Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 01:52 am GMT

PDB ID	:	5DED
Title	:	Crystal structure of the small alarmone synthethase 1 from Bacillus subtilis bound to its product pppGpp
Authors	:	Steinchen, W.; Schuhmacher, J.S.; Altegoer, F.; Bange, G.
Deposited on	:	2015-08-25
Resolution	:	2.94 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

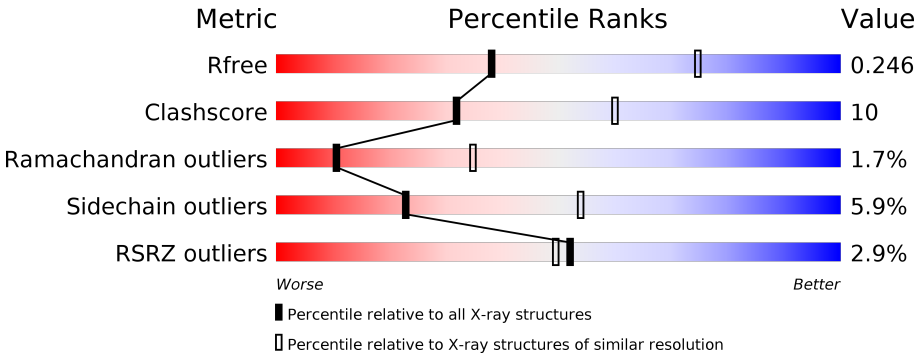
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2289 (2.98-2.90)
Clashscore	112137	2543 (2.98-2.90)
Ramachandran outliers	110173	2475 (2.98-2.90)
Sidechain outliers	110143	2477 (2.98-2.90)
RSRZ outliers	101464	2301 (2.98-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	218	5% 58% 28% • 10%
1	B	218	% 62% 23% • 12%
1	C	218	3% 63% 25% • 11%
1	D	218	2% 70% 15% • 14%
1	E	218	% 64% 21% • 13%
1	F	218	2% 66% 19% • • 12%

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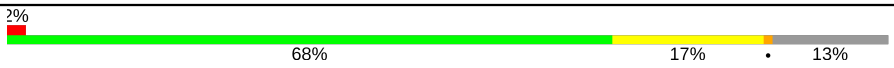
Mol	Chain	Length	Quality of chain
1	G	218	
1	H	218	

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	0O2	A	301	X	-	-	-
2	0O2	A	302	X	-	-	-
2	0O2	B	301	X	-	-	-
2	0O2	C	301	X	-	-	-
2	0O2	D	301	X	-	-	-
2	0O2	D	302	X	-	-	-
2	0O2	E	301	X	-	-	-
2	0O2	F	301	X	-	-	-
2	0O2	G	301	X	-	-	-
2	0O2	G	302	X	-	-	X
2	0O2	H	301	X	-	-	-
2	0O2	H	302	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13016 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 GTP pyrophosphokinase YjbM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	188	Total	C	N	O	S	0	0	0
			1544	984	269	285	6			
1	A	196	Total	C	N	O	S	0	0	0
			1608	1023	280	299	6			
1	B	191	Total	C	N	O	S	0	0	0
			1559	991	274	288	6			
1	C	194	Total	C	N	O	S	0	0	0
			1591	1014	278	293	6			
1	E	190	Total	C	N	O	S	0	0	0
			1551	990	269	286	6			
1	F	192	Total	C	N	O	S	0	0	0
			1563	995	271	291	6			
1	G	190	Total	C	N	O	S	0	0	0
			1533	977	267	283	6			
1	H	194	Total	C	N	O	S	0	0	0
			1583	1010	277	290	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	initiating methionine	UNP O31611
D	-5	GLY	-	expression tag	UNP O31611
D	-4	HIS	-	expression tag	UNP O31611
D	-3	HIS	-	expression tag	UNP O31611
D	-2	HIS	-	expression tag	UNP O31611
D	-1	HIS	-	expression tag	UNP O31611
D	0	HIS	-	expression tag	UNP O31611
D	1	HIS	-	expression tag	UNP O31611
A	-6	MET	-	initiating methionine	UNP O31611
A	-5	GLY	-	expression tag	UNP O31611
A	-4	HIS	-	expression tag	UNP O31611
A	-3	HIS	-	expression tag	UNP O31611
A	-2	HIS	-	expression tag	UNP O31611

