



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:41 PM UTC

PDB ID : 6DRH / pdb_00006drh
Title : ADP-ribosyltransferase toxin/immunity pair
Authors : Bosch, D.E.; Ting, S.; Allaire, M.; Mougous, J.D.
Deposited on : 2018-06-11
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

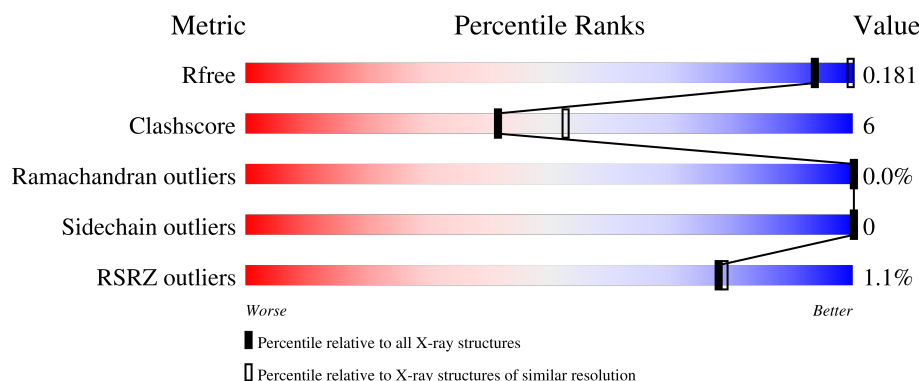
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

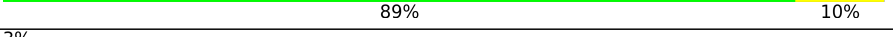
The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	366	 89% 11%
1	C	366	 90% 10%
1	E	366	 91% 9%
1	G	366	 89% 10%
2	B	188	 86% 12% 3%

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Mol	Chain	Length	Quality of chain
2	D	188	2% 83% 14% ••
2	F	188	3% 82% 12% 5%
2	H	188	2% 86% 12% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18940 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 ADP-ribosyl-(Dinitrogen reductase) hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	1	0
			2878	1812	498	555	13			
1	C	365	Total	C	N	O	S	0	0	0
			2872	1809	497	553	13			
1	E	366	Total	C	N	O	S	0	0	0
			2880	1814	498	554	14			
1	G	365	Total	C	N	O	S	0	1	0
			2878	1812	498	555	13			

- Molecule 2 is a protein called PAAR repeat-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	185	Total	C	N	O	S	0	0	0
			1443	899	252	291	1			
2	D	185	Total	C	N	O	S	0	0	0
			1443	899	252	291	1			
2	F	178	Total	C	N	O	S	0	0	0
			1382	859	242	280	1			
2	H	185	Total	C	N	O	S	0	0	0
			1443	899	252	291	1			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	expression tag	UNP A8GG78
B	6	HIS	-	expression tag	UNP A8GG78
B	7	HIS	-	expression tag	UNP A8GG78
B	8	HIS	-	expression tag	UNP A8GG78
B	9	HIS	-	expression tag	UNP A8GG78
B	10	HIS	-	expression tag	UNP A8GG78
B	11	SER	-	expression tag	UNP A8GG78
B	12	GLN	-	expression tag	UNP A8GG78

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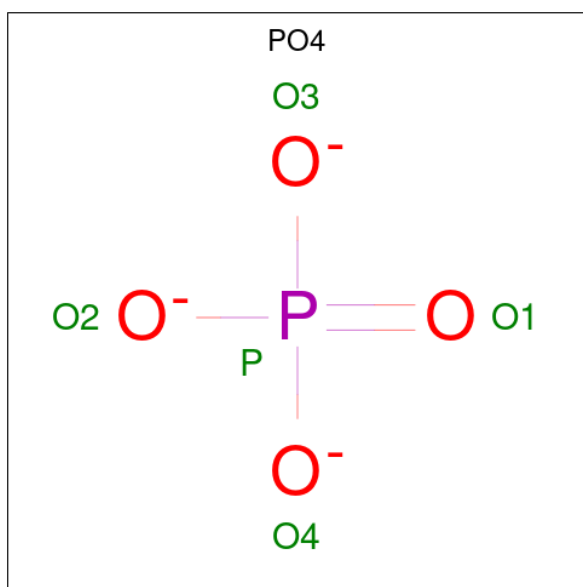
Chain	Residue	Modelled	Actual	Comment	Reference
B	13	ASP	-	expression tag	UNP A8GG78
B	14	PRO	-	expression tag	UNP A8GG78
B	15	GLU	-	expression tag	UNP A8GG78
B	16	ASN	-	expression tag	UNP A8GG78
B	17	LEU	-	expression tag	UNP A8GG78
B	18	TYR	-	expression tag	UNP A8GG78
B	19	PHE	-	expression tag	UNP A8GG78
B	20	GLN	-	expression tag	UNP A8GG78
B	190	GLU	-	expression tag	UNP A8GG78
B	191	ILE	-	expression tag	UNP A8GG78
B	192	PRO	-	expression tag	UNP A8GG78
D	5	HIS	-	expression tag	UNP A8GG78
D	6	HIS	-	expression tag	UNP A8GG78
D	7	HIS	-	expression tag	UNP A8GG78
D	8	HIS	-	expression tag	UNP A8GG78
D	9	HIS	-	expression tag	UNP A8GG78
D	10	HIS	-	expression tag	UNP A8GG78
D	11	SER	-	expression tag	UNP A8GG78
D	12	GLN	-	expression tag	UNP A8GG78
D	13	ASP	-	expression tag	UNP A8GG78
D	14	PRO	-	expression tag	UNP A8GG78
D	15	GLU	-	expression tag	UNP A8GG78
D	16	ASN	-	expression tag	UNP A8GG78
D	17	LEU	-	expression tag	UNP A8GG78
D	18	TYR	-	expression tag	UNP A8GG78
D	19	PHE	-	expression tag	UNP A8GG78
D	20	GLN	-	expression tag	UNP A8GG78
D	190	GLU	-	expression tag	UNP A8GG78
D	191	ILE	-	expression tag	UNP A8GG78
D	192	PRO	-	expression tag	UNP A8GG78
F	5	HIS	-	expression tag	UNP A8GG78
F	6	HIS	-	expression tag	UNP A8GG78
F	7	HIS	-	expression tag	UNP A8GG78
F	8	HIS	-	expression tag	UNP A8GG78
F	9	HIS	-	expression tag	UNP A8GG78
F	10	HIS	-	expression tag	UNP A8GG78
F	11	SER	-	expression tag	UNP A8GG78
F	12	GLN	-	expression tag	UNP A8GG78
F	13	ASP	-	expression tag	UNP A8GG78
F	14	PRO	-	expression tag	UNP A8GG78
F	15	GLU	-	expression tag	UNP A8GG78
F	16	ASN	-	expression tag	UNP A8GG78

