



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:06 am GMT

PDB ID : 2W6U  
Title : STRUCTURES OF P. AERUGINOSA FPVA BOUND TO HETEROLOGOUS PYOVERDINES: FPVA-PVD(G173)-FE COMPLEX  
Authors : Greenwald, J.; Nader, M.; Celia, H.; Gruffaz, C.; Meyer, J.-M.; Schalk, I.J.; Pattus, F.  
Deposited on : 2008-12-19  
Resolution : 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

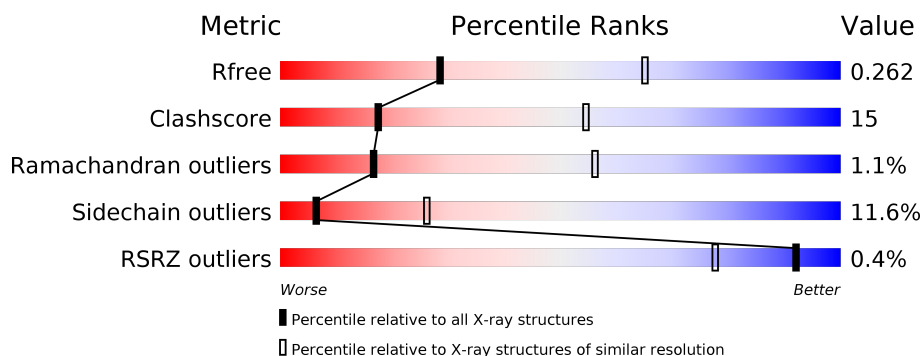
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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  $\geq 3$ , 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	 63% 30% 6% .
1	B	772	 65% 29% . . .
2	C	7	 71% 29%

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	DAS	C	7	-	-	X	-
3	N8E	A	1816	-	-	-	X
4	PO4	A	1822	-	-	-	X

## 2 Entry composition [i](#)

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.

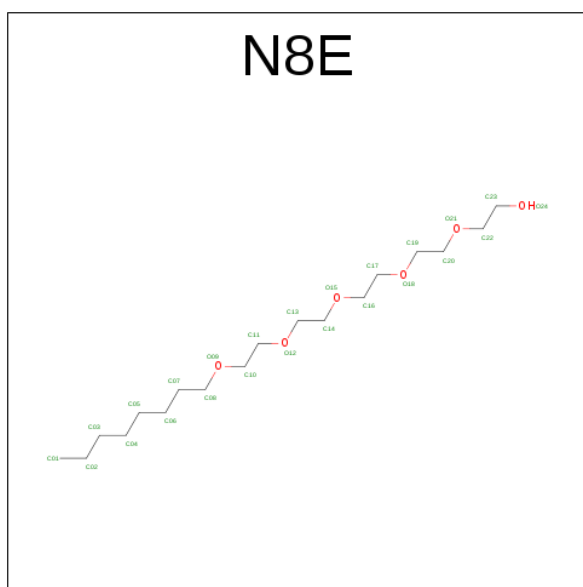
- Molecule 1 is a protein called FERRIPYOVERDINE RECEPTOR.

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 G173.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			57	32	10	15			

- Molecule 3 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (three-letter code: N8E) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>6</sub>).



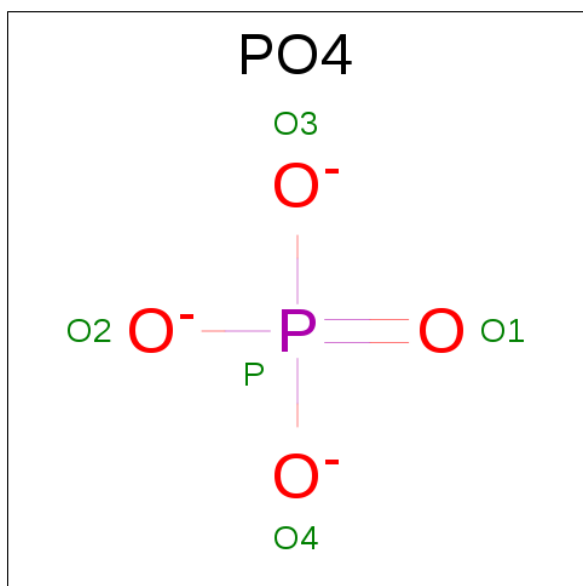
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	18	6		

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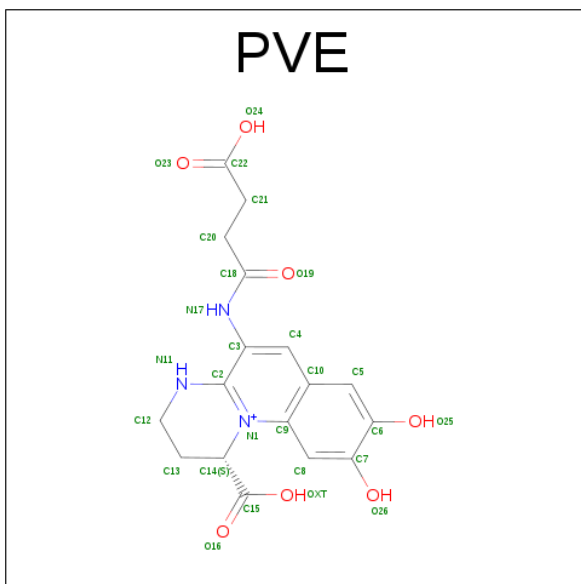
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			48	36	12		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 5 is (1S)-1-CARBOXY-5-[(3-CARBOXYPROPANOYL)AMINO]-8,9-DIHYDROXY-1,2,3,4-TETRAHYDROPYRIMIDO[1,2-A]QUINOLIN-11-IUM (three-letter code: PVE) (formula: C<sub>17</sub>H<sub>18</sub>N<sub>3</sub>O<sub>7</sub>).



