



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:35 PM GMT

PDB ID : 3ZWO  
Title : Crystal structure of ADP ribosyl cyclase complexed with reaction intermediate  
Authors : Kotaka, M.; Graeff, R.; Zhang, L.H.; Lee, H.C.; Hao, Q.  
Deposited on : 2011-08-02  
Resolution : 2.00 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

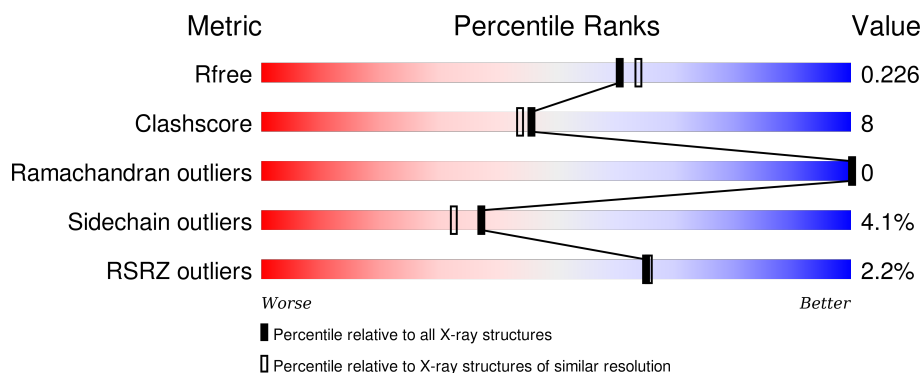
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	259	<div> <div>2%</div> <div>81% 13% . .</div> </div>
1	B	259	<div> <div>2%</div> <div>86% 10% . .</div> </div>
1	C	259	<div> <div>2%</div> <div>84% 10% . .</div> </div>
1	D	259	<div> <div>2%</div> <div>81% 14% . .</div> </div>
1	E	259	<div> <div>2%</div> <div>85% 11% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	259	
1	G	259	
1	H	259	

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	G2Q	A	301	-	-	X	-
2	G2Q	B	301	-	-	X	-
2	G2Q	C	301	-	-	X	-
2	G2Q	E	301	-	-	X	-
2	G2Q	G	301	-	-	X	-
3	NGD	F	5573	-	-	-	X

## 2 Entry composition

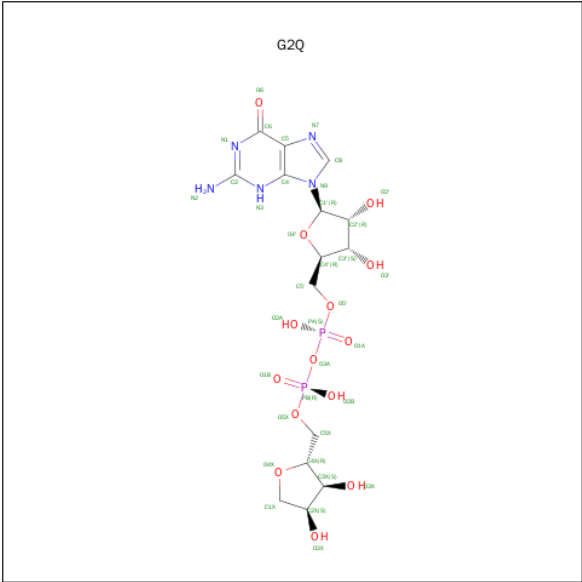
There are 4 unique types of molecules in this entry. The entry contains 17700 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYCLASE.

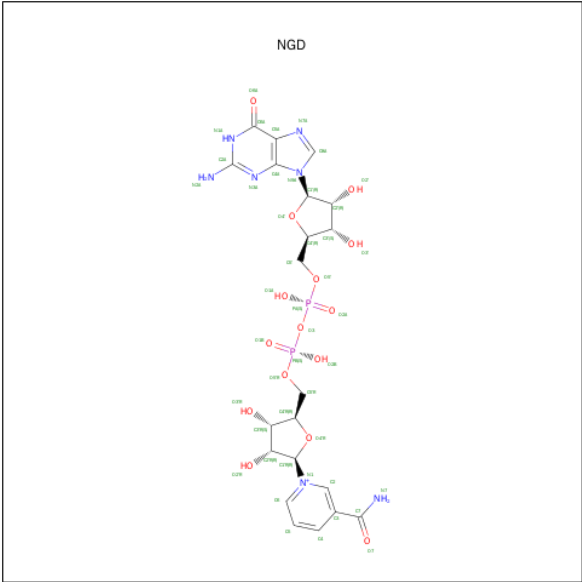
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2017	1291	343	369	14			
1	B	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	C	252	Total	C	N	O	S	0	0	0
			2017	1291	343	369	14			
1	D	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	E	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	F	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	G	252	Total	C	N	O	S	0	0	0
			2017	1291	343	369	14			
1	H	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			

- Molecule 2 is GUANOSINE DIPHOSPHATE RIBOSE (three-letter code: G2Q) (formula:  $C_{15}H_{23}N_5O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	C	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	E	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	G	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	H	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 3 is 3-(AMINOCARBONYL)-1-[(2R,3R,4S,5R)-5-({[(S)-{[(S)-{(2R,3S,4R,5R)-5-(2-AMINO-6-OXO-1,6-DIHYDRO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHOXY}(HYDROXY)PHOSPHORYL]OXY}(HYDROXY)PHOSPHORYL]OXY}METHYL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]PYRIDINIUM (three-letter code: NGD) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			45	21	7	15	2		

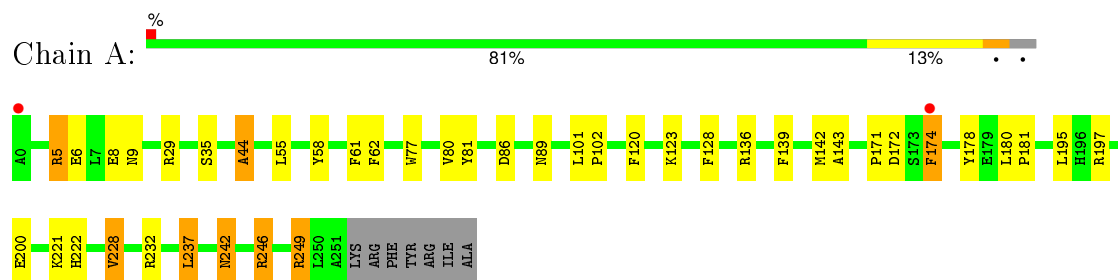
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		
4	B	194	Total	O	0	0
			194	194		
4	C	208	Total	O	0	0
			208	208		
4	D	204	Total	O	0	0
			204	204		
4	E	182	Total	O	0	0
			182	182		
4	F	138	Total	O	0	0
			138	138		
4	G	100	Total	O	0	0
			100	100		
4	H	98	Total	O	0	0
			98	98		