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Chain	Residue	Modelled	Actual	Comment	Reference
F	17	LEU	-	expression tag	UNP A8GG78
F	18	TYR	-	expression tag	UNP A8GG78
F	19	PHE	-	expression tag	UNP A8GG78
F	20	GLN	-	expression tag	UNP A8GG78
F	190	GLU	-	expression tag	UNP A8GG78
F	191	ILE	-	expression tag	UNP A8GG78
F	192	PRO	-	expression tag	UNP A8GG78
H	5	HIS	-	expression tag	UNP A8GG78
H	6	HIS	-	expression tag	UNP A8GG78
H	7	HIS	-	expression tag	UNP A8GG78
H	8	HIS	-	expression tag	UNP A8GG78
H	9	HIS	-	expression tag	UNP A8GG78
H	10	HIS	-	expression tag	UNP A8GG78
H	11	SER	-	expression tag	UNP A8GG78
H	12	GLN	-	expression tag	UNP A8GG78
H	13	ASP	-	expression tag	UNP A8GG78
H	14	PRO	-	expression tag	UNP A8GG78
H	15	GLU	-	expression tag	UNP A8GG78
H	16	ASN	-	expression tag	UNP A8GG78
H	17	LEU	-	expression tag	UNP A8GG78
H	18	TYR	-	expression tag	UNP A8GG78
H	19	PHE	-	expression tag	UNP A8GG78
H	20	GLN	-	expression tag	UNP A8GG78
H	190	GLU	-	expression tag	UNP A8GG78
H	191	ILE	-	expression tag	UNP A8GG78
H	192	PRO	-	expression tag	UNP A8GG78

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	267	Total	O	0	0
			267	267		
5	B	175	Total	O	0	0
			175	175		
5	C	278	Total	O	0	0
			278	278		
5	D	168	Total	O	0	0
			168	168		
5	E	265	Total	O	0	0
			265	265		

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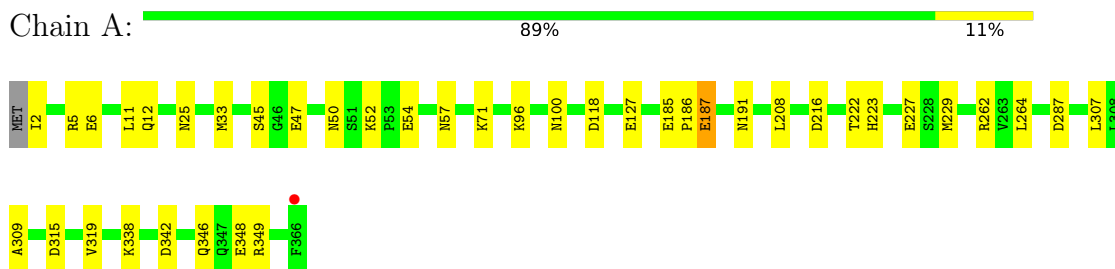
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	150	Total 150	O 150	0	0
5	G	272	Total 272	O 272	0	0
5	H	130	Total 130	O 130	0	0