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

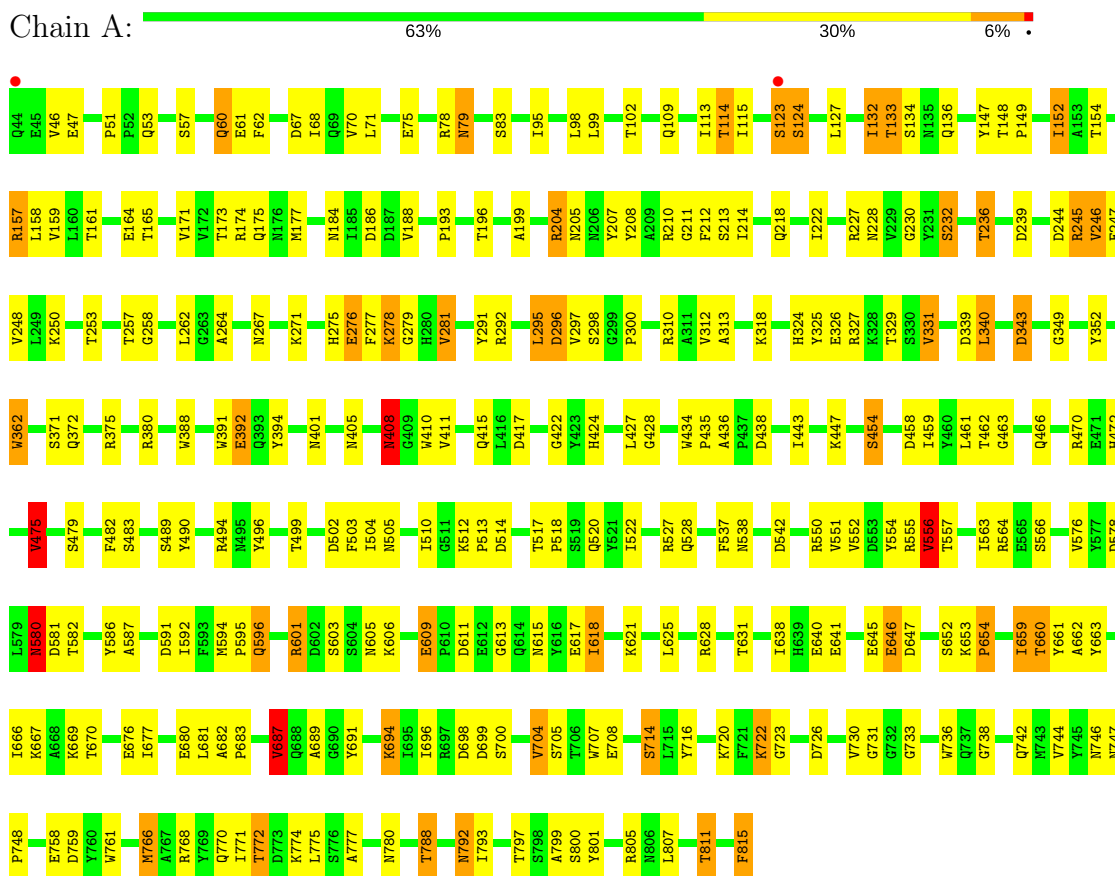
- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

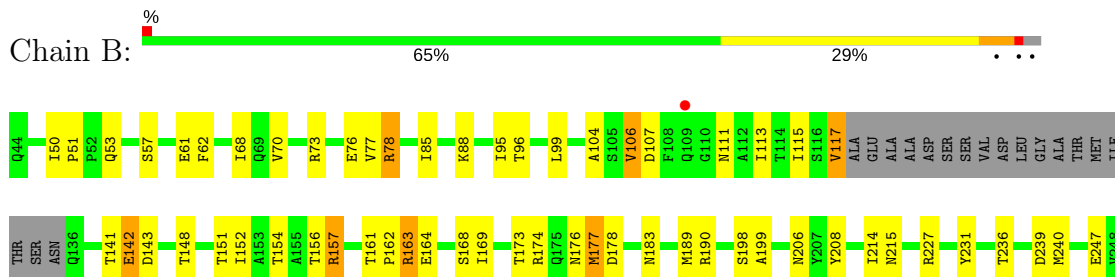
### 3 Residue-property plots

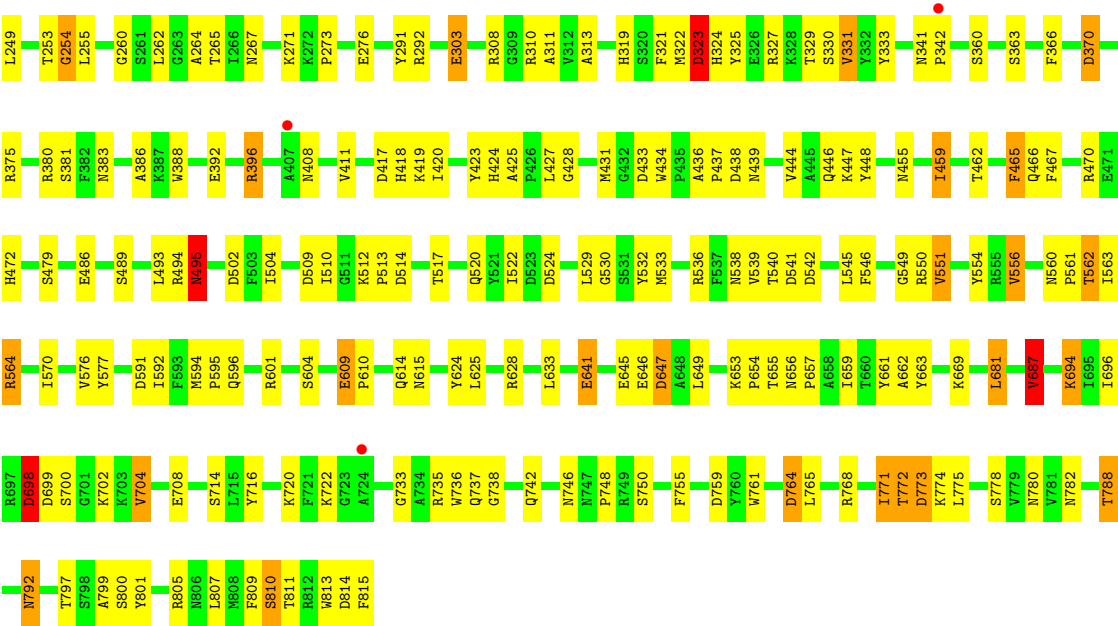
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.77Å 129.93Å 141.56Å 90.00° 130.36° 90.00°	Depositor
Resolution (Å)	97.59 – 3.00 27.52 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.4 (97.59-3.00) 89.6 (27.52-3.00)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.209 , 0.266 0.210 , 0.262	Depositor DCC
$R_{free}$ test set	2449 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12314	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.03	3/6266 (0.0%)	1.05	12/8514 (0.1%)
1	B	0.90	3/6145 (0.0%)	0.96	13/8347 (0.2%)
2	C	1.31	0/9	1.92	1/9 (11.1%)
All	All	0.97	6/12420 (0.0%)	1.01	26/16870 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
2	C	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	GLU	CG-CD	6.14	1.61	1.51
1	B	773	ASP	CB-CG	5.47	1.63	1.51
1	B	267	ASN	CB-CG	5.42	1.63	1.51
1	B	323	ASP	CB-CG	-5.39	1.40	1.51
1	A	276	GLU	CG-CD	5.21	1.59	1.51
1	A	362	TRP	CE3-CZ3	5.19	1.47	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	VAL	CB-CA-C	-8.02	96.17	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ASP	CB-CG-OD1	7.88	125.39	118.30
1	B	323	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	A	295	LEU	CA-CB-CG	6.59	130.46	115.30
1	B	768	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	580	ASN	CB-CA-C	-6.06	98.29	110.40
1	B	687	VAL	CB-CA-C	-5.92	100.15	111.40
1	A	768	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	B	773	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	765	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	71	LEU	CA-CB-CG	5.73	128.47	115.30
1	B	545	LEU	CA-CB-CG	5.72	128.46	115.30
1	B	698	ASP	CB-CA-C	-5.71	98.99	110.40
1	B	239	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	A	362	TRP	CA-CB-CG	5.48	124.11	113.70
1	A	475	VAL	CB-CA-C	-5.38	101.18	111.40
1	A	556	VAL	CB-CA-C	5.35	121.56	111.40
2	C	4	ALA	N-CA-C	5.34	125.43	111.00
1	B	768	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	281	VAL	N-CA-C	-5.26	96.79	111.00
1	B	681	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	514	ASP	CB-CG-OD1	5.23	123.00	118.30
1	B	649	LEU	CB-CG-CD1	5.20	119.83	111.00
1	B	764	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	A	67	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	514	ASP	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ILE	Peptide
1	B	208	TYR	Peptide
1	B	698	ASP	Peptide
2	C	3	DSN	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	190	0
1	B	5994	0	5675	173	0
2	C	57	0	43	11	0
3	A	72	0	114	17	0
4	A	30	0	0	2	0
4	B	20	0	0	2	0
5	C	26	0	14	1	0
6	C	1	0	0	0	0
All	All	12314	0	11634	368	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 15.