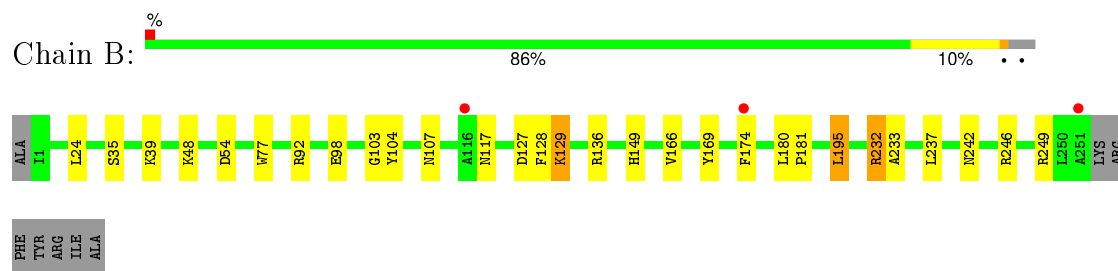
### 3 Residue-property plots

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

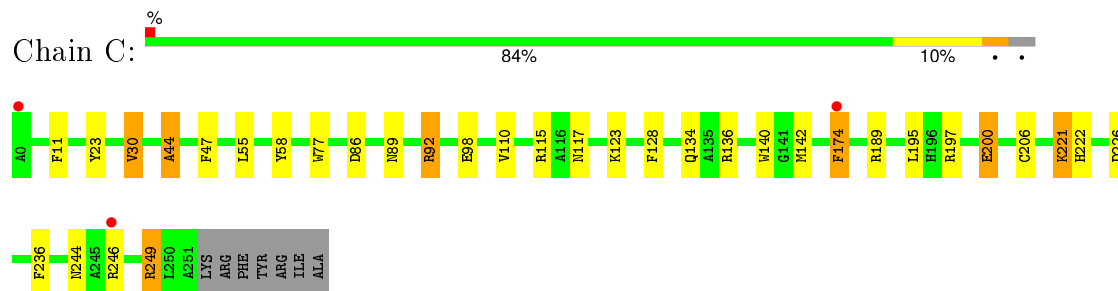
- Molecule 1: ADP-RIBOSYL CYCLASE



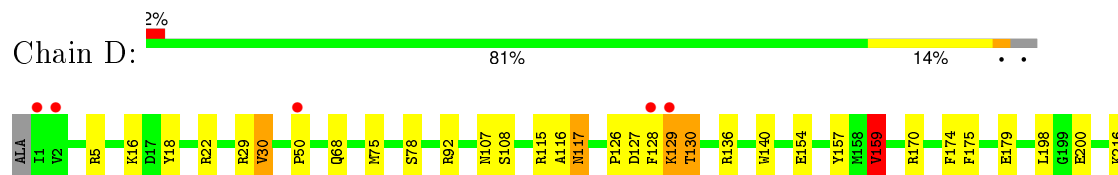
- Molecule 1: ADP-RIBOSYL CYCLASE



- Molecule 1: ADP-RIBOSYL CYCLASE

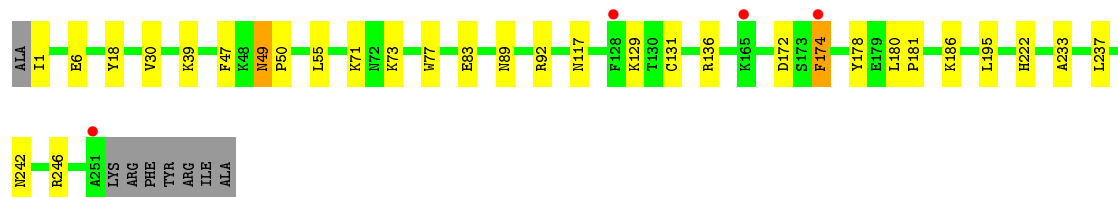
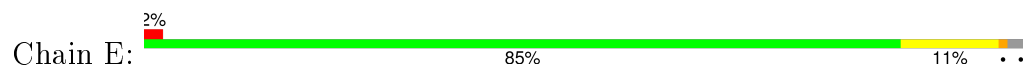


- Molecule 1: ADP-RIBOSYL CYCLASE

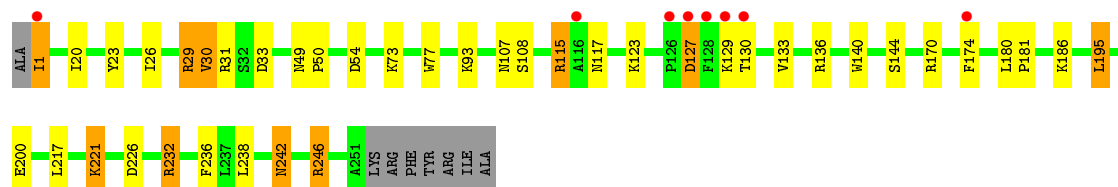
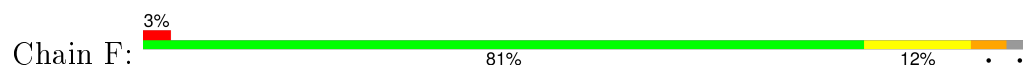




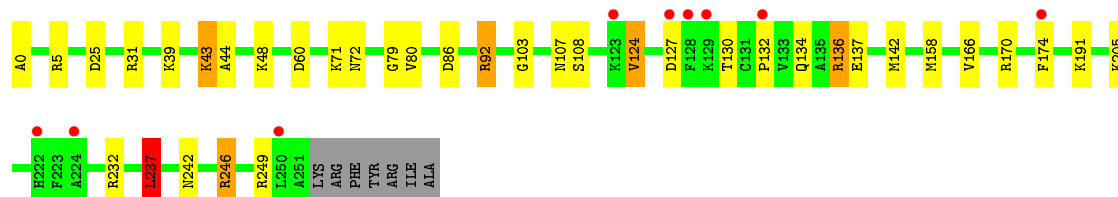
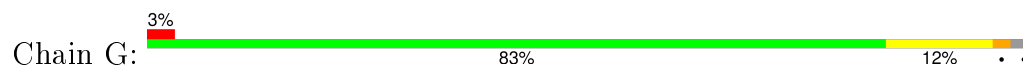
• Molecule 1: ADP-RIBOSYL CYCLASE



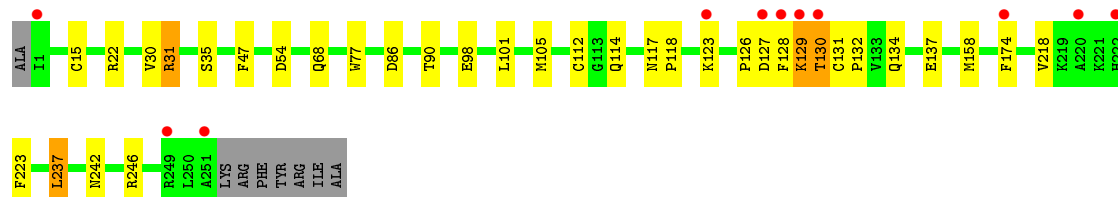
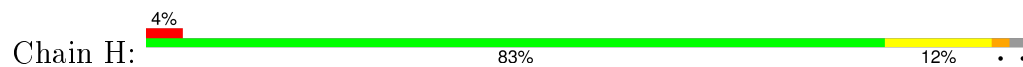
• Molecule 1: ADP-RIBOSYL CYCLASE



• Molecule 1: ADP-RIBOSYL CYCLASE



• Molecule 1: ADP-RIBOSYL CYCLASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.57Å 76.42Å 139.71Å 87.80° 89.09° 89.32°	Depositor
Resolution (Å)	30.00 – 2.00 29.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-2.00) 82.4 (29.69-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.177 , 0.228 0.177 , 0.226	Depositor DCC
$R_{free}$ test set	7075 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.5	EDS
Estimated twinning fraction	0.059 for h,-k,-l 0.015 for -h,k,-l 0.004 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 140698 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17700	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NGD, G2Q