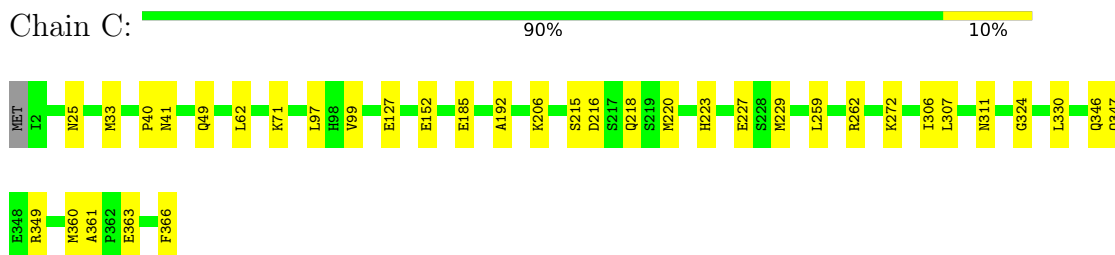
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

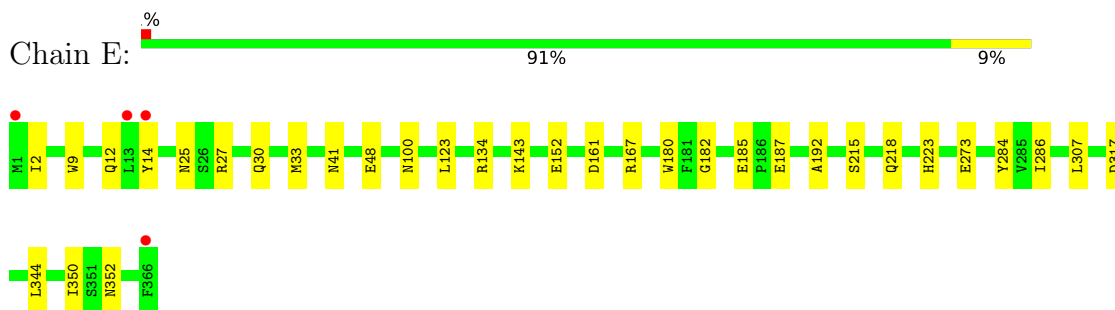
- Molecule 1: ADP-ribosyl-(Dinitrogen reductase) hydrolase



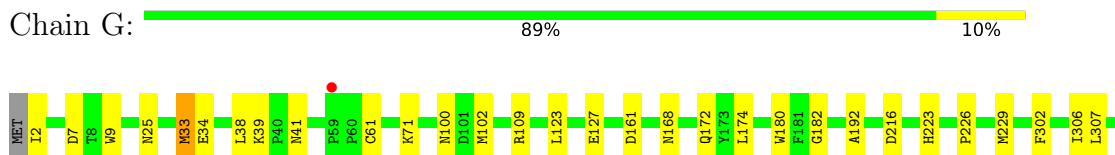
- Molecule 1: ADP-ribosyl-(Dinitrogen reductase) hydrolase



- Molecule 1: ADP-ribosyl-(Dinitrogen reductase) hydrolase

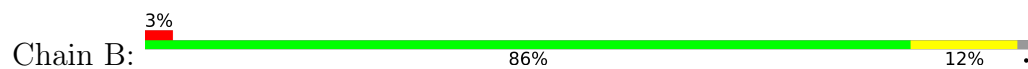


- Molecule 1: ADP-ribosyl-(Dinitrogen reductase) hydrolase

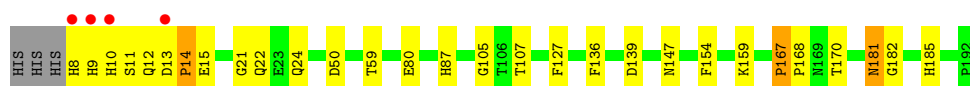
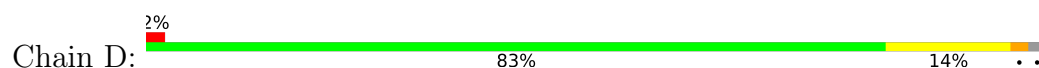




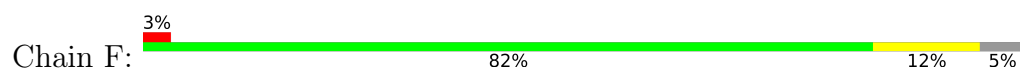
- Molecule 2: PAAR repeat-containing protein



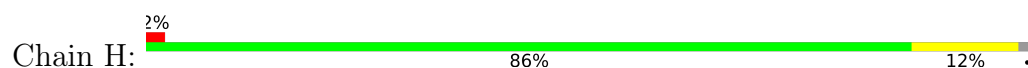
- Molecule 2: PAAR repeat-containing protein



- Molecule 2: PAAR repeat-containing protein



- Molecule 2: PAAR repeat-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.17Å 151.01Å 196.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.53 – 2.30 49.53 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.53-2.30) 99.6 (49.53-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.152 , 0.206 (Not available) , 0.181	Depositor DCC
R_{free} test set	2000 reflections (1.72%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18940	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7329e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4