All (368) 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:396:ARG:HG2	1:B:396:ARG:HH11	1.18	1.02
1:B:696:ILE:HG23	1:B:704:VAL:HG12	1.42	1.01
1:B:772:THR:HG22	1:B:774:LYS:H	1.20	0.99
1:B:189:MET:HE2	1:B:189:MET:HA	1.45	0.98
1:B:363:SER:HB3	1:B:431:MET:CE	1.98	0.94
1:A:53:GLN:OE1	1:A:57:SER:HB2	1.68	0.93
1:B:698:ASP:HB3	1:B:700:SER:H	1.33	0.91
1:A:805:ARG:HD2	3:A:1817[A]:N8E:H031	1.52	0.90
1:B:396:ARG:HG2	1:B:396:ARG:NH1	1.83	0.89
1:B:536:ARG:HD2	1:B:546:PHE:CZ	2.09	0.88
1:A:772:THR:HG21	1:B:291:TYR:OH	1.78	0.83
1:A:777:ALA:HB1	3:A:1817[B]:N8E:H192	1.61	0.82
1:A:133:THR:HG21	1:A:159:VAL:HG21	1.62	0.81
1:B:154:THR:OG1	1:B:247:GLU:OE1	1.99	0.81
1:B:363:SER:HB2	2:C:8:AHO:HC71	1.60	0.81
1:B:363:SER:HB3	1:B:431:MET:HE1	1.64	0.78
1:B:792:ASN:HB3	1:B:800:SER:HB2	1.65	0.77
1:A:694:LYS:HE2	1:A:708:GLU:OE1	1.85	0.77
1:B:772:THR:HG22	1:B:774:LYS:N	2.00	0.76
3:A:1817[B]:N8E:H031	1:B:805:ARG:HD2	1.66	0.76
1:B:560:ASN:HB3	1:B:561:PRO:HD2	1.68	0.75
2:C:6:ORN:HG3	2:C:7:DAS:N	1.99	0.75
1:A:694:LYS:HE2	1:A:708:GLU:CD	2.06	0.75
1:A:443:ILE:HG13	1:A:510:ILE:CD1	2.16	0.75
1:B:646:GLU:O	1:B:662:ALA:O	2.04	0.75
1:A:722:LYS:HG3	1:A:723:GLY:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:ARG:NH1	3:A:1817[A]:N8E:H013	2.01	0.74
1:A:603:SER:O	1:A:659:ILE:HD11	1.88	0.74
1:B:363:SER:CB	1:B:431:MET:CE	2.66	0.74
1:A:811:THR:CG2	3:A:1817[A]:N8E:H232	2.17	0.74
1:A:291:TYR:OH	1:B:772:THR:HG21	1.86	0.74
1:B:370:ASP:HA	1:B:434:TRP:O	1.88	0.73
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.70	0.73
1:A:443:ILE:HG13	1:A:510:ILE:HD13	1.69	0.72
1:B:255:LEU:O	1:B:550:ARG:HD2	1.88	0.72
1:B:470:ARG:HH12	1:B:540:THR:HA	1.54	0.72
1:B:540:THR:HG22	1:B:541:ASP:H	1.55	0.72
1:B:189:MET:CE	1:B:189:MET:HA	2.18	0.71
1:A:204:ARG:HG3	1:A:391:TRP:CH2	2.25	0.71
1:B:142:GLU:HB2	1:B:174:ARG:HG2	1.71	0.71
1:A:527:ARG:HH21	1:A:555:ARG:HD2	1.56	0.70
1:A:805:ARG:HH11	3:A:1817[A]:N8E:H013	1.56	0.70
1:A:262:LEU:HD21	1:A:613:GLY:HA3	1.74	0.70
1:A:244:ASP:O	1:A:245:ARG:HB3	1.91	0.70
1:A:792:ASN:HB3	1:A:800:SER:HB2	1.72	0.69
1:A:214:ILE:HG12	1:A:264:ALA:HB3	1.74	0.69
1:A:222:ILE:HD11	1:A:415:GLN:NE2	2.08	0.69
1:A:165:THR:O	1:A:621:LYS:NZ	2.25	0.68
1:A:188:VAL:HG11	1:A:246:VAL:CG1	2.24	0.68
1:B:681:LEU:HD22	1:B:687:VAL:HG13	1.76	0.68
1:B:698:ASP:HB3	1:B:700:SER:N	2.06	0.68
1:B:737:GLN:O	1:B:759:ASP:HB2	1.94	0.68
1:A:742:GLN:HG3	1:A:793:ILE:O	1.94	0.67
1:B:696:ILE:CG2	1:B:704:VAL:HG12	2.22	0.67
1:B:363:SER:CB	1:B:431:MET:HE1	2.24	0.67
1:A:615:ASN:HD21	1:A:617:GLU:HB2	1.60	0.67
1:A:392:GLU:HG2	1:A:424:HIS:HB3	1.77	0.66
1:A:554:TYR:CD2	1:A:595:PRO:HG2	2.30	0.66
1:B:418:HIS:HE1	4:B:1821:PO4:O1	1.79	0.66
1:A:99:LEU:O	1:A:102:THR:HG23	1.96	0.65
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.31	0.65
1:A:157:ARG:HB3	1:A:475:VAL:HG11	1.77	0.65
1:B:152:ILE:HD12	1:B:169:ILE:HG12	1.78	0.64
1:A:454:SER:OG	1:A:483:SER:HB2	1.98	0.64
1:A:411:VAL:HG13	1:A:462:THR:HG22	1.80	0.64
1:B:564:ARG:HH11	1:B:564:ARG:CG	2.11	0.64
1:A:722:LYS:HG3	1:A:723:GLY:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ILE:O	1:B:459:ILE:HG13	1.98	0.63
1:A:371:SER:OG	1:A:436:ALA:HA	1.97	0.63
1:A:281:VAL:HG23	1:A:815:PHE:CZ	2.33	0.63
1:A:208:TYR:HA	1:A:212:PHE:O	1.99	0.63
1:A:297:VAL:HG12	3:A:1816:N8E:H162	1.81	0.63
3:A:1817[B]:N8E:H052	1:B:805:ARG:HD2	1.81	0.63
2:C:7:DAS:HA	2:C:9:SER:HB3	1.81	0.62
1:A:53:GLN:OE1	1:A:57:SER:CB	2.45	0.62
1:B:323:ASP:HB2	1:B:381:SER:O	1.98	0.62
1:A:186:ASP:OD1	1:A:207:TYR:OH	2.13	0.62
1:A:771:ILE:HG12	1:B:809:PHE:CD1	2.34	0.62
1:B:540:THR:HG22	1:B:541:ASP:N	2.14	0.61
3:A:1817[A]:N8E:H221	1:B:811:THR:OG1	1.99	0.61
1:A:158:LEU:CD2	1:A:475:VAL:HG22	2.31	0.61
1:A:188:VAL:HG11	1:A:246:VAL:HG11	1.82	0.61
1:A:132:ILE:HG23	1:A:133:THR:H	1.66	0.61
1:A:410:TRP:CD2	1:A:463:GLY:HA3	2.36	0.61
1:A:811:THR:HG21	3:A:1817[A]:N8E:H232	1.83	0.60
1:B:772:THR:CG2	1:B:773:ASP:N	2.64	0.60
1:A:470:ARG:NH1	1:A:538:ASN:OD1	2.33	0.60
1:B:694:LYS:HE3	1:B:708:GLU:OE1	2.01	0.60
1:B:669:LYS:O	1:B:696:ILE:HA	2.02	0.60
1:A:777:ALA:HB1	3:A:1817[B]:N8E:C19	2.32	0.60
