



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:18 am BST

PDB ID : 6DRH  
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](mailto: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.

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

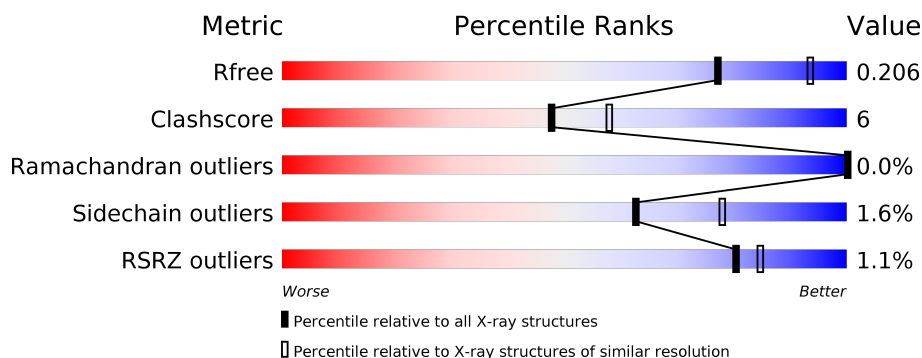
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	C	366	<div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	E	366	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	G	366	<div> <div>%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	B	188	<div> <div>3%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
2	D	188	<div> <div>4%</div> <div>82%</div> <div>13%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	188	<div><div></div><div>3%</div><div>82%</div><div>11%</div><div>• 5%</div></div>
2	H	188	<div><div></div><div>2%</div><div>85%</div><div>13%</div><div>• •</div></div>

## 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 (three-letter code: PO4) (formula: O<sub>4</sub>P).



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 (three-letter code: 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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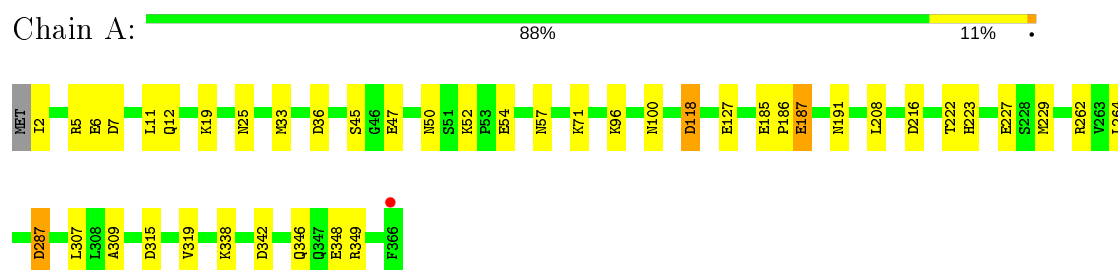
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	150	Total 150	O 150	0	0
5	G	272	Total 272	O 272	0	0
5	H	130	Total 130	O 130	0	0



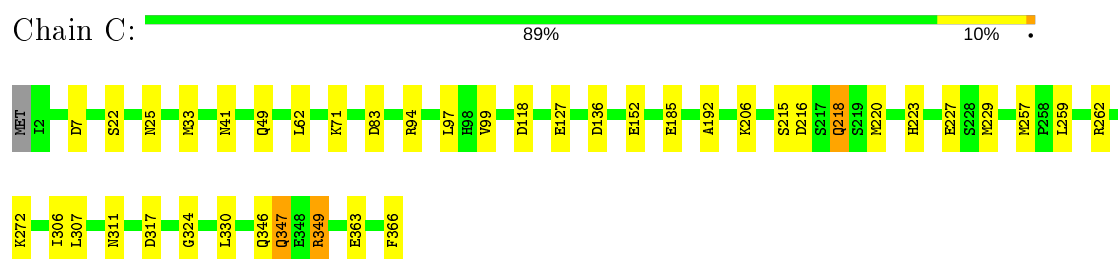
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

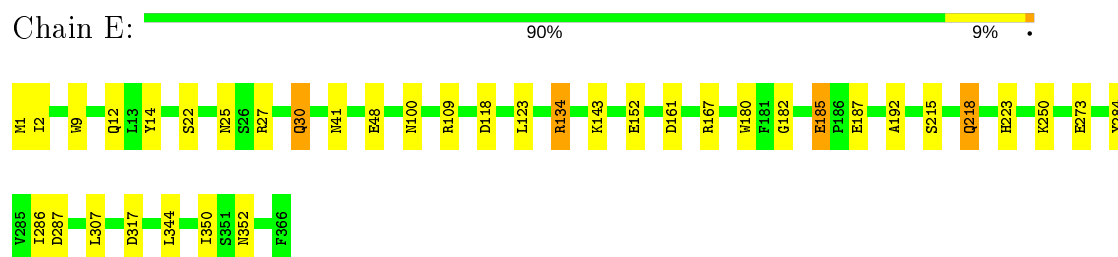
- Molecule 1: ADP-ribosyl-(Dinitrogen reductase) hydrolase