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	0.68	0/2944	0.84	3/3996 (0.1%)
1	C	0.73	0/2938	0.83	2/3987 (0.1%)
1	E	0.70	1/2946 (0.0%)	0.82	0/3997
1	G	0.70	0/2944	0.79	1/3996 (0.0%)
2	B	0.66	0/1475	0.86	2/2008 (0.1%)
2	D	0.69	0/1475	0.88	3/2008 (0.1%)
2	F	0.69	0/1411	0.84	1/1920 (0.1%)
2	H	0.66	0/1475	0.82	0/2008
All	All	0.69	1/17608 (0.0%)	0.83	12/23920 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	41	ASN	CB-CG	-6.13	1.36	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	167	PRO	CA-N-CD	-8.74	99.76	112.00
2	B	181	ASN	CA-C-N	-8.69	100.11	122.78
2	B	181	ASN	C-N-CA	-8.69	100.11	122.78
2	D	181	ASN	CA-C-N	-8.15	101.50	122.78
2	D	181	ASN	C-N-CA	-8.15	101.50	122.78
1	A	50	ASN	CB-CA-C	-7.91	95.09	110.11
1	G	33	MET	CB-CG-SD	5.78	130.05	112.70
1	A	187	GLU	CA-CB-CG	5.58	125.27	114.10
2	F	62	GLU	CA-CB-CG	5.58	125.27	114.10
1	A	187	GLU	CB-CA-C	-5.18	100.42	110.46
1	C	40	PRO	CA-C-N	5.05	131.35	122.42
1	C	40	PRO	C-N-CA	5.05	131.35	122.42

There are no chirality outliers.

There are no planarity outliers.

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	2878	0	2802	40	0
1	C	2872	0	2797	29	0
1	E	2880	0	2809	30	0
1	G	2878	0	2802	38	0
2	B	1443	0	1376	20	0
2	D	1443	0	1376	33	0
2	F	1382	0	1321	20	0
2	H	1443	0	1376	22	0
3	A	5	0	0	1	0
3	C	5	0	0	0	0
3	G	5	0	0	0	0
4	C	1	0	0	0	0
5	A	267	0	0	8	0
5	B	175	0	0	4	0
5	C	278	0	0	4	0
5	D	168	0	0	8	2
5	E	265	0	0	15	1
5	F	150	0	0	4	0
5	G	272	0	0	10	1
5	H	130	0	0	5	0
All	All	18940	0	16659	217	2

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 6.

