HH11	1.86	0.40
1:A:521:TYR:CD1	1:A:521:TYR:N	2.89	0.40
1:A:244:ASP:O	1:A:245:ARG:HB3	2.21	0.40
1:A:281:VAL:HG23	1:A:815:PHE:CE1	2.57	0.40
1:B:706:THR:OG1	1:B:741:TRP:O	2.31	0.40
1:A:274:THR:O	1:A:299:GLY:HA2	2.21	0.40
1:B:764:ASP:HA	1:B:784:VAL:HG23	2.03	0.40
1:A:645:GLU:HG3	1:A:666:ILE:HD11	2.02	0.40
1:B:117:VAL:HG12	1:B:117:VAL:O	2.20	0.40
1:A:98:LEU:C	1:A:98:LEU:HD23	2.42	0.40
1:A:491:TRP:CE2	1:A:519:SER:HB3	2.56	0.40
1:B:99:LEU:O	1:B:102:THR:HG23	2.21	0.40
1:B:395:THR:O	1:B:396:ARG:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	770/772 (100%)	714 (93%)	46 (6%)	10 (1%)	15	44
1	B	750/772 (97%)	694 (92%)	48 (6%)	8 (1%)	17	50
2	C	1/7 (14%)	0	1 (100%)	0	100	100
All	All	1521/1551 (98%)	1408 (93%)	95 (6%)	18 (1%)	16	47

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	SER
1	A	227	ARG

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Mol	Chain	Res	Type
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%)	575 (88%)	75 (12%)	7	21
1	B	637/650 (98%)	569 (89%)	68 (11%)	8	24
2	C	1/1 (100%)	0	1 (100%)	0	0
All	All	1288/1301 (99%)	1144 (89%)	144 (11%)	7	22

All (144) 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

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Mol	Chain	Res	Type
1	A	109	GLN
1	A	114	THR
1	A	123	SER
1	A	132	ILE
1	A	142	GLU
1	A	152	ILE
1	A	157	ARG
1	A	191	HIS
1	A	204	ARG
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
1	A	401	ASN
1	A	408	ASN
1	A	411	VAL
1	A	417	ASP
1	A	459	ILE
1	A	461	LEU
1	A	462	THR
1	A	470	ARG
1	A	475	VAL
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

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Mol	Chain	Res	Type
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	645	GLU
1	A	652	SER
1	A	659	ILE
1	A	660	THR
1	A	683	PRO
1	A	694	LYS
1	A	704	VAL
1	A	713	LEU
1	A	714	SER
1	A	720	LYS
1	A	722	LYS
1	A	725	LEU
1	A	744	VAL
1	A	766	MET
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	148	THR
1	B	157	ARG
1	B	163	ARG
1	B	168	SER
1	B	176	ASN
1	B	195	ILE

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Mol	Chain	Res	Type
1	B	201	ASP
1	B	227	ARG
1	B	229	VAL
1	B	232	SER
1	B	236	THR
1	B	245	ARG
1	B	278	LYS
1	B	297	VAL
1	B	319	HIS
1	B	326	GLU
1	B	329	THR
1	B	360	SER
1	B	396	ARG
1	B	411	VAL
1	B	416	LEU
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	509	ASP
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	564	ARG
1	B	596	GLN
1	B	609	GLU
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	699	ASP
1	B	702	LYS
1	B	704	VAL

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Mol	Chain	Res	Type
1	B	705	SER
1	B	720	LYS
1	B	730	VAL
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

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	136	GLN
1	A	205	ASN
1	A	218	GLN
1	A	372	GLN
1	A	401	ASN
1	A	408	ASN
1	A	415	GLN
1	A	492	ASN
1	A	580	ASN
1	A	596	GLN
1	A	710	GLN
1	B	176	ASN
1	B	205	ASN
1	B	418	HIS
1	B	472	HIS
1	B	615	ASN
1	B	630	ASN
1	B	688	GLN
1	B	710	GLN
1	B	742	GLN
1	B	780	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	DSN	C	3	2,5	3,4,6	3.26	1 (33%)	0,4,7	0.00	-
2	DAB	C	4	2	5,6,7	0.45	0	3,6,8	2.78	1 (33%)
2	FHO	C	5	2,6	7,10,11	0.88	0	6,11,13	1.31	1 (16%)
2	DGN	C	7	2	7,8,9	0.99	0	6,9,11	0.92	1 (16%)
2	FHO	C	8	2,6	7,10,11	0.68	0	6,11,13	1.18	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	DSN	C	3	2,5	1/1/1/2	0/0/2/6	0/0/0/0
2	DAB	C	4	2	-	0/3/5/7	0/0/0/0
2	FHO	C	5	2,6	-	0/5/10/12	0/0/0/0
2	DGN	C	7	2	-	0/5/7/9	0/0/0/0
2	FHO	C	8	2,6	-	0/5/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	DSN	O-C	5.58	1.45	1.19

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	DAB	O-C-CA	-4.64	113.40	125.49
2	C	5	FHO	O-C-CA	-2.77	118.28	125.49
2	C	7	DGN	O-C-CA	-2.10	120.01	125.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	DSN	CA