1:A:132:ILE:CG2	1:A:133:THR:H	2.15	0.60
1:A:680:GLU:HG3	1:A:682:ALA:O	2.02	0.60
1:A:631:THR:HG22	1:A:677:ILE:HG13	1.84	0.59
1:B:694:LYS:NZ	1:B:708:GLU:O	2.35	0.59
1:A:747:ASN:HB3	1:A:748:PRO:HD3	1.84	0.59
1:B:646:GLU:O	1:B:663:TYR:HA	2.01	0.59
1:A:158:LEU:HD21	1:A:475:VAL:HG22	1.84	0.59
1:A:797:THR:HG22	1:A:797:THR:O	2.02	0.59
1:B:324:HIS:CE1	1:B:383:ASN:HB3	2.38	0.59
1:A:807:LEU:HD11	3:A:1817[A]:N8E:H061	1.84	0.59
1:A:646:GLU:O	1:A:662:ALA:O	2.21	0.59
1:A:210:ARG:O	1:A:670:THR:HG21	2.02	0.59
1:A:707:TRP:CH2	1:A:793:ILE:HG13	2.38	0.59
1:B:470:ARG:NH1	1:B:540:THR:HA	2.17	0.59
1:A:132:ILE:CG2	1:A:133:THR:N	2.66	0.58
1:A:601:ARG:NH1	1:A:605:ASN:O	2.37	0.58
1:A:392:GLU:CG	1:A:424:HIS:HB3	2.33	0.58
1:A:277:PHE:O	1:A:278:LYS:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:ASN:O	1:A:799:ALA:HA	2.02	0.58
1:A:805:ARG:HD3	3:A:1817[A]:N8E:H052	1.85	0.58
1:A:127:LEU:HD11	1:A:581:ASP:HA	1.85	0.58
1:B:542:ASP:O	1:B:577:TYR:HA	2.03	0.58
1:A:512:LYS:HD2	4:A:1818:PO4:O1	2.03	0.58
1:A:79:ASN:OD1	1:A:79:ASN:N	2.37	0.57
1:B:50:ILE:HG23	1:B:53:GLN:NE2	2.19	0.57
1:B:141:THR:HG21	1:B:173:THR:HG22	1.87	0.57
1:A:443:ILE:CG1	1:A:510:ILE:CD1	2.82	0.57
1:B:536:ARG:HB2	1:B:546:PHE:CE1	2.39	0.57
1:A:587:ALA:HB2	1:A:618:ILE:HG13	1.87	0.57
1:B:363:SER:CB	1:B:431:MET:HE2	2.35	0.57
1:B:694:LYS:HZ2	1:B:708:GLU:HG2	1.69	0.57
1:B:380:ARG:HD3	1:B:788:THR:HB	1.85	0.57
1:A:738:GLY:HA2	1:A:759:ASP:HB3	1.86	0.56
1:A:46:VAL:HG12	1:A:47:GLU:N	2.19	0.56
1:B:554:TYR:CD2	1:B:595:PRO:HG2	2.40	0.56
2:C:3:DSN:OG	2:C:4:ALA:N	2.33	0.56
1:A:435:PRO:HD3	1:A:503:PHE:CE1	2.40	0.56
1:A:380:ARG:HD3	1:A:788:THR:HB	1.88	0.56
1:A:60:GLN:HE21	1:A:134:SER:HA	1.71	0.56
1:B:62:PHE:CZ	1:B:95:ILE:HB	2.40	0.56
1:B:174:ARG:NH2	1:B:178:ASP:OD1	2.38	0.56
1:B:262:LEU:HD23	1:B:592:ILE:HG22	1.87	0.55
1:B:375:ARG:NE	1:B:755:PHE:CZ	2.74	0.55
1:A:580:ASN:HB2	1:A:582:THR:H	1.70	0.55
1:A:391:TRP:HB2	1:A:427:LEU:HD21	1.87	0.55
1:B:156:THR:O	1:B:157:ARG:HB2	2.06	0.55
1:B:659:ILE:HG23	1:B:659:ILE:O	2.06	0.55
1:A:738:GLY:HA2	1:A:759:ASP:CB	2.37	0.55
1:B:303:GLU:H	1:B:303:GLU:CD	2.10	0.55
1:B:738:GLY:HA2	1:B:759:ASP:CB	2.37	0.55
1:B:311:ALA:HA	1:B:333:TYR:O	2.06	0.55
1:B:775:LEU:HD13	1:B:813:TRP:HB2	1.89	0.55
1:A:109:GLN:OE1	1:A:114:THR:HG22	2.07	0.54
1:A:408:ASN:HB3	1:A:410:TRP:H	1.71	0.54
1:A:736:TRP:HB2	1:A:761:TRP:CE3	2.43	0.54
1:A:75:GLU:HB2	1:A:78:ARG:NH2	2.22	0.54
1:A:75:GLU:OE1	1:A:75:GLU:N	2.40	0.54
2:C:3:DSN:N	5:C:1:PVE:H8	2.22	0.54
3:A:1817[B]:N8E:H052	1:B:805:ARG:CD	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:TYR:OH	1:B:772:THR:CG2	2.54	0.54
1:A:253:THR:O	1:A:257:THR:HB	2.06	0.54
1:A:410:TRP:CE2	1:A:463:GLY:HA3	2.43	0.54
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.42	0.54
1:A:133:THR:HG21	1:A:159:VAL:CG2	2.34	0.53
1:A:458:ASP:OD2	1:A:479:SER:HB3	2.07	0.53
1:B:425:ALA:HB1	1:B:427:LEU:HD21	1.89	0.53
1:B:646:GLU:HA	1:B:663:TYR:CD2	2.44	0.53
1:B:772:THR:CG2	1:B:774:LYS:H	2.08	0.53
2:C:7:DAS:HA	2:C:9:SER:CB	2.39	0.53
1:A:199:ALA:HA	1:A:205:ASN:HD22	1.74	0.53
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.44	0.53
1:B:512:LYS:HG3	1:B:513:PRO:HD2	1.90	0.53
1:A:646:GLU:HG3	1:A:661:TYR:OH	2.08	0.52
1:A:722:LYS:HA	1:A:726:ASP:HB3	1.90	0.52
1:A:380:ARG:HA	1:A:801:TYR:CD2	2.45	0.52
1:A:556:VAL:HG22	1:A:563:ILE:HD12	1.91	0.52
1:B:446:GLN:OE1	1:B:448:TYR:OH	2.25	0.52
1:A:447:LYS:HB3	1:A:490:TYR:HB2	1.91	0.52
1:A:723:GLY:O	1:A:726:ASP:OD2	2.27	0.52
1:A:51:PRO:O	1:A:53:GLN:HG2	2.09	0.52
1:A:772:THR:HG22	1:A:774:LYS:H	1.73	0.52
1:B:494:ARG:O	1:B:495:ASN:C	2.48	0.52
1:B:76:GLU:HG2	1:B:117:VAL:HB	1.92	0.52
1:B:151:THR:HG22	1:B:161:THR:HG22	1.91	0.52
1:B:341:ASN:HB2	1:B:342:PRO:CD	2.38	0.52
1:B:198:SER:OG	1:B:206:ASN:HB3	2.10	0.51
1:B:50:ILE:HG12	1:B:61:GLU:HG2	1.92	0.51
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.46	0.51
1:A:527:ARG:NH2	1:A:555:ARG:HD2	2.25	0.51
1:B:764:ASP:CB	1:B:782:ASN:HA	2.41	0.51
1:A:193:PRO:O	1:A:250:LYS:HE2	2.11	0.51
1:A:228:ASN:OD1	1:A:230:GLY:N	2.44	0.51
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.46	0.51