All (217) 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)
2:B:10:HIS:O	2:B:14:PRO:HD2	1.66	0.94
2:D:10:HIS:O	2:D:14:PRO:HD3	1.72	0.90
2:D:167:PRO:HD2	2:D:170:THR:OG1	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:LEU:HD12	2:H:74:GLN:HE21	1.38	0.88
2:B:192:PRO:O	5:B:201:HOH:O	1.93	0.87
1:A:342:ASP:O	5:A:501:HOH:O	1.93	0.86
1:A:346:GLN:HE22	1:A:349:ARG:HH11	1.27	0.83
1:A:346:GLN:NE2	1:A:349:ARG:HH11	1.79	0.80
1:G:25:ASN:HD21	1:G:33:MET:HE2	1.47	0.80
2:D:147:ASN:O	5:D:201:HOH:O	2.00	0.78
1:A:222:THR:OG1	1:A:223:HIS:HD2	1.67	0.78
2:B:22:GLN:O	5:B:202:HOH:O	2.01	0.77
2:B:124:ASP:OD1	5:B:203:HOH:O	2.03	0.77
1:G:2:ILE:N	5:G:502:HOH:O	2.17	0.76
1:E:33:MET:HE2	2:F:104:ARG:HA	1.67	0.76
2:D:9:HIS:ND1	5:D:202:HOH:O	2.18	0.75
1:E:161:ASP:N	5:E:403:HOH:O	2.16	0.75
1:E:317:ASP:OD2	5:E:401:HOH:O	2.05	0.74
1:A:127:GLU:OE2	5:A:502:HOH:O	2.04	0.74
2:D:9:HIS:CD2	2:D:11:SER:H	2.04	0.74
1:A:348:GLU:OE2	5:A:503:HOH:O	2.05	0.74
1:G:346:GLN:HE21	1:G:349:ARG:HD3	1.52	0.74
1:E:185:GLU:OE2	5:E:402:HOH:O	2.06	0.74
1:A:346:GLN:HE21	1:A:349:ARG:HD3	1.53	0.73
2:D:107:THR:HG22	2:D:139:ASP:H	1.53	0.73
1:E:30:GLN:HE21	1:E:30:GLN:HA	1.55	0.71
1:G:346:GLN:HE22	1:G:349:ARG:HH11	1.40	0.70
1:C:33:MET:HE3	2:D:105:GLY:O	1.92	0.69
1:A:25:ASN:HD21	1:A:33:MET:HE2	1.56	0.68
1:C:346:GLN:HE21	1:C:349:ARG:HD3	1.59	0.68
1:G:352:ASN:HB2	5:G:724:HOH:O	1.93	0.68
1:E:167:ARG:NE	5:E:407:HOH:O	2.26	0.68
1:G:346:GLN:NE2	1:G:349:ARG:HH11	1.91	0.67
1:C:346:GLN:NE2	1:C:349:ARG:HH11	1.92	0.67
1:C:99:VAL:H	1:C:311:ASN:HD21	1.42	0.67
1:C:127:GLU:OE1	1:C:349:ARG:NH2	2.26	0.67
2:F:10:HIS:O	2:F:14:PRO:HD3	1.93	0.67
1:C:25:ASN:HD21	1:C:33:MET:HE2	1.60	0.66
1:A:54:GLU:OE1	1:A:57:ASN:ND2	2.28	0.66
1:A:2:ILE:N	5:A:505:HOH:O	2.29	0.65
2:D:22:GLN:N	5:D:203:HOH:O	2.30	0.65
1:C:272:LYS:O	5:C:501:HOH:O	2.14	0.65
1:G:33:MET:HE3	2:H:105:GLY:H	1.61	0.64
2:F:181:ASN:O	5:F:201:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:LYS:O	2:F:30:GLN:HG3	1.99	0.63
2:H:127:PHE:HB3	2:H:165:LEU:HD11	1.80	0.63
2:D:11:SER:OG	2:D:22:GLN:HG3	1.99	0.62
1:E:161:ASP:OD2	5:E:401:HOH:O	2.16	0.62
1:G:100:ASN:HA	1:G:307:LEU:HD22	1.82	0.62
1:C:346:GLN:HE22	1:C:349:ARG:HH11	1.48	0.61
1:A:346:GLN:HE22	1:A:349:ARG:NH1	1.99	0.61
1:E:344:LEU:O	5:E:404:HOH:O	2.16	0.60
2:B:13:ASP:OD2	2:B:83:ALA:HB3	2.01	0.60
2:D:167:PRO:HD2	2:D:170:THR:HG1	1.67	0.60
2:F:192:PRO:HD2	5:F:321:HOH:O	2.01	0.59
2:H:32:ALA:HB1	2:H:52:ILE:HG12	1.84	0.59
1:C:25:ASN:HD21	1:C:33:MET:CE	2.14	0.59
1:E:167:ARG:CD	5:E:407:HOH:O	2.51	0.59
1:G:338:LYS:HE3	5:G:737:HOH:O	2.03	0.59
2:F:65:THR:HG21	5:F:337:HOH:O	2.03	0.58
1:A:127:GLU:OE1	1:A:349:ARG:NH2	2.36	0.58
1:E:167:ARG:HD2	5:E:407:HOH:O	2.03	0.58
2:F:11:SER:O	2:F:14:PRO:HD2	2.03	0.58
2:B:182:GLY:HA3	2:D:136:PHE:CE2	2.39	0.57
1:A:12:GLN:HE21	1:A:12:GLN:HA	1.69	0.57
1:C:25:ASN:ND2	1:C:33:MET:HE2	2.18	0.57
1:A:25:ASN:ND2	1:A:33:MET:HE2	2.20	0.57
2:H:192:PRO:HD2	5:H:270:HOH:O	2.04	0.57
1:G:109:ARG:NH1	5:G:505:HOH:O	2.28	0.57
2:F:13:ASP:HB3	2:F:14:PRO:HD3	1.85	0.57
1:E:352:ASN:ND2	5:E:412:HOH:O	2.37	0.56
1:A:222:THR:OG1	1:A:223:HIS:CD2	2.54	0.56
1:E:30:GLN:HA	1:E:30:GLN:NE2	2.20	0.56
2:D:87:HIS:HD2	5:D:338:HOH:O	1.88	0.56
2:D:9:HIS:HD2	2:D:10:HIS:N	2.04	0.56
2:F:9:HIS:CE1	2:F:12:GLN:HB2	2.41	0.55
1:E:25:ASN:HD22	1:E:30:GLN:NE2	2.05	0.54