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	1.29	10/2069 (0.5%)	1.06	7/2800 (0.2%)
1	B	1.24	4/2064 (0.2%)	0.98	4/2793 (0.1%)
1	C	1.31	8/2069 (0.4%)	1.00	4/2800 (0.1%)
1	D	1.17	1/2064 (0.0%)	0.98	5/2793 (0.2%)
1	E	1.27	10/2064 (0.5%)	0.98	2/2793 (0.1%)
1	F	1.09	1/2064 (0.0%)	0.96	4/2793 (0.1%)
1	G	0.96	0/2069	0.87	4/2800 (0.1%)
1	H	0.94	0/2064	0.90	5/2793 (0.2%)
All	All	1.17	34/16527 (0.2%)	0.97	35/22365 (0.2%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	110	VAL	CB-CG2	8.40	1.70	1.52
1	B	166	VAL	CB-CG1	7.39	1.68	1.52
1	E	174	PHE	CE1-CZ	7.19	1.51	1.37
1	E	131	CYS	CB-SG	7.18	1.94	1.82
1	C	140	TRP	CE3-CZ3	6.95	1.50	1.38
1	A	44	ALA	CA-CB	6.49	1.66	1.52
1	A	139	PHE	CE1-CZ	6.34	1.49	1.37
1	E	174	PHE	CD1-CE1	6.27	1.51	1.39
1	A	174	PHE	CE1-CZ	6.21	1.49	1.37
1	C	174	PHE	CE1-CZ	6.18	1.49	1.37
1	C	174	PHE	CG-CD2	6.17	1.48	1.38
1	E	174	PHE	CD2-CE2	6.17	1.51	1.39
1	A	174	PHE	CD2-CE2	6.10	1.51	1.39
1	A	174	PHE	CG-CD2	6.10	1.47	1.38
1	E	49	ASN	CB-CG	6.06	1.65	1.51
1	A	8	GLU	CD-OE1	-6.04	1.19	1.25
1	B	233	ALA	CA-CB	6.03	1.65	1.52
1	A	6	GLU	CD-OE2	-6.01	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	TYR	CD2-CE2	6.00	1.48	1.39
1	C	44	ALA	CA-CB	6.00	1.65	1.52
1	C	23	TYR	CE1-CZ	5.88	1.46	1.38
1	F	23	TYR	CD1-CE1	5.77	1.48	1.39
1	A	61	PHE	CE1-CZ	5.71	1.48	1.37
1	D	159	VAL	CB-CG1	-5.69	1.40	1.52
1	B	104	TYR	CE1-CZ	5.69	1.46	1.38
1	E	174	PHE	CG-CD2	5.47	1.47	1.38
1	C	206	CYS	CB-SG	5.37	1.91	1.82
1	B	169	TYR	CG-CD1	5.34	1.46	1.39
1	E	18	TYR	CD2-CE2	5.34	1.47	1.39
1	E	174	PHE	CE2-CZ	5.30	1.47	1.37
1	A	120	PHE	CE1-CZ	5.29	1.47	1.37
1	C	11	PHE	CE2-CZ	5.21	1.47	1.37
1	E	178	TYR	CD1-CE1	-5.08	1.31	1.39
1	E	83	GLU	CB-CG	5.03	1.61	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	172	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	A	172	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	172	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	H	237	LEU	CA-CB-CG	7.40	132.33	115.30
1	A	29	ARG	NE-CZ-NH1	-7.21	116.70	120.30
1	B	195	LEU	CB-CG-CD2	-6.96	99.17	111.00
1	F	30	VAL	CG1-CB-CG2	6.51	121.31	110.90
1	G	60	ASP	CB-CG-OD1	6.46	124.11	118.30
1	C	30	VAL	CG1-CB-CG2	6.23	120.86	110.90
1	D	5	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	G	43	LYS	CB-CA-C	-6.08	98.23	110.40
1	H	237	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	F	29	ARG	NE-CZ-NH1	-6.01	117.30	120.30
1	D	29	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	B	48	LYS	CD-CE-NZ	-5.98	97.94	111.70
1	A	197	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	G	5	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	F	54	ASP	CB-CG-OD1	5.89	123.60	118.30
1	C	249	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	E	136	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	249	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	5	ARG	NE-CZ-NH1	5.36	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	75	MET	CG-SD-CE	-5.31	91.70	100.20
1	G	237	LEU	CB-CG-CD1	-5.30	101.99	111.00
1	C	30	VAL	N-CA-CB	-5.27	99.90	111.50
1	B	24	LEU	C-N-CA	-5.26	108.56	121.70
1	D	30	VAL	N-CA-CB	-5.23	100.00	111.50
1	A	123	LYS	CD-CE-NZ	-5.19	99.77	111.70
1	H	31	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	H	31	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	142	MET	CG-SD-CE	-5.03	92.15	100.20
1	D	170	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	H	22	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	F	226	ASP	CB-CG-OD1	-5.01	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	2017	0	1973	24	0
1	B	2012	0	1968	13	0
1	C	2017	0	1973	26	0
1	D	2012	0	1968	35	1
1	E	2012	0	1968	25	0
1	F	2012	0	1968	34	1
1	G	2017	0	1973	28	0
1	H	2012	0	1968	27	0
2	A	36	0	21	10	0
2	B	36	0	21	12	0
2	C	36	0	21	13	0
2	E	36	0	21	11	0
2	G	36	0	21	9	0
2	H	36	0	21	5	0
3	F	45	0	26	5	0
4	A	204	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	194	0	0	9	0
4	C	208	0	0	13	0
4	D	204	0	0	11	1
4	E	182	0	0	14	0
4	F	138	0	0	8	1
4	G	100	0	0	6	0
4	H	98	0	0	3	0
All	All	17700	0	15911	247	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 8.