1:A:770:GLN:NE2	1:A:772:THR:O	2.34	0.51
1:B:396:ARG:CG	1:B:396:ARG:HH11	2.00	0.51
1:A:174:ARG:CZ	1:A:177:MET:HE2	2.40	0.51
1:B:77:VAL:O	1:B:78:ARG:C	2.49	0.50
1:A:517:THR:O	1:A:518:PRO:C	2.47	0.50
1:B:156:THR:O	1:B:157:ARG:CB	2.60	0.50
1:B:736:TRP:HB2	1:B:761:TRP:CE3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:ORN:CG	2:C:7:DAS:N	2.68	0.50
1:A:434:TRP:HB3	1:A:435:PRO:HA	1.92	0.50
1:A:438:ASP:OD1	1:A:438:ASP:C	2.50	0.50
1:B:646:GLU:HG3	1:B:661:TYR:OH	2.10	0.50
1:A:211:GLY:HA2	1:A:708:GLU:OE1	2.10	0.50
1:B:439:ASN:ND2	1:B:502:ASP:HA	2.27	0.50
1:A:218:GLN:NE2	1:A:267:ASN:HB2	2.27	0.50
1:A:611:ASP:OD1	1:A:640:GLU:OE2	2.30	0.50
1:B:174:ARG:NH2	1:B:177:MET:HB3	2.27	0.50
1:B:694:LYS:NZ	1:B:708:GLU:HG2	2.27	0.50
1:A:228:ASN:O	1:A:232:SER:HB2	2.12	0.50
1:A:646:GLU:O	1:A:647:ASP:HB3	2.12	0.50
1:B:556:VAL:HG13	1:B:563:ILE:HB	1.94	0.49
1:B:625:LEU:O	1:B:628:ARG:HD3	2.12	0.49
1:A:147:TYR:HA	1:A:173:THR:OG1	2.12	0.49
1:B:467:PHE:HB3	1:B:472:HIS:CE1	2.47	0.49
1:B:249:LEU:O	1:B:264:ALA:HA	2.13	0.49
1:A:343:ASP:HB2	1:A:405:ASN:HB2	1.94	0.49
1:B:370:ASP:O	1:B:433:ASP:HB3	2.13	0.49
1:B:152:ILE:CD1	1:B:169:ILE:HG12	2.42	0.49
1:B:321:PHE:CE1	1:B:322:MET:HG3	2.46	0.49
1:A:401:ASN:ND2	1:A:415:GLN:HG2	2.27	0.49
1:B:70:VAL:HG13	1:B:113:ILE:CG1	2.43	0.49
1:B:363:SER:HB2	2:C:8:AHO:C7	2.35	0.48
1:A:811:THR:HG23	3:A:1817[A]:N8E:H232	1.95	0.48
1:A:199:ALA:HA	1:A:205:ASN:ND2	2.28	0.48
1:B:436:ALA:HB1	1:B:437:PRO:CD	2.43	0.48
1:B:774:LYS:HE2	1:B:814:ASP:O	2.13	0.48
3:A:1817[B]:N8E:H031	1:B:805:ARG:HH11	1.78	0.48
1:A:352:TYR:CD1	1:A:352:TYR:C	2.87	0.48
1:B:470:ARG:HH12	1:B:540:THR:CA	2.25	0.48
1:A:666:ILE:HD12	1:A:698:ASP:HB2	1.94	0.48
1:B:735:ARG:NH2	1:B:737:GLN:OE1	2.30	0.48
1:B:50:ILE:HD12	1:B:85:ILE:HD11	1.94	0.48
1:B:50:ILE:HG23	1:B:53:GLN:HE21	1.78	0.48
1:B:470:ARG:NH2	1:B:541:ASP:OD1	2.43	0.48
1:B:609:GLU:HG3	1:B:610:PRO:HD2	1.96	0.48
1:A:46:VAL:CG1	1:A:47:GLU:N	2.76	0.47
1:B:214:ILE:CD1	1:B:264:ALA:HB3	2.44	0.47
1:B:532:TYR:HA	1:B:549:GLY:O	2.15	0.47
1:A:123:SER:O	1:A:124:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:PRO:HG3	1:A:660:THR:O	2.15	0.47
1:A:576:VAL:HG22	1:A:586:TYR:HB3	1.96	0.47
1:A:275:HIS:O	1:A:300:PRO:HD3	2.14	0.47
1:A:435:PRO:HD3	1:A:503:PHE:CD1	2.49	0.47
1:A:496:TYR:CG	1:A:513:PRO:HB3	2.49	0.47
1:A:638:ILE:HB	1:A:670:THR:HB	1.95	0.47
1:A:775:LEU:C	1:A:775:LEU:HD23	2.34	0.47
1:A:502:ASP:OD2	1:A:505:ASN:HB2	2.14	0.47
1:A:98:LEU:C	1:A:98:LEU:HD23	2.35	0.47
1:B:764:ASP:HB3	1:B:782:ASN:HA	1.97	0.47
1:B:106:VAL:HG13	1:B:115:ILE:HD13	1.97	0.47
1:B:772:THR:HG22	1:B:773:ASP:N	2.30	0.47
1:B:653:LYS:HA	1:B:654:PRO:HD2	1.66	0.47
1:B:262:LEU:CD2	1:B:592:ILE:HG22	2.45	0.47
1:A:239:ASP:OD2	1:A:292:ARG:NH2	2.48	0.46
1:A:472:HIS:ND1	1:A:537:PHE:HA	2.31	0.46
1:B:417:ASP:O	1:B:455:ASN:HA	2.15	0.46
1:A:161:THR:OG1	1:A:164:GLU:HG3	2.16	0.46
1:A:174:ARG:NH1	1:A:177:MET:CE	2.79	0.46
1:A:443:ILE:HG13	1:A:510:ILE:HD12	1.96	0.46
1:A:435:PRO:HB3	1:A:503:PHE:CB	2.45	0.46
1:B:530:GLY:HA2	1:B:551:VAL:O	2.16	0.46
1:B:646:GLU:O	1:B:647:ASP:CB	2.64	0.46
1:A:271:LYS:NZ	1:A:296:ASP:OD2	2.44	0.46
1:B:313:ALA:HA	1:B:331:VAL:O	2.16	0.46
1:B:50:ILE:HA	1:B:51:PRO:HD3	1.62	0.46
1:A:313:ALA:HA	1:A:331:VAL:O	2.16	0.45
1:B:260:GLY:O	1:B:594:MET:HB2	2.16	0.45
1:A:698:ASP:OD1	1:A:700:SER:OG	2.26	0.45
1:A:772:THR:HG22	1:A:774:LYS:N	2.31	0.45
1:B:538:ASN:ND2	1:B:540:THR:O	2.49	0.45
1:A:443:ILE:CG1	1:A:510:ILE:HD12	2.47	0.45
1:B:564:ARG:HG3	1:B:564:ARG:HH11	1.82	0.45
1:B:614:GLN:OE1	1:B:641:GLU:OE2	2.33	0.45
1:A:681:LEU:HG	1:A:687:VAL:HG22	1.99	0.45
1:A:388:TRP:CH2	1:A:428:GLY:HA3	2.52	0.45
1:B:142:GLU:O	1:B:143:ASP:HB2	2.17	0.45
1:A:489:SER:HB2	1:A:520:GLN:HB3	1.99	0.45
1:A:325:TYR:OH	1:A:327:ARG:NH1	2.50	0.44
1:A:339:ASP:O	1:A:340:LEU:C	2.55	0.44
1:B:231:TYR:HB3	1:B:423:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ARG:HG2	1:A:552:VAL:CG2	2.47	0.44
1:B:189:MET:CE	1:B:189:MET:CA	2.92	0.44
1:B:746:ASN:OD1	1:B:748:PRO:HD2	2.17	0.44
2:C:7:DAS:HA	2:C:9:SER:CA	2.47	0.44
1:B:694:LYS:HD2	1:B:694:LYS:C	2.38	0.44