1:G:39:LYS:O	1:G:39:LYS:HG3	2.07	0.54
1:A:338:LYS:HE3	5:A:735:HOH:O	2.07	0.54
1:A:71:LYS:HE3	5:A:612:HOH:O	2.07	0.53
1:A:223:HIS:HE1	3:A:401:PO4:O4	1.92	0.53
2:F:125:GLY:O	2:F:168:PRO:HB3	2.09	0.53
2:D:181:ASN:HB3	5:D:257:HOH:O	2.09	0.52
2:H:13:ASP:HB2	2:H:14:PRO:HD3	1.92	0.52
1:G:61:CYS:N	5:G:501:HOH:O	1.81	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:GLN:NE2	1:G:349:ARG:HD3	2.24	0.52
2:D:9:HIS:H	2:D:12:GLN:NE2	2.08	0.51
1:C:306:ILE:HD11	1:C:324:GLY:HA2	1.92	0.51
2:H:9:HIS:CD2	2:H:10:HIS:N	2.79	0.51
1:C:216:ASP:HB2	1:C:229:MET:HB3	1.92	0.51
1:E:192:ALA:HB3	1:E:223:HIS:CE1	2.45	0.51
1:A:185:GLU:HB3	1:A:187:GLU:OE2	2.11	0.50
2:D:8:HIS:HA	2:D:12:GLN:HE22	1.76	0.50
1:G:25:ASN:HD21	1:G:33:MET:CE	2.20	0.50
1:G:7:ASP:OD2	1:G:9:TRP:HB3	2.11	0.50
1:A:47:GLU:HG3	5:A:749:HOH:O	2.11	0.50
1:A:186:PRO:HD3	2:B:99:ASN:ND2	2.27	0.50
1:G:100:ASN:ND2	5:G:514:HOH:O	2.40	0.50
2:F:127:PHE:HB3	2:F:165:LEU:HD11	1.93	0.50
1:G:342:ASP:O	5:G:503:HOH:O	2.19	0.50
1:G:346:GLN:HE22	1:G:349:ARG:NH1	2.09	0.49
2:B:9:HIS:CE1	2:B:11:SER:H	2.30	0.49
1:E:152:GLU:OE2	5:E:405:HOH:O	2.20	0.49
1:A:45:SER:HB3	1:C:41:ASN:OD1	2.12	0.49
1:E:180:TRP:CZ2	1:E:182:GLY:HA3	2.47	0.49
1:A:346:GLN:NE2	1:A:349:ARG:HD3	2.26	0.49
1:G:352:ASN:HB2	5:G:726:HOH:O	2.12	0.49
1:G:33:MET:HE1	5:G:659:HOH:O	2.13	0.49
2:H:10:HIS:O	2:H:14:PRO:HD3	2.12	0.48
1:A:25:ASN:HD21	1:A:33:MET:CE	2.25	0.48
1:A:100:ASN:HA	1:A:307:LEU:HD22	1.96	0.48
2:B:182:GLY:HA3	2:D:136:PHE:HE2	1.77	0.48
2:D:127:PHE:CD2	2:D:168:PRO:HD3	2.49	0.48
1:E:187:GLU:CD	1:E:187:GLU:H	2.22	0.48
1:G:102:MET:HB3	1:G:343:LYS:HD3	1.96	0.48
1:C:49:GLN:HE22	2:D:59:THR:HB	1.79	0.48
2:D:185:HIS:HE1	5:D:240:HOH:O	1.97	0.48
1:E:27:ARG:HD2	5:E:420:HOH:O	2.13	0.47
2:H:8:HIS:HB2	2:H:13:ASP:OD2	2.15	0.47
2:D:9:HIS:CD2	2:D:10:HIS:N	2.81	0.47
2:D:167:PRO:HD2	2:D:167:PRO:O	2.13	0.47
2:B:16:ASN:ND2	5:B:204:HOH:O	2.27	0.47
2:D:9:HIS:HD2	2:D:11:SER:H	1.57	0.47
1:E:143:LYS:NZ	5:E:419:HOH:O	2.48	0.47
1:G:127:GLU:OE2	1:G:349:ARG:NH2	2.48	0.46
1:G:25:ASN:ND2	1:G:33:MET:HE2	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:10:HIS:O	2:H:14:PRO:CD	2.63	0.46
1:A:52:LYS:HE2	1:A:57:ASN:OD1	2.14	0.46
2:D:9:HIS:NE2	5:D:206:HOH:O	2.36	0.46
1:E:100:ASN:HA	1:E:307:LEU:HD22	1.97	0.46
2:F:8:HIS:N	2:F:8:HIS:CD2	2.83	0.46
1:G:192:ALA:HB3	1:G:223:HIS:CE1	2.51	0.46
2:H:169:ASN:ND2	5:H:201:HOH:O	2.20	0.46
1:A:5:ARG:NH2	1:A:287:ASP:OD2	2.48	0.46
1:C:227:GLU:OE1	1:C:262:ARG:HD2	2.16	0.46
1:A:227:GLU:OE2	1:A:262:ARG:HD2	2.15	0.45
1:A:222:THR:HG1	1:A:223:HIS:HD2	1.62	0.45
1:G:302:PHE:CE1	1:G:306:ILE:HG13	2.50	0.45
1:A:12:GLN:HA	1:A:12:GLN:NE2	2.30	0.45
1:E:9:TRP:O	1:E:12:GLN:HB3	2.17	0.45
1:A:96:LYS:HG3	2:F:118:ILE:HD13	1.97	0.45
1:G:216:ASP:HB2	1:G:229:MET:HB3	1.98	0.45
2:H:9:HIS:CD2	2:H:11:SER:H	2.34	0.45
1:A:264:LEU:HD11	5:A:512:HOH:O	2.17	0.45
2:D:11:SER:O	2:D:14:PRO:HD2	2.17	0.45
2:F:163:GLU:OE2	5:F:202:HOH:O	2.21	0.45
1:E:134:ARG:HG2	1:E:134:ARG:HH11	1.82	0.44
1:G:174:LEU:HD23	1:G:174:LEU:HA	1.76	0.44
2:D:24:GLN:HB3	5:D:203:HOH:O	2.17	0.44
2:F:10:HIS:CD2	2:F:25:ALA:HB1	2.53	0.44
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.68	0.44
2:D:13:ASP:OD1	2:D:80:GLU:O	2.35	0.44
1:E:48:GLU:OE2	5:E:406:HOH:O	2.20	0.44
2:D:15:GLU:O	2:D:21:GLY:HA3	2.17	0.44
1:A:309:ALA:HB1	1:A:319:VAL:HG22	2.00	0.44