All (247) 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:C:301:G2Q:H1XA	4:C:2106:HOH:O	1.25	1.33
1:A:86:ASP:HB3	4:A:2108:HOH:O	1.26	1.30
1:C:86:ASP:HB3	4:C:2116:HOH:O	1.24	1.25
1:D:200:GLU:HG2	4:D:2168:HOH:O	1.41	1.19
1:F:49:ASN:HB2	1:F:115:ARG:HH22	1.05	1.13
1:G:127:ASP:O	1:G:130:THR:HG22	1.49	1.13
1:D:174:PHE:HZ	4:D:2055:HOH:O	1.34	1.10
1:F:200:GLU:HG2	4:F:2120:HOH:O	1.50	1.10
2:C:301:G2Q:C1X	4:C:2106:HOH:O	1.86	1.09
1:F:246:ARG:HG2	1:F:246:ARG:HH11	1.14	1.06
1:A:232:ARG:NH1	4:A:2187:HOH:O	1.85	1.06
1:E:92:ARG:HD2	4:E:2101:HOH:O	1.58	1.03
1:F:246:ARG:CG	1:F:246:ARG:HH11	1.71	1.02
1:D:68:GLN:CG	4:D:2081:HOH:O	2.13	0.95
1:F:49:ASN:HB2	1:F:115:ARG:NH2	1.80	0.95
1:D:68:GLN:HG3	4:D:2081:HOH:O	1.67	0.94
1:G:174:PHE:CZ	4:G:2100:HOH:O	2.19	0.94
1:C:55:LEU:HD22	4:C:2080:HOH:O	1.71	0.90
1:D:117:ASN:HD22	1:D:117:ASN:H	1.14	0.89
1:C:55:LEU:CD2	4:C:2080:HOH:O	2.21	0.88
1:H:132:PRO:HB2	1:H:134:GLN:HE22	1.39	0.88
1:H:132:PRO:HB2	1:H:134:GLN:NE2	1.89	0.87
1:G:174:PHE:HZ	4:G:2100:HOH:O	1.52	0.87
1:H:174:PHE:CE2	2:H:301:G2Q:O2'	2.28	0.86
1:E:174:PHE:CE1	4:E:2129:HOH:O	2.28	0.86
1:F:93:LYS:HE2	4:F:2079:HOH:O	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:TRP:O	2:E:301:G2Q:H5XA	1.77	0.84
2:C:301:G2Q:C2X	4:C:2106:HOH:O	2.19	0.82
1:C:92:ARG:HG3	1:C:92:ARG:HH11	1.44	0.81
1:H:117:ASN:HD22	1:H:118:PRO:HA	1.45	0.81
1:F:246:ARG:CG	1:F:246:ARG:NH1	2.38	0.79
1:F:26:ILE:HG13	4:F:2026:HOH:O	1.82	0.78
1:G:127:ASP:O	1:G:130:THR:CG2	2.30	0.77
1:B:77:TRP:O	2:B:301:G2Q:H5XA	1.83	0.77
1:E:222:HIS:ND1	4:E:2171:HOH:O	2.18	0.76
1:E:233:ALA:O	4:E:2177:HOH:O	2.03	0.76
2:A:301:G2Q:O4X	2:A:301:G2Q:O3'	2.02	0.75
1:B:246:ARG:HG3	4:B:2194:HOH:O	1.84	0.75
1:E:49:ASN:HB2	4:E:2059:HOH:O	1.85	0.75
1:H:54:ASP:HB2	4:H:2044:HOH:O	1.86	0.75
1:H:137:GLU:HG2	1:H:174:PHE:CE1	2.23	0.74
1:B:127:ASP:OD1	1:B:129:LYS:HG2	1.86	0.74
2:B:301:G2Q:H1XA	2:B:301:G2Q:O3'	1.90	0.72
1:H:132:PRO:CB	1:H:134:GLN:HE22	2.02	0.72
4:B:2193:HOH:O	1:G:232:ARG:NH2	2.23	0.71
1:B:92:ARG:NH1	4:B:2109:HOH:O	2.22	0.71
2:E:301:G2Q:O3'	2:E:301:G2Q:O4X	2.07	0.71
1:C:77:TRP:O	2:C:301:G2Q:H5XA	1.90	0.71
1:C:142:MET:HE1	4:C:2156:HOH:O	1.91	0.71
1:A:77:TRP:O	2:A:301:G2Q:H5XA	1.89	0.70
2:C:301:G2Q:H2X	4:C:2106:HOH:O	1.88	0.70
1:E:47:PHE:HE1	1:E:117:ASN:HD22	1.37	0.69
1:H:126:PRO:HB2	1:H:130:THR:HG23	1.76	0.68
1:F:246:ARG:NH2	4:F:2137:HOH:O	2.14	0.68
1:E:174:PHE:CD1	4:E:2129:HOH:O	2.46	0.68
1:D:117:ASN:H	1:D:117:ASN:ND2	1.89	0.68
1:C:244:ASN:OD1	1:F:232:ARG:NH2	2.26	0.68
2:E:301:G2Q:O3'	2:E:301:G2Q:C1X	2.43	0.66
2:B:301:G2Q:C1X	2:B:301:G2Q:O3'	2.43	0.66
1:E:47:PHE:HE1	1:E:117:ASN:ND2	1.94	0.65
1:D:117:ASN:ND2	4:D:2123:HOH:O	2.29	0.65
1:F:246:ARG:HG2	1:F:246:ARG:NH1	1.97	0.65
1:H:137:GLU:HG2	1:H:174:PHE:CZ	2.31	0.65
1:A:86:ASP:CB	4:A:2108:HOH:O	2.06	0.65
1:H:127:ASP:O	1:H:130:THR:HG22	1.96	0.65
1:D:154:GLU:OE2	4:D:2136:HOH:O	2.14	0.65
1:G:25:ASP:HB2	4:G:2022:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:G2Q:HN3	2:C:301:G2Q:H2'	1.62	0.64
1:C:92:ARG:HG3	1:C:92:ARG:NH1	2.06	0.64
1:E:6:GLU:OE1	4:E:2011:HOH:O	2.15	0.64
1:D:128:PHE:O	1:D:136:ARG:HD3	1.98	0.64
1:G:79:GLY:N	2:G:301:G2Q:O2A	2.31	0.63
1:F:246:ARG:NH1	4:F:2137:HOH:O	2.22	0.63
1:H:127:ASP:O	1:H:130:THR:CG2	2.47	0.63
1:F:242:ASN:ND2	4:F:2134:HOH:O	2.21	0.63
2:C:301:G2Q:H5X	2:C:301:G2Q:O3'	1.98	0.63
1:D:127:ASP:O	1:D:130:THR:CG2	2.47	0.63
1:B:174:PHE:CD2	2:B:301:G2Q:O2'	2.51	0.62
1:F:174:PHE:CD2	3:F:5573:NGD:H6	2.35	0.61
1:D:127:ASP:O	1:D:129:LYS:N	2.31	0.61
1:F:127:ASP:O	1:F:130:THR:HG23	2.00	0.61
1:H:174:PHE:CZ	2:H:301:G2Q:O2'	2.51	0.61
1:E:186:LYS:HD2	4:E:2132:HOH:O	2.01	0.61
1:F:200:GLU:CG	4:F:2120:HOH:O	2.24	0.60
1:F:77:TRP:O	3:F:5573:NGD:H5'1	2.01	0.60
1:C:92:ARG:HH11	1:C:92:ARG:CG	2.13	0.59
1:G:31:ARG:HD3	4:G:2027:HOH:O	2.02	0.59
1:D:78:SER:HB2	1:D:159:VAL:HG12	1.83	0.59
1:A:5:ARG:HD2	4:A:2011:HOH:O	2.02	0.59
1:G:174:PHE:CD2	2:G:301:G2Q:H2'	2.38	0.59
1:C:115:ARG:NH1	4:C:2072:HOH:O	2.36	0.58
1:F:174:PHE:HB2	3:F:5573:NGD:PB	2.43	0.58
1:G:80:VAL:HG21	1:G:158:MET:HG2	1.85	0.58
1:H:68:GLN:HG3	4:H:2049:HOH:O	2.04	0.57
2:C:301:G2Q:N3	2:C:301:G2Q:H2'	2.18	0.57
2:G:301:G2Q:H1XA	2:G:301:G2Q:N7	2.20	0.56
2:A:301:G2Q:O3'	2:A:301:G2Q:C5X	2.53	0.56
1:C:244:ASN:HB2	4:C:2202:HOH:O	2.05	0.56
2:E:301:G2Q:O3'	2:E:301:G2Q:H1XA	2.06	0.56
1:G:103:GLY:O	1:G:107:ASN:HB2	2.06	0.56
1:A:174:PHE:CD2	2:A:301:G2Q:O2'	2.57	0.55
1:C:55:LEU:H	1:C:55:LEU:HD22	1.71	0.55
1:A:237:LEU:HD13	1:D:240:SER:CB	2.36	0.55
1:D:127:ASP:O	1:D:130:THR:HG22	2.07	0.55
2:C:301:G2Q:C5X	2:C:301:G2Q:O3'	2.54	0.55
1:A:237:LEU:HD13	1:D:240:SER:HB2	1.88	0.55
1:E:49:ASN:CG	1:E:50:PRO:HD2	2.27	0.55
1:E:92:ARG:CD	4:E:2101:HOH:O	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:ARG:O	1:G:249:ARG:HG3	2.08	0.54
1:C:98:GLU:OE2	2:C:301:G2Q:N2	2.41	0.54
1:E:174:PHE:CD1	2:E:301:G2Q:H4'	2.43	0.54
1:G:0:ALA:HB1	1:G:124:VAL:HG22	1.90	0.54
1:D:127:ASP:O	1:D:130:THR:HG23	2.07	0.54
1:B:180:LEU:HB3	1:B:181:PRO:HD3	1.90	0.53
1:F:217:LEU:O	1:F:221:LYS:HG2	2.07	0.53
1:B:128:PHE:HD2	1:B:136:ARG:HA	1.74	0.53
1:C:197:ARG:HB2	1:C:200:GLU:HG3	1.91	0.53
1:D:117:ASN:HD22	1:D:117:ASN:N	1.95	0.53
2:A:301:G2Q:O3'	2:A:301:G2Q:C1X	2.57	0.53
2:G:301:G2Q:H1XA	2:G:301:G2Q:C8	2.40	0.52
2:B:301:G2Q:C2'	2:B:301:G2Q:HN3	2.22	0.52
1:D:200:GLU:CG	4:D:2168:HOH:O	2.22	0.52
1:A:246:ARG:O	1:A:249:ARG:HG3	2.10	0.52
1:F:49:ASN:OD1	1:F:50:PRO:HD2	2.10	0.52
1:G:136:ARG:HG2	1:G:137:GLU:HG3	1.92	0.52
1:E:174:PHE:CZ	2:E:301:G2Q:H1'	2.46	0.51
1:F:144:SER:HG	1:F:174:PHE:HD2	1.58	0.51
1:G:44:ALA:O	1:G:48:LYS:NZ	2.43	0.51
1:B:232:ARG:NH1	4:B:2188:HOH:O	2.44	0.50
1:G:86:ASP:HB3	1:G:237:LEU:HD21	1.94	0.50
1:G:174:PHE:CG	2:G:301:G2Q:H2'	2.47	0.50
2:B:301:G2Q:C3'	2:B:301:G2Q:HN3	2.25	0.50
4:B:2101:HOH:O	1:G:92:ARG:CD	2.59	0.50
2:B:301:G2Q:H2'	2:B:301:G2Q:HN3	1.77	0.49
4:B:2101:HOH:O	1:G:92:ARG:HD3	2.12	0.49
1:H:218:VAL:HG13	1:H:223:PHE:HB2	1.94	0.49
1:B:149:HIS:ND1	4:B:2142:HOH:O	2.34	0.49
2:B:301:G2Q:O3'	2:B:301:G2Q:O4X	2.30	0.49
1:C:142:MET:CE	4:C:2156:HOH:O	2.52	0.49
2:H:301:G2Q:H8	2:H:301:G2Q:H1XA	1.95	0.49
1:E:246:ARG:HG3	4:E:2182:HOH:O	2.12	0.49
1:C:47:PHE:HE1	1:C:117:ASN:HD22	1.59	0.48
1:A:171:PRO:HG3	1:E:129:LYS:HD3	1.95	0.48
1:D:117:ASN:CG	4:D:2124:HOH:O	2.51	0.48
1:H:35:SER:HB3	4:H:2004:HOH:O	2.13	0.48
1:H:47:PHE:HA	1:H:114:GLN:O	2.13	0.48
2:H:301:G2Q:C8	2:H:301:G2Q:H1XA	2.44	0.48
1:D:127:ASP:C	1:D:129:LYS:H	2.17	0.48
2:B:301:G2Q:H3'	2:B:301:G2Q:HN3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128:PHE:O	1:H:131:CYS:N	2.42	0.47
1:G:166:VAL:HG13	1:G:170:ARG:HD3	1.95	0.47
1:A:128:PHE:HD2	1:A:136:ARG:HA	1.79	0.47
1:F:246:ARG:HG3	1:F:246:ARG:NH1	2.23	0.47
1:G:132:PRO:HB2	1:G:134:GLN:NE2	2.30	0.47
1:C:55:LEU:CD2	1:C:134:GLN:HB2	2.45	0.47
1:D:175:PHE:HA	1:D:179:GLU:HB2	1.97	0.47
1:F:195:LEU:HD11	1:F:238:LEU:HD21	1.97	0.47
1:C:174:PHE:HZ	4:C:2153:HOH:O	1.97	0.47
2:B:301:G2Q:H2'	2:B:301:G2Q:N3	2.30	0.47
1:E:49:ASN:CB	4:E:2059:HOH:O	2.54	0.47
1:C:55:LEU:HD23	4:C:2080:HOH:O	2.04	0.47
2:A:301:G2Q:C2'	2:A:301:G2Q:HN3	2.28	0.47
1:C:128:PHE:HD2	1:C:136:ARG:HA	1.80	0.46
2:A:301:G2Q:N3	2:A:301:G2Q:H2'	2.29	0.46
2:G:301:G2Q:H5'A	2:G:301:G2Q:O5X	2.16	0.46
2:A:301:G2Q:H2'	2:A:301:G2Q:HN3	1.80	0.46
1:B:98:GLU:OE2	2:B:301:G2Q:N2	2.49	0.46
2:E:301:G2Q:HN3	2:E:301:G2Q:C2'	2.29	0.46
1:D:129:LYS:HB2	1:D:129:LYS:HE2	1.37	0.46
1:C:189:ARG:HD3	1:C:226:ASP:OD2	2.16	0.46
1:A:44:ALA:HB3	1:A:58:TYR:CE1	2.51	0.46
1:H:98:GLU:OE2	2:H:301:G2Q:O6	2.34	0.45
1:D:50:PRO:HG3	4:D:2121:HOH:O	2.16	0.45
1:D:222:HIS:ND1	4:D:2179:HOH:O	2.36	0.45
1:A:55:LEU:HB2	4:A:2075:HOH:O	2.16	0.45
1:F:174:PHE:HB2	3:F:5573:NGD:O5'R	2.17	0.45
1:A:62:PHE:CZ	1:A:143:ALA:HB2	2.51	0.45
2:G:301:G2Q:H3'	2:G:301:G2Q:O2B	2.16	0.44
1:C:246:ARG:O	1:C:249:ARG:HG3	2.17	0.44
1:H:126:PRO:HB2	1:H:130:THR:CG2	2.44	0.44
2:C:301:G2Q:HN3	2:C:301:G2Q:C2'	2.28	0.44
1:D:68:GLN:HG2	4:D:2081:HOH:O	1.98	0.44
1:A:242:ASN:ND2	4:A:2196:HOH:O	2.40	0.44
1:H:127:ASP:OD2	1:H:129:LYS:HB3	2.18	0.44
1:D:107:ASN:O	1:D:108:SER:HB2	2.18	0.44
2:E:301:G2Q:HN3	2:E:301:G2Q:H3'	1.82	0.44
1:D:157:TYR:CZ	1:D:159:VAL:CG1	3.01	0.44
1:H:117:ASN:ND2	1:H:118:PRO:HA	2.23	0.43
1:E:55:LEU:HB2	4:E:2067:HOH:O	2.17	0.43
1:G:39:LYS:O	1:G:43:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:TRP:NE1	2:E:301:G2Q:H2X	2.33	0.43
1:F:107:ASN:O	1:F:108:SER:HB2	2.19	0.43
1:E:180:LEU:HB3	1:E:181:PRO:HD3	2.00	0.43
1:G:174:PHE:CE2	4:G:2100:HOH:O	2.60	0.43
1:F:73:LYS:HD3	1:F:73:LYS:HA	1.82	0.43
1:H:101:LEU:O	1:H:105:MET:HG3	2.19	0.43
1:H:86:ASP:HB3	1:H:237:LEU:HD11	1.99	0.43
1:F:170:ARG:HH22	3:F:5573:NGD:H2A2	1.66	0.43
2:E:301:G2Q:HN3	2:E:301:G2Q:H2'	1.83	0.43
1:C:174:PHE:CD2	2:C:301:G2Q:O2'	2.71	0.43
1:C:236:PHE:HB3	1:F:236:PHE:O	2.19	0.43
1:A:9:ASN:HB3	1:D:16:LYS:HG2	1.99	0.43
1:A:174:PHE:CE2	4:A:2147:HOH:O	2.69	0.43
1:B:54:ASP:HB2	4:B:2065:HOH:O	2.18	0.43
1:G:132:PRO:HB2	1:G:134:GLN:HE22	1.84	0.43
2:G:301:G2Q:H3'	2:G:301:G2Q:PB	2.59	0.42
1:E:174:PHE:HZ	4:E:2126:HOH:O	1.97	0.42
1:F:49:ASN:CB	1:F:115:ARG:NH2	2.67	0.42
1:B:117:ASN:HB2	4:B:2124:HOH:O	2.18	0.42
1:C:221:LYS:O	1:C:222:HIS:HB2	2.20	0.42
1:D:140:TRP:HB3	1:D:174:PHE:HE2	1.84	0.42
1:D:126:PRO:O	1:D:128:PHE:CD1	2.72	0.42
1:H:15:CYS:HB2	1:H:105:MET:SD	2.60	0.42
1:F:246:ARG:CZ	4:F:2137:HOH:O	2.51	0.42
2:E:301:G2Q:H2'	2:E:301:G2Q:N3	2.35	0.42
1:G:71:LYS:O	1:G:72:ASN:HB2	2.20	0.42
1:D:128:PHE:HB3	1:D:136:ARG:CG	2.50	0.42
2:B:301:G2Q:C2'	2:B:301:G2Q:N3	2.81	0.42
2:A:301:G2Q:H3'	2:A:301:G2Q:HN3	1.84	0.42
1:F:180:LEU:HB3	1:F:181:PRO:HD3	2.01	0.42
1:H:127:ASP:O	1:H:130:THR:HG23	2.17	0.42
1:A:44:ALA:CB	1:A:58:TYR:CD1	3.03	0.41
1:D:18:TYR:HA	1:D:22:ARG:CG	2.51	0.41
1:G:191:LYS:HE3	1:G:191:LYS:HB3	1.76	0.41
1:A:232:ARG:NH2	4:A:2188:HOH:O	2.53	0.41
1:F:140:TRP:C	1:F:174:PHE:HE2	2.24	0.41
2:C:301:G2Q:H1XA	2:C:301:G2Q:O3'	2.21	0.41
1:H:112:CYS:HB3	1:H:128:PHE:HZ	1.84	0.41
1:F:1:ILE:HG13	1:F:1:ILE:O	2.20	0.41
1:B:103:GLY:O	1:B:107:ASN:HB2	2.21	0.41
1:F:133:VAL:HB	1:F:136:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ASN:O	1:D:245:ALA:C	2.58	0.41
2:A:301:G2Q:C3'	2:A:301:G2Q:HN3	2.33	0.41
1:A:101:LEU:HB3	1:A:102:PRO:HD3	2.01	0.41
1:H:77:TRP:HA	1:H:158:MET:O	2.20	0.41
1:A:180:LEU:HB3	1:A:181:PRO:HD3	2.03	0.41
1:G:174:PHE:CE2	2:G:301:G2Q:H2'	2.55	0.41
1:A:228:VAL:HG22	4:A:2171:HOH:O	2.21	0.41
1:C:44:ALA:HB3	1:C:58:TYR:CE1	2.56	0.41
1:G:142:MET:HE2	4:G:2040:HOH:O	2.20	0.41
1:E:71:LYS:HG2	1:E:71:LYS:H	1.71	0.40
1:E:71:LYS:HG2	4:E:2082:HOH:O	2.20	0.40
1:D:116:ALA:O	1:D:117:ASN:C	2.60	0.40
1:E:73:LYS:HD3	1:E:73:LYS:HA	1.86	0.40
1:A:80:VAL:O	1:A:81:TYR:C	2.60	0.40
1:A:221:LYS:O	1:A:222:HIS:HB2	2.20	0.40
1:D:198:LEU:HD22	1:D:247:GLU:HB2	2.04	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)
1:D:154:GLU:OE1	1:F:31:ARG:NH1[1_565]	1.48	0.72
4:D:2183:HOH:O	4:F:2025:HOH:O[1_565]	2.12	0.08