1:A:174:ARG:NH1	1:A:177:MET:HE2	2.33	0.44
1:A:318:LYS:HG3	1:A:318:LYS:O	2.18	0.44
1:A:731:GLY:O	1:A:766:MET:N	2.50	0.44
1:B:396:ARG:CG	1:B:396:ARG:NH1	2.61	0.44
1:B:470:ARG:NH1	1:B:539:VAL:O	2.48	0.44
1:A:147:TYR:HA	1:A:173:THR:HG1	1.82	0.44
1:B:50:ILE:CG2	1:B:53:GLN:HE21	2.31	0.44
1:B:570:ILE:HG23	1:B:591:ASP:HB3	1.99	0.44
1:A:258:GLY:HA2	1:A:550:ARG:HD3	2.00	0.44
1:A:392:GLU:O	1:A:392:GLU:HG3	2.18	0.44
1:A:262:LEU:HD23	1:A:592:ILE:HG22	2.00	0.44
1:B:366:PHE:CE2	1:B:799:ALA:HB3	2.52	0.44
1:B:646:GLU:O	1:B:647:ASP:HB3	2.18	0.44
1:B:681:LEU:HD13	1:B:687:VAL:HG22	1.99	0.44
1:A:295:LEU:O	1:A:312:VAL:HA	2.18	0.43
1:A:408:ASN:HB3	1:A:410:TRP:HB2	2.00	0.43
1:A:482:PHE:CD2	1:A:527:ARG:HG3	2.54	0.43
1:A:152:ILE:HA	1:A:152:ILE:HD13	1.68	0.43
1:B:392:GLU:HB2	1:B:424:HIS:O	2.17	0.43
1:B:419:LYS:HG3	1:B:420:ILE:N	2.33	0.43
1:A:171:VAL:HG22	1:A:247:GLU:HB3	1.99	0.43
1:B:386:ALA:N	1:B:428:GLY:O	2.46	0.43
1:A:174:ARG:CZ	4:A:1823:PO4:O2	2.67	0.43
1:A:615:ASN:ND2	1:A:617:GLU:HB2	2.32	0.43
1:B:199:ALA:O	1:B:792:ASN:HB2	2.19	0.43
1:A:148:THR:OG1	1:A:149:PRO:HD2	2.19	0.43
1:A:207:TYR:O	1:A:214:ILE:HD12	2.18	0.43
1:A:550:ARG:HG2	1:A:552:VAL:HG22	2.01	0.43
1:A:646:GLU:O	1:A:647:ASP:CB	2.67	0.43
1:A:236:THR:H	1:A:236:THR:HG22	1.53	0.43
1:A:175:GLN:HG3	1:A:175:GLN:O	2.18	0.42
1:A:746:ASN:C	1:A:746:ASN:OD1	2.57	0.42
1:B:738:GLY:HA2	1:B:759:ASP:HB2	2.01	0.42
1:B:772:THR:HG23	1:B:773:ASP:H	1.83	0.42
1:A:411:VAL:HG13	1:A:462:THR:CG2	2.48	0.42
1:A:667:LYS:HB2	1:A:699:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ASN:ND2	1:B:227:ARG:O	2.42	0.42
1:B:183:ASN:O	1:B:240:MET:HB2	2.19	0.42
1:B:771:ILE:HG13	1:B:771:ILE:H	1.26	0.42
1:B:772:THR:HB	1:B:775:LEU:HB3	2.00	0.42
2:C:5:AHO:HC73	2:C:5:AHO:HC52	1.91	0.42
1:A:298:SER:HB2	1:A:310:ARG:HG3	2.01	0.42
1:B:797:THR:O	1:B:797:THR:HG22	2.19	0.42
1:A:349:GLY:HA2	3:A:1816:N8E:H051	2.00	0.42
1:B:681:LEU:HD13	1:B:687:VAL:CG2	2.49	0.42
1:B:778:SER:HB2	1:B:810:SER:HB3	2.01	0.42
1:B:479:SER:O	1:B:529:LEU:HA	2.20	0.42
1:A:184:ASN:C	1:A:184:ASN:OD1	2.57	0.42
1:A:691:TYR:CD2	1:A:691:TYR:C	2.93	0.42
1:A:62:PHE:CZ	1:A:95:ILE:HB	2.55	0.42
1:A:279:GLY:HA3	1:A:296:ASP:O	2.20	0.42
1:B:273:PRO:HB2	1:B:308:ARG:HB3	2.01	0.42
1:A:70:VAL:CG1	1:A:115:ILE:HD13	2.50	0.41
1:A:591:ASP:CG	1:A:592:ILE:N	2.73	0.41
1:A:704:VAL:O	1:A:705:SER:C	2.59	0.41
1:A:689:ALA:HA	1:A:714:SER:O	2.19	0.41
1:B:764:ASP:HB2	1:B:782:ASN:HA	2.02	0.41
1:A:132:ILE:HG22	1:A:133:THR:N	2.35	0.41
1:B:472:HIS:HD2	1:B:538:ASN:H	1.68	0.41
1:B:388:TRP:CZ2	1:B:513:PRO:HD3	2.55	0.41
1:B:465:PHE:CD1	1:B:465:PHE:N	2.89	0.41
2:C:7:DAS:HA	2:C:9:SER:O	2.21	0.41
1:A:646:GLU:HA	1:A:663:TYR:CD2	2.54	0.41
1:B:162:PRO:O	1:B:163:ARG:C	2.57	0.41
1:B:271:LYS:HD3	1:B:310:ARG:NH2	2.35	0.41
1:B:540:THR:CG2	1:B:541:ASP:H	2.28	0.41
1:A:132:ILE:HD13	1:A:132:ILE:HA	1.94	0.41
1:B:363:SER:HB3	1:B:431:MET:HE2	1.92	0.41
1:B:99:LEU:HD22	1:B:104:ALA:HB3	2.03	0.41
1:B:780:ASN:O	1:B:807:LEU:HA	2.20	0.41
1:A:596:GLN:NE2	1:A:609:GLU:O	2.53	0.41
1:A:625:LEU:O	1:A:628:ARG:HB2	2.21	0.41
1:B:431:MET:HG3	1:B:444:VAL:CG2	2.50	0.41
1:A:594:MET:HA	1:A:595:PRO:HD3	1.90	0.41
1:B:375:ARG:HE	1:B:755:PHE:HZ	1.60	0.41
1:B:438:ASP:OD1	1:B:438:ASP:N	2.48	0.41
1:B:418:HIS:CD2	1:B:455:ASN:HD21	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:GLN:NE2	1:B:641:GLU:OE2	2.53	0.41
1:B:111:ASN:HB2	1:B:276:GLU:OE1	2.21	0.41
1:B:254:GLY:N	1:B:592:ILE:HD12	2.35	0.41
1:A:188:VAL:HG11	1:A:246:VAL:HG13	2.01	0.40
1:A:669:LYS:O	1:A:696:ILE:HA	2.21	0.40
1:B:190:ARG:NH2	4:B:1819:PO4:O3	2.55	0.40
1:A:136:GLN:HE22	1:A:462:THR:HG21	1.86	0.40
1:B:325:TYR:OH	1:B:327:ARG:HD3	2.21	0.40
1:A:716:TYR:CE1	1:A:733:GLY:HA3	2.57	0.40
1:B:489:SER:HB2	1:B:520:GLN:HB3	2.03	0.40
1:B:656:ASN:HA	1:B:657:PRO:HD2	1.93	0.40
1:A:470:ARG:HD3	1:A:538:ASN:O	2.22	0.40
1:B:161:THR:HG23	1:B:164:GLU:OE1	2.22	0.40
1:B:486:GLU:HA	1:B:522:ILE:O	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%)	706 (92%)	57 (7%)	7 (1%)	20	62
1	B	750/772 (97%)	689 (92%)	52 (7%)	9 (1%)	15	53
All	All	1520/1544 (98%)	1395 (92%)	109 (7%)	16 (1%)	17	56