1:E:273:GLU:N	5:E:410:HOH:O	2.37	0.43
1:E:284:TYR:CE2	1:E:286:ILE:HB	2.53	0.43
2:F:9:HIS:CE1	2:F:12:GLN:CB	3.01	0.43
2:F:13:ASP:OD1	2:F:84:PHE:HB2	2.19	0.43
1:G:71:LYS:NZ	1:G:330:LEU:O	2.51	0.43
1:A:6:GLU:HB2	1:A:11:LEU:HD21	2.01	0.43
1:E:185:GLU:H	1:E:185:GLU:CD	2.27	0.43
1:C:185:GLU:CD	1:C:185:GLU:H	2.27	0.43
2:F:10:HIS:HD2	2:F:25:ALA:HB1	1.83	0.43
1:C:215:SER:O	1:C:218:GLN:HG3	2.19	0.43
1:E:273:GLU:HB2	5:E:410:HOH:O	2.19	0.43
2:H:9:HIS:HD2	2:H:10:HIS:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LEU:HD23	5:C:527:HOH:O	2.18	0.42
1:A:191:ASN:ND2	1:A:315:ASP:OD2	2.52	0.42
2:B:20:GLN:H	2:B:20:GLN:CD	2.20	0.42
2:D:127:PHE:CE2	2:D:168:PRO:HD3	2.53	0.42
1:E:123:LEU:HD21	1:E:350:ILE:HG12	2.01	0.42
2:F:13:ASP:OD1	2:F:84:PHE:CA	2.68	0.42
2:H:9:HIS:HB3	2:H:12:GLN:CD	2.44	0.42
1:C:192:ALA:HB3	1:C:223:HIS:CE1	2.55	0.42
1:C:307:LEU:HD23	1:C:307:LEU:HA	1.86	0.42
1:A:118:ASP:OD1	1:A:118:ASP:N	2.49	0.42
2:B:9:HIS:ND1	2:B:10:HIS:N	2.68	0.42
2:B:109:PRO:HG2	2:B:112:ILE:HG13	2.02	0.42
2:B:125:GLY:O	2:B:168:PRO:HB3	2.20	0.42
2:B:136:PHE:HE2	2:D:182:GLY:HA3	1.84	0.42
2:H:43:LEU:HD23	2:H:43:LEU:HA	1.90	0.42
1:C:152:GLU:OE2	5:C:502:HOH:O	2.22	0.42
2:H:157:LYS:HG2	2:H:158:TYR:CE2	2.55	0.42
2:D:154:PHE:HA	2:D:159:LYS:HG3	2.02	0.42
1:G:34:GLU:CD	1:G:41:ASN:H	2.28	0.42
2:H:87:HIS:HD2	5:H:310:HOH:O	2.01	0.42
1:G:123:LEU:HD21	1:G:350:ILE:HG12	2.02	0.42
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.80	0.42
2:B:136:PHE:CE2	2:D:182:GLY:HA3	2.54	0.41
1:C:71:LYS:NZ	1:C:330:LEU:O	2.52	0.41
2:D:10:HIS:HB2	2:D:50:ASP:CG	2.45	0.41
2:H:135:PRO:HG2	5:H:282:HOH:O	2.19	0.41
2:B:8:HIS:HD1	2:B:8:HIS:N	2.18	0.41
1:G:180:TRP:CZ2	1:G:182:GLY:HA3	2.54	0.41
1:A:33:MET:HE3	2:B:105:GLY:H	1.85	0.41
1:C:206:LYS:NZ	1:C:363:GLU:OE1	2.50	0.41
1:C:62:LEU:HB2	5:C:617:HOH:O	2.20	0.41
2:F:61:ASN:O	2:F:65:THR:HG23	2.20	0.41
1:G:226:PRO:HD3	5:H:239:HOH:O	2.21	0.41
1:A:216:ASP:HB2	1:A:229:MET:HB3	2.03	0.41
1:C:97:LEU:HD12	1:C:97:LEU:HA	1.78	0.41
1:G:38:LEU:HD12	2:H:74:GLN:NE2	2.20	0.41
1:C:347:GLN:HE21	1:C:347:GLN:HB3	1.72	0.41
1:C:366:PHE:CD2	1:C:366:PHE:C	2.99	0.41
2:H:36:ALA:HB1	2:H:44:SER:HB2	2.03	0.41
1:E:215:SER:O	1:E:218:GLN:HG3	2.21	0.41
2:H:175:ILE:HD13	2:H:175:ILE:HG21	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ILE:HD11	1:E:14:TYR:CE1	2.55	0.40
1:G:127:GLU:HG2	5:G:744:HOH:O	2.20	0.40
1:C:216:ASP:O	1:C:220:MET:HG3	2.21	0.40
1:G:33:MET:HE3	2:H:105:GLY:N	2.31	0.40
2:B:26:LYS:O	2:B:30:GLN:HG3	2.22	0.40
1:C:360:MET:O	1:C:361:ALA:C	2.65	0.40
1:G:161:ASP:O	1:G:161:ASP:CG	2.63	0.40
2:B:8:HIS:N	2:B:8:HIS:ND1	2.69	0.40
1:G:168:ASN:O	1:G:172:GLN:HG2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:287:HOH:O	5:E:602:HOH:O[2_555]	1.88	0.32
5:D:340:HOH:O	5:G:699:HOH:O[4_455]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/366 (100%)	359 (99%)	5 (1%)	0	100	100
1	C	363/366 (99%)	356 (98%)	7 (2%)	0	100	100
1	E	364/366 (100%)	357 (98%)	7 (2%)	0	100	100
1	G	364/366 (100%)	358 (98%)	6 (2%)	0	100	100
2	B	183/188 (97%)	177 (97%)	6 (3%)	0	100	100
2	D	183/188 (97%)	174 (95%)	8 (4%)	1 (0%)	24	31
2	F	174/188 (93%)	168 (97%)	6 (3%)	0	100	100
2	H	183/188 (97%)	177 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2178/2216 (98%)	2126 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	14	PRO