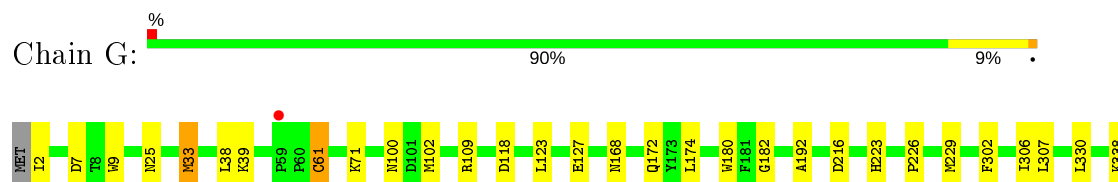
- Molecule 1: ADP-ribosyl-(Dinitrogen reductase) hydrolase



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

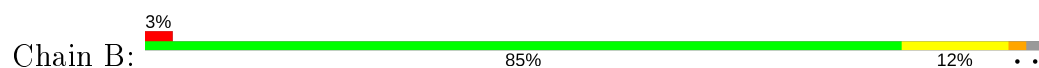


- Molecule 1: ADP-ribosyl-(Dinitrogen reductase) hydrolase

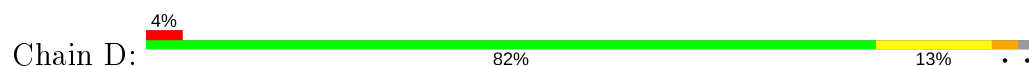




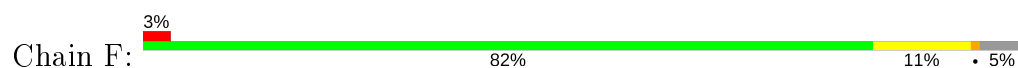
- Molecule 2: PAAR repeat-containing protein



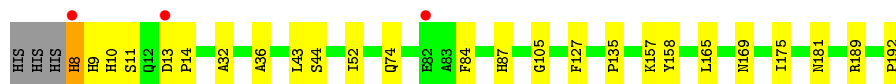
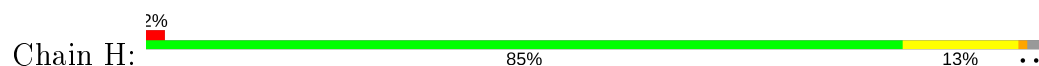
- Molecule 2: PAAR repeat-containing protein



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, $R_{free}$	0.152 , 0.206 0.152 , 0.206	Depositor DCC
$R_{free}$ test set	1999 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.72	0/2944	0.85	5/3996 (0.1%)
1	C	0.77	2/2938 (0.1%)	0.85	7/3987 (0.2%)
1	E	0.74	2/2946 (0.1%)	0.83	2/3997 (0.1%)
1	G	0.74	1/2944 (0.0%)	0.78	2/3996 (0.1%)
2	B	0.70	0/1475	0.83	3/2008 (0.1%)
2	D	0.71	0/1475	0.86	3/2008 (0.1%)
2	F	0.71	0/1411	0.86	4/1920 (0.2%)
2	H	0.70	0/1475	0.80	2/2008 (0.1%)
All	All	0.73	5/17608 (0.0%)	0.83	28/23920 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185	GLU	CG-CD	6.89	1.62	1.51
1	E	41	ASN	CB-CG	-6.23	1.36	1.51
1	E	185	GLU	CG-CD	5.80	1.60	1.51
1	C	317	ASP	CB-CG	-5.53	1.40	1.51
1	G	61	CYS	CB-SG	-5.30	1.73	1.81

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	181	ASN	C-N-CA	-10.57	100.11	122.30
2	D	181	ASN	C-N-CA	-9.90	101.50	122.30
2	D	167	PRO	CA-N-CD	-8.39	99.76	111.50
1	C	94	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	C	94	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	50	ASN	CB-CA-C	-7.66	95.09	110.40
2	H	189	ARG	NE-CZ-NH2	-7.58	116.51	120.30
2	D	189	ARG	NE-CZ-NH2	-7.39	116.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	ASP	CB-CG-OD1	-6.67	112.30	118.30
2	F	13	ASP	CB-CG-OD1	-6.53	112.43	118.30
1	A	287	ASP	CB-CG-OD1	6.42	124.08	118.30
1	C	83	ASP	CB-CG-OD1	6.20	123.88	118.30
2	F	13	ASP	CB-CG-OD2	6.18	123.86	118.30
1	C	349	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	G	33	MET	CB-CG-SD	5.88	130.05	112.40
2	F	181	ASN	C-N-CA	-5.76	110.21	122.30
2	H	181	ASN	C-N-CA	-5.69	110.35	122.30
1	G	33	MET	CG-SD-CE	5.64	109.22	100.20
1	E	287	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	257	MET	CG-SD-CE	5.52	109.03	100.20
1	C	83	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	187	GLU	CA-CB-CG	5.40	125.27	113.40
2	F	62	GLU	CA-CB-CG	5.39	125.27	113.40
1	C	136	ASP	CB-CG-OD2	5.36	123.12	118.30
2	B	189	ARG	NE-CZ-NH2	-5.19	117.70	120.30
2	B	192	PRO	CA-C-O	-5.14	107.87	120.20
1	E	109	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	36	ASP	CB-CG-OD2	5.03	122.83	118.30