## 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	250/259 (96%)	243 (97%)	7 (3%)	0	100	100
1	B	249/259 (96%)	247 (99%)	2 (1%)	0	100	100
1	C	250/259 (96%)	241 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	249/259 (96%)	242 (97%)	7 (3%)	0	100	100
1	E	249/259 (96%)	245 (98%)	4 (2%)	0	100	100
1	F	249/259 (96%)	241 (97%)	8 (3%)	0	100	100
1	G	250/259 (96%)	243 (97%)	7 (3%)	0	100	100
1	H	249/259 (96%)	240 (96%)	9 (4%)	0	100	100
All	All	1995/2072 (96%)	1942 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	220/226 (97%)	211 (96%)	9 (4%)	37	32
1	B	220/226 (97%)	213 (97%)	7 (3%)	46	44
1	C	220/226 (97%)	213 (97%)	7 (3%)	46	44
1	D	220/226 (97%)	210 (96%)	10 (4%)	34	29
1	E	220/226 (97%)	213 (97%)	7 (3%)	46	44
1	F	220/226 (97%)	204 (93%)	16 (7%)	17	11
1	G	220/226 (97%)	212 (96%)	8 (4%)	42	39
1	H	220/226 (97%)	212 (96%)	8 (4%)	42	39
All	All	1760/1808 (97%)	1688 (96%)	72 (4%)	37	32