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	DSN	1	0
2	C	4	DAB	2	0
2	C	5	FHO	1	0
2	C	7	DGN	2	0
2	C	8	FHO	1	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	$\# Z > 2$
3	N8E	A	1816	-	23,23,23	0.55	0	22,22,22	0.42	0
3	N8E	A	1817[A]	-	23,23,23	0.72	0	22,22,22	0.78	0
3	N8E	A	1817[B]	-	23,23,23	0.87	0	22,22,22	0.98	1 (4%)
4	PO4	A	1818	-	4,4,4	0.37	0	6,6,6	0.34	0
4	PO4	A	1819	-	4,4,4	0.50	0	6,6,6	0.30	0
4	PO4	A	1820	-	4,4,4	0.75	0	6,6,6	0.29	0
4	PO4	A	1821	-	4,4,4	0.47	0	6,6,6	0.28	0
4	PO4	A	1822	-	4,4,4	0.59	0	6,6,6	0.26	0
4	PO4	A	1823	-	4,4,4	0.62	0	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	B	1816	-	4,4,4	0.32	0	6,6,6	0.32	0
4	PO4	B	1817	-	4,4,4	0.27	0	6,6,6	0.30	0
4	PO4	B	1818	-	4,4,4	0.51	0	6,6,6	0.30	0
4	PO4	B	1819	-	4,4,4	0.36	0	6,6,6	0.27	0
5	PVE	C	1	2,6	24,28,29	2.05	5 (20%)	24,40,42	1.43	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N8E	A	1816	-	-	0/21/21/21	0/0/0/0
3	N8E	A	1817[A]	-	-	0/21/21/21	0/0/0/0
3	N8E	A	1817[B]	-	-	0/21/21/21	0/0/0/0
4	PO4	A	1818	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1819	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1820	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1821	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1822	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1823	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1816	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1817	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1818	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1819	-	-	0/0/0/0	0/0/0/0
5	PVE	C	1	2,6	-	0/7/21/23	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	-5.46	1.40	1.51
5	C	1	PVE	C9-N1	-3.13	1.36	1.40
5	C	1	PVE	C8-C7	3.37	1.40	1.37
5	C	1	PVE	C14-C15	3.57	1.54	1.50
5	C	1	PVE	C5-C6	4.84	1.42	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	PVE	C21-C20-C18	-3.30	104.93	113.01
5	C	1	PVE	C8-C7-C6	-2.29	118.63	119.97
5	C	1	PVE	C7-C8-C9	2.58	121.75	117.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1817[B]	N8E	O18-C19-C20	3.13	124.27	110.36
5	C	1	PVE	C12-C13-C14	3.68	118.08	110.13

There are no chirality outliers.

There are no torsion outliers.

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
3	A	1817[B]	N8E	4	0
4	A	1818	PO4	1	0
4	A	1821	PO4	1	0
4	B	1818	PO4	1	0
4	B	1819	PO4	1	0

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%)	-0.50	6 (0%) 87 81	12, 26, 41, 62	0
1	B	754/772 (97%)	-0.27	14 (1%) 70 59	19, 34, 54, 65	0
2	C	2/7 (28%)	0.09	0 100 100	50, 50, 50, 56	0
All	All	1528/1551 (98%)	-0.39	20 (1%) 79 71	12, 29, 49, 65	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	ALA	5.8
1	A	44	GLN	4.6
1	A	123	SER	4.3
1	B	78	ARG	4.0
1	B	44	GLN	3.8
1	A	724	ALA	3.4
1	B	683	PRO	2.8
1	B	110	GLY	2.8
1	B	467	PHE	2.4
1	B	109	GLN	2.4
1	B	344	THR	2.4
1	B	581	ASP	2.3
1	B	343	ASP	2.3
1	A	407	ALA	2.3
1	B	538	ASN	2.2
1	B	566	SER	2.1
1	A	645	GLU	2.1
1	A	566	SER	2.1
1	B	699	ASP	2.1
1	B	404	HIS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	FHO	C	5	11/12	0.98	0.13	-	47,50,55,56	0
2	DAB	C	4	7/8	0.91	0.17	-	56,57,58,58	0
2	DSN	C	3	5/7	0.90	0.19	-	57,57,58,58	0
2	DGN	C	7	9/10	0.84	0.20	-	49,53,54,54	0
2	FHO	C	8	11/12	0.95	0.16	-	41,44,50,52	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	N8E	A	1816	24/24	0.87	0.29	7.62	47,57,75,76	0
3	N8E	A	1817[A]	24/24	0.87	0.26	5.69	2,6,16,17	24
4	PO4	A	1823	5/5	0.94	0.20	3.51	54,55,55,56	0
4	PO4	B	1816	5/5	0.96	0.27	2.70	58,58,58,59	0
4	PO4	A	1822	5/5	0.97	0.14	1.56	57,59,60,61	0
3	N8E	A	1817[B]	24/24	0.87	0.26	1.54	2,7,12,13	24
4	PO4	A	1818	5/5	0.99	0.15	-0.43	33,34,34,34	0
5	PVE	C	1	26/27	0.94	0.14	-0.51	44,48,60,63	5
4	PO4	B	1818	5/5	0.97	0.12	-0.63	50,51,54,54	0
4	PO4	A	1820	5/5	0.99	0.09	-2.59	36,38,39,39	0
4	PO4	B	1817	5/5	0.98	0.10	-2.73	27,27,29,29	0
4	PO4	A	1819	5/5	0.98	0.08	-4.46	24,25,29,30	0
6	FE	C	2	1/1	0.99	0.06	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	PO4	B	1819	5/5	0.97	0.22	-	46,46,50,51	0
4	PO4	A	1821	5/5	0.96	0.24	-	53,53,53,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.