5.3.2 Protein sidechains [i](#)

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	308/308 (100%)	308 (100%)	0	100	100
1	C	307/308 (100%)	307 (100%)	0	100	100
1	E	308/308 (100%)	308 (100%)	0	100	100
1	G	308/308 (100%)	308 (100%)	0	100	100
2	B	155/158 (98%)	155 (100%)	0	100	100
2	D	155/158 (98%)	155 (100%)	0	100	100
2	F	149/158 (94%)	149 (100%)	0	100	100
2	H	155/158 (98%)	155 (100%)	0	100	100
All	All	1845/1864 (99%)	1845 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	49	GLN
1	A	150	HIS
1	A	191	ASN
1	A	223	HIS
1	A	346	GLN

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Mol	Chain	Res	Type
1	A	352	ASN
2	B	99	ASN
2	B	111	HIS
1	C	49	GLN
1	C	150	HIS
1	C	168	ASN
1	C	244	ASN
1	C	311	ASN
1	C	346	GLN
1	C	347	GLN
1	C	356	GLN
2	D	9	HIS
2	D	12	GLN
2	D	20	GLN
2	D	24	GLN
2	D	87	HIS
2	D	185	HIS
1	E	30	GLN
1	E	111	GLN
1	E	168	ASN
1	E	347	GLN
2	F	8	HIS
2	F	10	HIS
2	F	35	ASN
2	F	151	GLN
1	G	49	GLN
1	G	100	ASN
1	G	325	GLN
1	G	346	GLN
2	H	61	ASN
2	H	74	GLN
2	H	111	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	PO4	A	401	-	4,4,4	1.42	1 (25%)	6,6,6	0.81	0
3	PO4	G	401	-	4,4,4	1.05	1 (25%)	6,6,6	0.97	0
3	PO4	C	401	-	4,4,4	0.68	0	6,6,6	1.25	1 (16%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	PO4	P-O1	2.65	1.56	1.50
3	G	401	PO4	P-O1	2.04	1.55	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	401	PO4	O4-P-O3	2.30	115.08	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	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	365/366 (99%)	-0.78	1 (0%) 90 90	14, 24, 41, 62	1 (0%)
1	C	365/366 (99%)	-0.86	0 100 100	14, 21, 36, 55	0
1	E	366/366 (100%)	-0.76	4 (1%) 78 79	15, 23, 40, 63	0
1	G	365/366 (99%)	-0.75	1 (0%) 90 90	14, 23, 40, 62	1 (0%)
2	B	185/188 (98%)	-0.52	6 (3%) 50 52	19, 27, 54, 66	0
2	D	185/188 (98%)	-0.55	4 (2%) 62 64	16, 24, 51, 72	0
2	F	178/188 (94%)	-0.58	5 (2%) 55 57	17, 25, 60, 92	0
2	H	185/188 (98%)	-0.34	4 (2%) 62 64	19, 29, 60, 84	0
All	All	2194/2216 (99%)	-0.69	25 (1%) 78 79	14, 24, 44, 92	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	13	ASP	6.3
2	F	13	ASP	4.7
2	B	13	ASP	4.6
2	D	8	HIS	4.2
2	H	13	ASP	3.8
2	B	9	HIS	3.7
2	D	10	HIS	3.7
2	F	8	HIS	3.6
2	H	8	HIS	3.4
2	B	8	HIS	3.3
2	F	9	HIS	3.2
2	H	10	HIS	3.2
1	E	13	LEU	3.1
2	F	10	HIS	2.9
1	A	366	PHE	2.7
2	B	10	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	9	HIS	2.6
1	E	14	TYR	2.6
2	B	20	GLN	2.3
1	G	59	PRO	2.2
2	B	21	GLY	2.2
2	H	9	HIS	2.2
1	E	366	PHE	2.2
2	F	15	GLU	2.2
1	E	1	MET	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	C	401	5/5	0.91	0.14	44,49,58,63	0
4	MG	C	400	1/1	0.94	0.08	39,39,39,39	0
3	PO4	G	401	5/5	0.97	0.09	27,27,41,46	0
3	PO4	A	401	5/5	0.97	0.06	24,24,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.