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	89	ASN
1	A	195	LEU
1	A	200	GLU
1	A	228	VAL

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Mol	Chain	Res	Type
1	A	237	LEU
1	A	242	ASN
1	A	246	ARG
1	A	249	ARG
1	B	35	SER
1	B	39	LYS
1	B	129	LYS
1	B	195	LEU
1	B	232	ARG
1	B	237	LEU
1	B	242	ASN
1	C	30	VAL
1	C	89	ASN
1	C	92	ARG
1	C	123	LYS
1	C	195	LEU
1	C	200	GLU
1	C	221	LYS
1	D	30	VAL
1	D	92	ARG
1	D	115	ARG
1	D	117	ASN
1	D	129	LYS
1	D	130	THR
1	D	159	VAL
1	D	216	LYS
1	D	228	VAL
1	D	242	ASN
1	E	1	ILE
1	E	30	VAL
1	E	39	LYS
1	E	89	ASN
1	E	195	LEU
1	E	237	LEU
1	E	242	ASN
1	F	1	ILE
1	F	20	ILE
1	F	29	ARG
1	F	30	VAL
1	F	33	ASP
1	F	115	ARG
1	F	117	ASN

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Mol	Chain	Res	Type
1	F	123	LYS
1	F	127	ASP
1	F	129	LYS
1	F	186	LYS
1	F	195	LEU
1	F	221	LYS
1	F	232	ARG
1	F	242	ASN
1	F	246	ARG
1	G	92	ARG
1	G	108	SER
1	G	124	VAL
1	G	136	ARG
1	G	205	LYS
1	G	237	LEU
1	G	242	ASN
1	G	246	ARG
1	H	30	VAL
1	H	31	ARG
1	H	90	THR
1	H	123	LYS
1	H	129	LYS
1	H	130	THR
1	H	242	ASN
1	H	246	ARG

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	89	ASN
1	A	117	ASN
1	A	149	HIS
1	A	242	ASN
1	B	49	ASN
1	B	89	ASN
1	B	242	ASN
1	C	89	ASN
1	C	117	ASN
1	C	242	ASN
1	D	89	ASN
1	D	117	ASN
1	D	242	ASN

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Mol	Chain	Res	Type
1	E	89	ASN
1	E	117	ASN
1	E	242	ASN
1	F	89	ASN
1	F	117	ASN
1	G	89	ASN
1	G	242	ASN
1	H	89	ASN
1	H	117	ASN
1	H	134	GLN
1	H	242	ASN