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	SER
1	A	408	ASN
1	B	408	ASN
1	B	647	ASP

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Mol	Chain	Res	Type
1	B	699	ASP
1	A	324	HIS
1	A	340	LEU
1	A	646	GLU
1	B	78	ARG
1	B	323	ASP
1	A	245	ARG
1	B	370	ASP
1	B	562	THR
1	B	495	ASN
1	A	653	LYS
1	B	254	GLY

### 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%)	572 (88%)	78 (12%)	6	25
1	B	637/650 (98%)	566 (89%)	71 (11%)	7	28
2	C	1/1 (100%)	1 (100%)	0	100	100
All	All	1288/1301 (99%)	1139 (88%)	149 (12%)	6	26

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	68	ILE
1	A	79	ASN
1	A	83	SER
1	A	113	ILE
1	A	114	THR
1	A	123	SER
1	A	133	THR
1	A	152	ILE
1	A	154	THR

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Mol	Chain	Res	Type
1	A	157	ARG
1	A	196	THR
1	A	204	ARG
1	A	213	SER
1	A	227	ARG
1	A	232	SER
1	A	236	THR
1	A	246	VAL
1	A	248	VAL
1	A	276	GLU
1	A	278	LYS
1	A	326	GLU
1	A	329	THR
1	A	331	VAL
1	A	343	ASP
1	A	362	TRP
1	A	372	GLN
1	A	375	ARG
1	A	392	GLU
1	A	408	ASN
1	A	417	ASP
1	A	454	SER
1	A	459	ILE
1	A	461	LEU
1	A	466	GLN
1	A	475	VAL
1	A	494	ARG
1	A	499	THR
1	A	504	ILE
1	A	522	ILE
1	A	528	GLN
1	A	542	ASP
1	A	551	VAL
1	A	556	VAL
1	A	557	THR
1	A	564	ARG
1	A	566	SER
1	A	578	ASP
1	A	580	ASN
1	A	596	GLN
1	A	601	ARG
1	A	606	LYS

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Mol	Chain	Res	Type
1	A	609	GLU
1	A	618	ILE
1	A	641	GLU
1	A	645	GLU
1	A	652	SER
1	A	654	PRO
1	A	659	ILE
1	A	660	THR
1	A	676	GLU
1	A	683	PRO
1	A	687	VAL
1	A	694	LYS
1	A	704	VAL
1	A	714	SER
1	A	720	LYS
1	A	722	LYS
1	A	730	VAL
1	A	744	VAL
1	A	758	GLU
1	A	766	MET
1	A	772	THR
1	A	780	ASN
1	A	788	THR
1	A	792	ASN
1	A	811	THR
1	A	815	PHE
1	B	57	SER
1	B	68	ILE
1	B	73	ARG
1	B	88	LYS
1	B	96	THR
1	B	106	VAL
1	B	107	ASP
1	B	117	VAL
1	B	142	GLU
1	B	148	THR
1	B	157	ARG
1	B	163	ARG
1	B	168	SER
1	B	176	ASN
1	B	177	MET
1	B	236	THR

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Mol	Chain	Res	Type
1	B	253	THR
1	B	265	THR
1	B	292	ARG
1	B	303	GLU
1	B	319	HIS
1	B	323	ASP
1	B	329	THR
1	B	330	SER
1	B	331	VAL
1	B	360	SER
1	B	396	ARG
1	B	411	VAL
1	B	447	LYS
1	B	459	ILE
1	B	462	THR
1	B	465	PHE
1	B	466	GLN
1	B	493	LEU
1	B	495	ASN
1	B	504	ILE
1	B	509	ASP
1	B	510	ILE
1	B	517	THR
1	B	524	ASP
1	B	533	MET
1	B	551	VAL
1	B	556	VAL
1	B	562	THR
1	B	564	ARG
1	B	576	VAL
1	B	596	GLN
1	B	601	ARG
1	B	604	SER
1	B	609	GLU
1	B	615	ASN
1	B	624	TYR
1	B	633	LEU
1	B	641	GLU
1	B	645	GLU
1	B	655	THR
1	B	687	VAL
1	B	694	LYS

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Mol	Chain	Res	Type
1	B	702	LYS
1	B	704	VAL
1	B	714	SER
1	B	720	LYS
1	B	722	LYS
1	B	742	GLN
1	B	750	SER
1	B	771	ILE
1	B	772	THR
1	B	788	THR
1	B	792	ASN
1	B	810	SER
1	B	815	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	109	GLN
1	A	136	GLN
1	A	205	ASN
1	A	218	GLN
1	A	401	ASN
1	A	408	ASN
1	A	415	GLN
1	A	424	HIS
1	A	455	ASN
1	A	492	ASN
1	A	505	ASN
1	A	580	ASN
1	A	596	GLN
1	A	615	ASN
1	B	53	GLN
1	B	176	ASN
1	B	183	ASN
1	B	418	HIS
1	B	455	ASN
1	B	472	HIS
1	B	538	ASN
1	B	560	ASN
1	B	596	GLN