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	25	0
1	E	2880	0	2809	28	0
1	G	2878	0	2802	36	0
2	B	1443	0	1376	20	0
2	D	1443	0	1376	32	0
2	F	1382	0	1321	19	0
2	H	1443	0	1376	21	0
3	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	0
All	All	18940	0	16659	206	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 (206) 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
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:G:33:MET:HE3	2:H:105:GLY:H	1.38	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:E:30:GLN:HE21	1.55	0.71
1:G:346:GLN:HE22	1:G:349:ARG:HH11	1.40	0.70
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:A:54:GLU:OE1	1:A:57:ASN:ND2	2.28	0.66
1:A:33:MET:HE3	2:B:105:GLY:H	1.60	0.65
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
2:F:181:ASN:O	5:F:201:HOH:O	2.15	0.64
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:33:MET:HE3	2:D:105:GLY:O	1.99	0.61
1:G:33:MET:HE3	2:H:105:GLY:N	2.14	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:25:ASN:HD21	1:G:33:MET:CE	2.20	0.55
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:HG3	1:G:39:LYS:O	2.07	0.54
1:A:338:LYS:HE3	5:A:735:HOH:O	2.07	0.54
1:A:223:HIS:HE1	3:A:401:PO4:O4	1.92	0.53
1:A:71:LYS:HE3	5:A:612:HOH:O	2.07	0.53
1:G:33:MET:HE1	5:G:659:HOH:O	2.09	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
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: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
1:A:25:ASN:HD21	1:A:33:MET:CE	2.25	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:C:25:ASN:HD21	1:C:33:MET:HE1	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:10:HIS:O	2:H:14:PRO:HD3	2.12	0.48
1:A:100:ASN:HA	1:A:307:LEU:HD22	1.96	0.48
2:D:127:PHE:CD2	2:D:168:PRO:HD3	2.49	0.48
2:B:182:GLY:HA3	2:D:136:PHE:HE2	1.77	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:O	2:D:167:PRO:HD2	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
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:CD2	2:F:8:HIS:N	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:G:302:PHE:CE1	1:G:306:ILE:HG13	2.50	0.45
1:A:12:GLN:NE2	1:A:12:GLN:HA	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:HH11	1:E:134:ARG:HG2	1.82	0.44
1:G:25:ASN:HD21	1:G:33:MET:HE1	1.83	0.44
1:G:174:LEU:HA	1:G:174:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.68	0.44
1:A:222:THR:HG1	1:A:223:HIS:HD2	1.63	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:E:187:GLU:H	1:E:187:GLU:CD	2.22	0.43
1:A:6:GLU:HB2	1:A:11:LEU:HD21	2.01	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
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: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
1:C:192:ALA:HB3	1:C:223:HIS:CE1	2.55	0.42
1:C:307:LEU:HA	1:C:307:LEU:HD23	1.86	0.42
1:C:206:LYS:NZ	1:C:363:GLU:OE1	2.50	0.42
1:A:118:ASP:N	1:A:118:ASP:OD1	2.49	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:9:HIS:ND1	2:B:10:HIS:N	2.68	0.42
2:B:136:PHE:HE2	2:D:182:GLY:HA3	1.84	0.42
2:H:43:LEU:HA	2:H:43:LEU:HD23	1.90	0.42
1:A:33:MET:HE3	2:B:105:GLY:N	2.33	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
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
1:G:33:MET:HE2	5:H:216:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:135:PRO:HG2	5:H:282:HOH:O	2.19	0.41
2:B:8:HIS:N	2:B:8:HIS:HD1	2.18	0.41
1:G:180:TRP:CZ2	1:G:182:GLY:HA3	2.54	0.41
1:C:62:LEU:HB2	5:C:617:HOH:O	2.20	0.41
1:A:25:ASN:HD21	1:A:33:MET:HE2	1.85	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:HB3	1:C:347:GLN:HE21	1.72	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:HG21	2:H:175:ILE:HD13	1.92	0.41
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
2:B:26:LYS:O	2:B:30:GLN:HG3	2.22	0.40
2:B:8:HIS:ND1	2:B:8:HIS:N	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%)	29	35
2	F	174/188 (93%)	168 (97%)	6 (3%)	0	100	100
2	H	183/188 (97%)	177 (97%)	6 (3%)	0	100	100
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 ⓘ