### 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](#)

7 ligands 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	G2Q	A	301	-	32,39,39	2.56	13 (40%)	42,60,60	2.57	16 (38%)
2	G2Q	B	301	-	32,39,39	2.79	10 (31%)	42,60,60	2.61	13 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	G2Q	C	301	-	32,39,39	2.62	9 (28%)	42,60,60	2.16	15 (35%)
2	G2Q	E	301	-	32,39,39	3.05	12 (37%)	42,60,60	2.35	13 (30%)
3	NGD	F	5573	-	39,49,49	1.73	6 (15%)	50,75,75	1.79	10 (20%)
2	G2Q	G	301	-	32,39,39	1.75	4 (12%)	42,60,60	2.65	12 (28%)
2	G2Q	H	301	-	32,39,39	1.30	3 (9%)	42,60,60	1.80	7 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G2Q	A	301	-	-	0/18/51/51	0/4/4/4
2	G2Q	B	301	-	-	0/18/51/51	0/4/4/4
2	G2Q	C	301	-	-	0/18/51/51	0/4/4/4
2	G2Q	E	301	-	-	0/18/51/51	0/4/4/4
3	NGD	F	5573	-	-	0/22/62/62	0/5/5/5
2	G2Q	G	301	-	-	0/18/51/51	0/4/4/4
2	G2Q	H	301	-	-	0/18/51/51	0/4/4/4

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	G2Q	PA-O2A	-2.34	1.45	1.54
2	C	301	G2Q	PA-O2A	-2.19	1.45	1.54
2	G	301	G2Q	PA-O2A	-2.08	1.46	1.54
2	E	301	G2Q	C6-C5	2.02	1.45	1.41
2	C	301	G2Q	PA-O5'	2.04	1.68	1.59
2	H	301	G2Q	PB-O5X	2.04	1.68	1.59
2	B	301	G2Q	C2-N1	2.09	1.39	1.35
2	A	301	G2Q	O5X-C5X	2.16	1.53	1.44
2	A	301	G2Q	C2-N1	2.17	1.39	1.35
2	A	301	G2Q	C5'-C4'	2.17	1.58	1.51
2	C	301	G2Q	PB-O5X	2.23	1.69	1.59
2	C	301	G2Q	C5'-C4'	2.34	1.59	1.51
2	A	301	G2Q	O4'-C4'	2.34	1.50	1.45
2	A	301	G2Q	PB-O5X	2.34	1.69	1.59
2	A	301	G2Q	C6-C5	2.55	1.46	1.41
2	B	301	G2Q	PB-O1B	2.60	1.60	1.51
2	C	301	G2Q	C2-N1	2.61	1.40	1.35
2	E	301	G2Q	O2'-C2'	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	G2Q	C1X-C2X	2.76	1.56	1.51
3	F	5573	NGD	O4'-C1'	2.79	1.44	1.41
2	B	301	G2Q	PB-O5X	2.81	1.71	1.59
2	G	301	G2Q	C2-N1	2.88	1.40	1.35
2	A	301	G2Q	PB-O1B	2.97	1.62	1.51
2	E	301	G2Q	PB-O5X	2.98	1.72	1.59
2	H	301	G2Q	C6-N1	3.01	1.38	1.33
2	B	301	G2Q	C5'-C4'	3.19	1.62	1.51
2	A	301	G2Q	C2X-C3X	3.20	1.58	1.53
2	B	301	G2Q	PA-O5'	3.23	1.73	1.59
3	F	5573	NGD	C6-N1	3.25	1.44	1.35
3	F	5573	NGD	O4'R-C1'R	3.30	1.45	1.41
2	E	301	G2Q	C1X-C2X	3.39	1.57	1.51
2	E	301	G2Q	C2-N1	3.62	1.41	1.35
2	E	301	G2Q	C5'-C4'	3.75	1.63	1.51
2	A	301	G2Q	O4X-C4X	3.81	1.51	1.44
2	E	301	G2Q	PA-O5'	3.98	1.77	1.59
2	H	301	G2Q	O4'-C1'	3.99	1.46	1.41
2	B	301	G2Q	C2X-C3X	4.27	1.59	1.53
2	E	301	G2Q	C2X-C3X	4.42	1.60	1.53
3	F	5573	NGD	C6A-C5A	4.44	1.50	1.41
2	G	301	G2Q	C6-N1	4.51	1.41	1.33
2	C	301	G2Q	O4X-C4X	4.73	1.52	1.44
3	F	5573	NGD	O7-C7	4.80	1.34	1.24
2	A	301	G2Q	C6-N1	4.83	1.42	1.33
2	C	301	G2Q	C6-N1	4.91	1.42	1.33
2	B	301	G2Q	C6-N1	5.11	1.42	1.33
3	F	5573	NGD	O6A-C6A	5.13	1.37	1.24
2	E	301	G2Q	C6-N1	5.39	1.43	1.33
2	E	301	G2Q	O4X-C1X	5.78	1.57	1.43
2	A	301	G2Q	O4'-C1'	6.45	1.49	1.41
2	B	301	G2Q	O4X-C1X	6.54	1.59	1.43
2	G	301	G2Q	O4'-C1'	6.66	1.49	1.41
2	E	301	G2Q	O4X-C4X	6.77	1.56	1.44
2	B	301	G2Q	O4X-C4X	7.22	1.57	1.44
2	B	301	G2Q	O4'-C1'	7.46	1.50	1.41
2	A	301	G2Q	O4X-C1X	7.55	1.61	1.43
2	E	301	G2Q	O4'-C1'	8.55	1.52	1.41
2	C	301	G2Q	O4'-C1'	10.82	1.54	1.41