### 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	5,5,6	1.12	1 (20%)	1,5,7	2.09	1 (100%)
2	AHO	C	5	2,6	10,11,12	6.83	2 (20%)	5,13,15	1.71	1 (20%)
2	ORN	C	6	2	7,7,8	1.09	0	4,7,9	1.33	0
2	DAS	C	7	2	4,7,8	1.87	1 (25%)	3,8,10	1.60	1 (33%)
2	AHO	C	8	2,6	10,11,12	7.13	2 (20%)	5,13,15	2.46	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DSN	C	3	2,5	-	0/2/4/6	0/0/0/0
2	AHO	C	5	2,6	-	0/10/12/14	0/0/0/0
2	ORN	C	6	2	-	0/4/6/8	0/0/0/0
2	DAS	C	7	2	-	0/2/6/8	0/0/0/0
2	AHO	C	8	2,6	-	0/10/12/14	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	8	AHO	O2-N2	-22.37	1.22	1.40
2	C	5	AHO	O2-N2	-21.35	1.23	1.40
2	C	3	DSN	CA-C	2.01	1.52	1.50
2	C	5	AHO	C2-C1	2.16	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	8	AHO	C2-C1	2.22	1.53	1.50
2	C	7	DAS	CA-C	3.12	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	AHO	C3-C2-C1	-3.10	106.54	111.65
2	C	3	DSN	O-C-CA	-2.09	119.24	125.02
2	C	7	DAS	CB-CA-C	2.55	116.32	111.41
2	C	8	AHO	C3-C2-C1	5.30	120.39	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	DSN	2	0
2	C	5	AHO	1	0
2	C	6	ORN	2	0
2	C	7	DAS	6	0
2	C	8	AHO	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
3	N8E	A	1816	-	23,23,23	0.62	0	22,22,22	0.56	0
3	N8E	A	1817[A]	-	23,23,23	0.81	0	22,22,22	0.68	0
3	N8E	A	1817[B]	-	23,23,23	0.78	0	22,22,22	0.72	0
4	PO4	A	1818	-	4,4,4	0.65	0	6,6,6	0.82	0
4	PO4	A	1819	-	4,4,4	1.00	0	6,6,6	1.05	1 (16%)
4	PO4	A	1820	-	4,4,4	0.62	0	6,6,6	0.88	0
4	PO4	A	1821	-	4,4,4	0.52	0	6,6,6	1.22	0
4	PO4	A	1822	-	4,4,4	0.78	0	6,6,6	0.49	0
4	PO4	A	1823	-	4,4,4	0.99	0	6,6,6	0.44	0
4	PO4	B	1818	-	4,4,4	0.28	0	6,6,6	1.26	1 (16%)
4	PO4	B	1819	-	4,4,4	1.11	0	6,6,6	0.55	0
4	PO4	B	1820	-	4,4,4	0.54	0	6,6,6	0.87	0
4	PO4	B	1821	-	4,4,4	0.72	0	6,6,6	0.56	0
5	PVE	C	1	2,6	24,28,29	2.74	4 (16%)	26,40,42	4.22	12 (46%)

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	1818	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1819	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1820	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1821	-	-	0/0/0/0	0/0/0/0
5	PVE	C	1	2,6	-	0/9/21/23	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	OXT-C15	-4.24	1.24	1.42
5	C	1	PVE	C9-N1	-2.70	1.37	1.40
5	C	1	PVE	C5-C6	4.20	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	PVE	C20-C18	11.03	1.72	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	PVE	C20-C18-N17	-13.72	90.01	114.53
5	C	1	PVE	C13-C12-N11	-6.63	100.39	110.28
5	C	1	PVE	C12-C13-C14	-3.21	107.88	110.37
5	C	1	PVE	C13-C14-C15	-3.13	106.70	111.89
5	C	1	PVE	C3-N17-C18	2.03	134.22	126.65
5	C	1	PVE	O19-C18-N17	2.07	127.56	123.67
5	C	1	PVE	C7-C8-C9	2.16	121.47	117.30
4	A	1819	PO4	O4-P-O2	2.20	115.99	107.90
5	C	1	PVE	C10-C9-N1	2.41	120.72	118.48
4	B	1818	PO4	O4-P-O3	2.50	117.09	107.90
5	C	1	PVE	OXT-C15-C14	2.66	124.57	112.96
5	C	1	PVE	C8-C7-C6	2.91	121.53	119.86
5	C	1	PVE	C20-C21-C22	8.14	126.57	112.66
5	C	1	PVE	O19-C18-C20	9.50	139.86	122.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1816	N8E	2	0
3	A	1817[A]	N8E	9	0
3	A	1817[B]	N8E	6	0
4	A	1818	PO4	1	0
4	A	1823	PO4	1	0
4	B	1819	PO4	1	0
4	B	1821	PO4	1	0
5	C	1	PVE	1	0

## 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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	772/772 (100%)	-0.69	2 (0%) 93 82	15, 27, 40, 58	0
1	B	754/772 (97%)	-0.59	4 (0%) 90 74	19, 33, 47, 58	0
2	C	2/7 (28%)	0.61	0 100 100	46, 46, 46, 50	0
All	All	1528/1551 (98%)	-0.64	6 (0%) 92 77	15, 30, 45, 58	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	724	ALA	3.7
1	A	44	GLN	3.4
1	A	123	SER	3.1
1	B	109	GLN	3.1
1	B	342	PRO	2.6
1	B	407	ALA	2.5

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ORN	C	6	8/9	0.92	0.23	-	47,48,48,50	0
2	AHO	C	8	12/13	0.96	0.21	-	36,40,49,49	0
2	AHO	C	5	12/13	0.99	0.11	-	37,41,46,46	0
2	DSN	C	3	6/7	0.96	0.16	-	44,44,44,45	0
2	DAS	C	7	8/9	0.82	0.36	-	45,49,49,52	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	N8E	A	1816	24/24	0.85	0.31	4.80	47,49,81,82	0
4	PO4	A	1822	5/5	0.91	0.23	3.20	84,84,86,87	0
4	PO4	B	1820	5/5	0.93	0.18	1.90	64,64,66,67	0
4	PO4	A	1818	5/5	0.97	0.16	1.58	48,49,51,51	0
3	N8E	A	1817[B]	24/24	0.87	0.25	1.36	2,7,12,14	24
4	PO4	B	1818	5/5	0.94	0.20	1.14	55,56,57,58	0
3	N8E	A	1817[A]	24/24	0.87	0.25	0.77	2,9,12,15	24
4	PO4	A	1823	5/5	0.95	0.14	-0.00	59,60,61,61	0
4	PO4	A	1820	5/5	0.98	0.13	-0.05	66,66,66,66	0
5	PVE	C	1	26/27	0.96	0.14	-0.15	35,37,52,53	5
4	PO4	B	1819	5/5	0.96	0.12	-0.31	40,43,44,45	0
4	PO4	A	1819	5/5	0.97	0.11	-1.41	28,29,33,34	0
4	PO4	B	1821	5/5	0.97	0.17	-	42,44,45,47	0
6	FE	C	2	1/1	0.99	0.05	-	33,33,33,33	0
4	PO4	A	1821	5/5	0.94	0.31	-	62,63,63,63	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.