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%)	306 (99%)	2 (1%)	86	94
1	C	307/308 (100%)	301 (98%)	6 (2%)	55	72
1	E	308/308 (100%)	301 (98%)	7 (2%)	50	67
1	G	308/308 (100%)	307 (100%)	1 (0%)	92	97
2	B	155/158 (98%)	150 (97%)	5 (3%)	39	54
2	D	155/158 (98%)	150 (97%)	5 (3%)	39	54
2	F	149/158 (94%)	148 (99%)	1 (1%)	84	92
2	H	155/158 (98%)	153 (99%)	2 (1%)	69	82
All	All	1845/1864 (99%)	1816 (98%)	29 (2%)	62	78

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	118	ASP
2	B	8	HIS
2	B	20	GLN
2	B	67	LEU
2	B	84	PHE
2	B	109	PRO
1	C	7	ASP
1	C	22	SER
1	C	118	ASP
1	C	218	GLN
1	C	347	GLN
1	C	366	PHE
2	D	11	SER
2	D	13	ASP
2	D	22	GLN
2	D	68	ASN
2	D	84	PHE
1	E	1	MET
1	E	22	SER
1	E	30	GLN
1	E	118	ASP
1	E	134	ARG
1	E	218	GLN
1	E	250	LYS
2	F	68	ASN
1	G	118	ASP
2	H	8	HIS
2	H	84	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	223	HIS
1	A	346	GLN
1	A	352	ASN
2	B	99	ASN
1	C	244	ASN
1	C	311	ASN
1	C	346	GLN
2	D	9	HIS
2	D	12	GLN

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Mol	Chain	Res	Type
2	D	87	HIS
2	D	185	HIS
1	E	30	GLN
2	F	8	HIS
2	F	10	HIS
2	F	35	ASN
1	G	16	GLN
1	G	325	GLN
1	G	346	GLN
2	H	61	ASN
2	H	74	GLN
2	H	87	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	G	401	-	4,4,4	0.99	0	6,6,6	0.93	0
3	PO4	A	401	-	4,4,4	1.36	1 (25%)	6,6,6	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	C	401	-	4,4,4	0.63	0	6,6,6	1.20	1 (16%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	PO4	P-O1	2.53	1.56	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	PO4	O4-P-O3	2.21	115.08	107.97

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, 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	365/366 (99%)	-0.67	1 (0%) 94 96	17, 24, 41, 62	0
1	C	365/366 (99%)	-0.74	0 100 100	14, 21, 36, 55	0
1	E	366/366 (100%)	-0.57	0 100 100	15, 23, 40, 63	0
1	G	365/366 (99%)	-0.66	2 (0%) 91 94	16, 23, 40, 62	0
2	B	185/188 (98%)	-0.47	5 (2%) 54 62	19, 27, 54, 66	0
2	D	185/188 (98%)	-0.43	7 (3%) 40 47	16, 24, 51, 72	0
2	F	178/188 (94%)	-0.37	6 (3%) 45 52	17, 25, 60, 92	0
2	H	185/188 (98%)	-0.40	3 (1%) 72 77	19, 29, 60, 84	0
All	All	2194/2216 (99%)	-0.58	24 (1%) 80 85	14, 24, 44, 92	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	13	ASP	4.2
2	F	9	HIS	4.1
2	H	13	ASP	4.0
2	H	8	HIS	3.9
2	F	13	ASP	3.9
2	F	8	HIS	3.8
1	G	59	PRO	3.5
2	D	8	HIS	3.5
2	B	9	HIS	3.4
2	B	13	ASP	3.2
2	D	21	GLY	3.1
2	F	12	GLN	3.0
2	B	8	HIS	3.0
2	D	9	HIS	2.8
1	A	366	PHE	2.8
2	F	15	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	21	GLY	2.4
2	F	11	SER	2.3
2	D	10	HIS	2.3
2	B	20	GLN	2.3
2	H	82	GLU	2.2
2	D	20	GLN	2.2
1	G	366	PHE	2.2
2	D	22	GLN	2.1

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	C	400	1/1	0.85	0.13	39,39,39,39	0
3	PO4	C	401	5/5	0.91	0.14	44,49,58,63	0
3	PO4	G	401	5/5	0.96	0.11	27,27,41,46	0
3	PO4	A	401	5/5	0.97	0.09	24,24,43,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.