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	G2Q	C5-C6-N1	-6.79	114.30	123.59
2	A	301	G2Q	N3-C2-N1	-6.07	118.20	127.44
2	B	301	G2Q	C5-C6-N1	-6.03	115.34	123.59
2	B	301	G2Q	N3-C2-N1	-5.44	119.16	127.44
2	C	301	G2Q	C2'-C1'-N9	-5.42	106.01	114.29
2	G	301	G2Q	C4-C5-N7	-5.25	104.65	109.48
2	H	301	G2Q	N3-C2-N1	-5.22	119.50	127.44
2	A	301	G2Q	O3A-PB-O5X	-5.15	89.28	102.94
2	E	301	G2Q	C5-C6-N1	-5.14	116.56	123.59
2	G	301	G2Q	C1'-N9-C4	-5.09	119.27	126.94
2	E	301	G2Q	N3-C2-N1	-5.05	119.75	127.44
3	F	5573	NGD	C2'-C1'-N9A	-4.90	106.80	114.29
2	C	301	G2Q	C5-C6-N1	-4.72	117.13	123.59
2	G	301	G2Q	C5'-C4'-C3'	-4.52	97.28	115.21
2	A	301	G2Q	C4-C5-N7	-4.41	105.42	109.48
2	B	301	G2Q	C5X-C4X-C3X	-4.31	98.11	115.21
2	G	301	G2Q	N3-C2-N1	-4.30	120.90	127.44
3	F	5573	NGD	N3A-C2A-N1A	-4.14	121.14	127.44
2	E	301	G2Q	PB-O3A-PA	-3.68	122.41	132.73
2	C	301	G2Q	O3A-PB-O5X	-3.59	93.42	102.94
2	G	301	G2Q	C5-C6-N1	-3.58	118.69	123.59
2	E	301	G2Q	O3A-PB-O5X	-3.37	94.00	102.94
2	E	301	G2Q	C4-C5-N7	-3.35	106.39	109.48
2	B	301	G2Q	PB-O3A-PA	-3.32	123.42	132.73
2	C	301	G2Q	N3-C2-N1	-3.31	122.41	127.44
2	B	301	G2Q	O3A-PB-O5X	-3.27	94.26	102.94
2	E	301	G2Q	O4X-C1X-C2X	-3.19	99.63	106.16
3	F	5573	NGD	C5A-C6A-N1A	-3.16	119.26	123.59
2	H	301	G2Q	N2-C2-N1	-3.15	111.99	117.20
2	B	301	G2Q	C4-C5-N7	-3.11	106.62	109.48
2	C	301	G2Q	O4'-C4'-C5'	-3.08	98.32	109.32
2	B	301	G2Q	C2'-C1'-N9	-3.07	109.60	114.29
2	E	301	G2Q	C5X-C4X-C3X	-3.06	103.07	115.21
2	E	301	G2Q	O4'-C4'-C3'	-2.92	99.26	105.15
2	A	301	G2Q	C2'-C1'-N9	-2.89	109.87	114.29
2	C	301	G2Q	C4-C5-N7	-2.86	106.85	109.48
2	G	301	G2Q	C6-C5-C4	-2.69	117.68	120.90
2	H	301	G2Q	C5-C6-N1	-2.65	119.97	123.59
2	B	301	G2Q	O4X-C1X-C2X	-2.60	100.83	106.16
2	A	301	G2Q	PB-O3A-PA	-2.54	125.59	132.73
3	F	5573	NGD	C6A-C5A-C4A	-2.52	117.88	120.90
2	A	301	G2Q	O4X-C1X-C2X	-2.49	101.06	106.16
2	A	301	G2Q	O3'-C3'-C2'	-2.34	104.20	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	G2Q	O3A-PB-O5X	-2.32	96.79	102.94
2	G	301	G2Q	PB-O3A-PA	-2.21	126.52	132.73
2	A	301	G2Q	C6-C5-C4	-2.18	118.29	120.90
2	H	301	G2Q	C2'-C1'-N9	-2.17	110.97	114.29
2	G	301	G2Q	O2A-PA-O5'	-2.17	97.52	108.46
2	C	301	G2Q	O3X-C3X-C4X	-2.17	104.55	111.05
3	F	5573	NGD	O7-C7-N7	-2.11	119.62	122.59
2	C	301	G2Q	O3'-C3'-C2'	-2.03	105.24	111.83
2	C	301	G2Q	O3'-C3'-C4'	2.01	117.09	111.05
2	C	301	G2Q	O2A-PA-O1A	2.10	123.90	112.53
3	F	5573	NGD	C4'R-O4'R-C1'R	2.11	112.04	109.72
2	A	301	G2Q	O2B-PB-O1B	2.26	124.75	112.53
2	A	301	G2Q	O4X-C4X-C5X	2.31	114.59	109.53
3	F	5573	NGD	C5-C6-N1	2.34	124.52	120.47
2	A	301	G2Q	O2X-C2X-C3X	2.35	115.74	111.23
2	C	301	G2Q	C6-N1-C2	2.41	119.28	115.94
2	C	301	G2Q	O3A-PA-O5'	2.41	109.33	102.94
2	A	301	G2Q	C1X-C2X-C3X	2.49	105.65	101.64
2	G	301	G2Q	C6-N1-C2	2.50	119.41	115.94
2	B	301	G2Q	O3A-PA-O5'	2.55	109.70	102.94
2	C	301	G2Q	C5'-C4'-C3'	2.59	125.48	115.21
2	B	301	G2Q	O2B-PB-O1B	2.61	126.65	112.53
2	C	301	G2Q	C1X-C2X-C3X	2.73	106.04	101.64
2	A	301	G2Q	N2-C2-N3	2.92	123.41	117.80
2	G	301	G2Q	N2-C2-N1	2.94	122.06	117.20
2	G	301	G2Q	O3A-PA-O5'	3.02	110.95	102.94
2	E	301	G2Q	O2B-PB-O1B	3.04	129.00	112.53
3	F	5573	NGD	O4'-C1'-N9A	3.09	114.57	108.10
2	E	301	G2Q	O3X-C3X-C2X	3.35	119.64	111.68
2	A	301	G2Q	O3A-PA-O5'	3.45	112.08	102.94
2	B	301	G2Q	C1X-C2X-C3X	3.49	107.25	101.64
3	F	5573	NGD	C6A-N1A-C2A	3.55	120.87	115.94
2	H	301	G2Q	C6-N1-C2	3.67	121.04	115.94
3	F	5573	NGD	C3-C7-N7	3.76	121.93	117.82
2	E	301	G2Q	O4X-C4X-C5X	4.10	118.50	109.53
2	E	301	G2Q	C6-N1-C2	4.12	121.66	115.94
2	E	301	G2Q	C1X-C2X-C3X	4.81	109.39	101.64
2	C	301	G2Q	O4'-C1'-N9	5.35	119.30	108.10
2	H	301	G2Q	N2-C2-N3	5.58	128.51	117.80
2	B	301	G2Q	C6-N1-C2	5.68	123.82	115.94
2	A	301	G2Q	C6-N1-C2	6.89	125.50	115.94
2	B	301	G2Q	O4X-C4X-C5X	7.24	125.38	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	G	301	G2Q	C2'-C1'-N9	10.62	130.53	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	G2Q	10	0
2	B	301	G2Q	12	0
2	C	301	G2Q	13	0
2	E	301	G2Q	11	0
3	F	5573	NGD	5	0
2	G	301	G2Q	9	0
2	H	301	G2Q	5	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	252/259 (97%)	-0.21	2 (0%) 87 88	15, 30, 48, 57	0
1	B	251/259 (96%)	-0.24	3 (1%) 81 81	19, 31, 49, 61	0
1	C	252/259 (97%)	-0.22	3 (1%) 81 81	17, 29, 48, 57	0
1	D	251/259 (96%)	-0.13	5 (1%) 68 69	18, 32, 53, 76	0
1	E	251/259 (96%)	-0.23	4 (1%) 74 75	19, 31, 47, 60	0
1	F	251/259 (96%)	-0.09	8 (3%) 51 52	19, 36, 56, 75	0
1	G	252/259 (97%)	0.05	9 (3%) 46 48	29, 46, 62, 76	0
1	H	251/259 (96%)	0.02	11 (4%) 38 39	30, 45, 63, 74	0
All	All	2011/2072 (97%)	-0.13	45 (2%) 65 66	15, 35, 56, 76	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	128	PHE	7.3
1	F	128	PHE	7.0
1	D	128	PHE	6.9
1	G	128	PHE	6.8
1	E	251	ALA	5.2
1	G	129	LYS	4.0
1	F	127	ASP	3.5
1	B	251	ALA	3.3
1	H	1	ILE	3.2
1	F	130	THR	3.1
1	H	129	LYS	3.1
1	D	50	PRO	2.9
1	C	0	ALA	2.9
1	H	123	LYS	2.8
1	G	222	HIS	2.8
1	A	174	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	1	ILE	2.8
1	H	222	HIS	2.7
1	G	174	PHE	2.7
1	H	220	ALA	2.7
1	F	174	PHE	2.6
1	C	174	PHE	2.6
1	E	174	PHE	2.5
1	H	251	ALA	2.5
1	G	132	PRO	2.5
1	H	127	ASP	2.5
1	G	250	LEU	2.5
1	F	126	PRO	2.3
1	G	123	LYS	2.3
1	D	129	LYS	2.3
1	G	127	ASP	2.3
1	H	249	ARG	2.3
1	E	128	PHE	2.3
1	H	174	PHE	2.2
1	F	129	LYS	2.2
1	D	2	VAL	2.2
1	B	174	PHE	2.2
1	G	224	ALA	2.2
1	C	246	ARG	2.1
1	D	1	ILE	2.1
1	A	0	ALA	2.1
1	H	130	THR	2.1
1	B	116	ALA	2.0
1	E	165	LYS	2.0
1	F	116	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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	NGD	F	5573	45/45	0.59	0.33	5.33	64,99,123,125	0
2	G2Q	A	301	36/36	0.87	0.16	0.91	20,43,54,56	0
2	G2Q	G	301	36/36	0.90	0.16	0.89	60,69,78,81	0
2	G2Q	B	301	36/36	0.88	0.16	0.81	31,48,54,56	0
2	G2Q	C	301	36/36	0.87	0.17	0.70	27,50,61,62	0
2	G2Q	E	301	36/36	0.89	0.15	0.60	27,51,57,59	0
2	G2Q	H	301	36/36	0.91	0.16	0.59	58,72,78,81	0

## 6.5 Other polymers

There are no such residues in this entry.