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP O31611
A	0	HIS	-	expression tag	UNP O31611
A	1	HIS	-	expression tag	UNP O31611
B	-6	MET	-	initiating methionine	UNP O31611
B	-5	GLY	-	expression tag	UNP O31611
B	-4	HIS	-	expression tag	UNP O31611
B	-3	HIS	-	expression tag	UNP O31611
B	-2	HIS	-	expression tag	UNP O31611
B	-1	HIS	-	expression tag	UNP O31611
B	0	HIS	-	expression tag	UNP O31611
B	1	HIS	-	expression tag	UNP O31611
C	-6	MET	-	initiating methionine	UNP O31611
C	-5	GLY	-	expression tag	UNP O31611
C	-4	HIS	-	expression tag	UNP O31611
C	-3	HIS	-	expression tag	UNP O31611
C	-2	HIS	-	expression tag	UNP O31611
C	-1	HIS	-	expression tag	UNP O31611
C	0	HIS	-	expression tag	UNP O31611
C	1	HIS	-	expression tag	UNP O31611
E	-6	MET	-	initiating methionine	UNP O31611
E	-5	GLY	-	expression tag	UNP O31611
E	-4	HIS	-	expression tag	UNP O31611
E	-3	HIS	-	expression tag	UNP O31611
E	-2	HIS	-	expression tag	UNP O31611
E	-1	HIS	-	expression tag	UNP O31611
E	0	HIS	-	expression tag	UNP O31611
E	1	HIS	-	expression tag	UNP O31611
F	-6	MET	-	initiating methionine	UNP O31611
F	-5	GLY	-	expression tag	UNP O31611
F	-4	HIS	-	expression tag	UNP O31611
F	-3	HIS	-	expression tag	UNP O31611
F	-2	HIS	-	expression tag	UNP O31611
F	-1	HIS	-	expression tag	UNP O31611
F	0	HIS	-	expression tag	UNP O31611
F	1	HIS	-	expression tag	UNP O31611
G	-6	MET	-	initiating methionine	UNP O31611
G	-5	GLY	-	expression tag	UNP O31611
G	-4	HIS	-	expression tag	UNP O31611
G	-3	HIS	-	expression tag	UNP O31611
G	-2	HIS	-	expression tag	UNP O31611
G	-1	HIS	-	expression tag	UNP O31611
G	0	HIS	-	expression tag	UNP O31611

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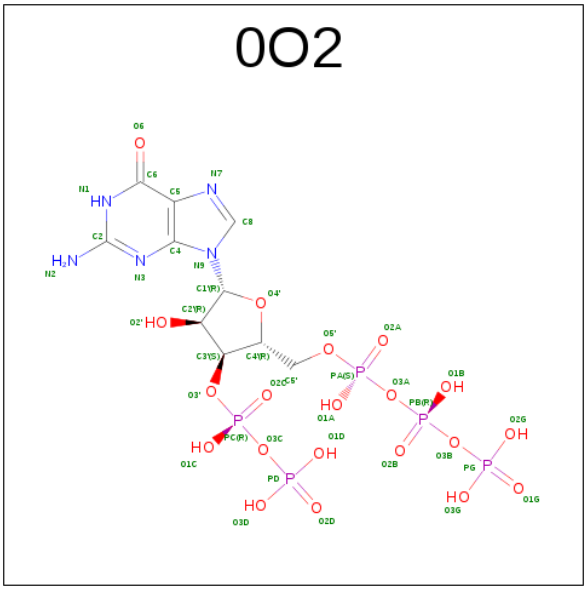
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	HIS	-	expression tag	UNP O31611
H	-6	MET	-	initiating methionine	UNP O31611
H	-5	GLY	-	expression tag	UNP O31611
H	-4	HIS	-	expression tag	UNP O31611
H	-3	HIS	-	expression tag	UNP O31611
H	-2	HIS	-	expression tag	UNP O31611
H	-1	HIS	-	expression tag	UNP O31611
H	0	HIS	-	expression tag	UNP O31611
H	1	HIS	-	expression tag	UNP O31611

- Molecule 2 is guanosine 5'-(tetrahydrogen triphosphate) 3'-(trihydrogen diphosphate) (three-letter code: 0O2) (formula: $C_{10}H_{18}N_5O_{20}P_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			40	10	5	20	5		
2	D	1	Total	C	N	O	P	0	0
			40	10	5	20	5		
2	A	1	Total	C	N	O	P	0	0
			40	10	5	20	5		
2	A	1	Total	C	N	O	P	0	0
			40	10	5	20	5		
2	B	1	Total	C	N	O	P	0	0
			40	10	5	20	5		
2	C	1	Total	C	N	O	P	0	0
			40	10	5	20	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			40	10	5	20	5		
2	F	1	Total	C	N	O	P	0	0
			40	10	5	20	5		
2	G	1	Total	C	N	O	P	0	0
			40	10	5	20	5		
2	G	1	Total	C	N	O	P	0	0
			40	10	5	20	5		
2	H	1	Total	C	N	O	P	0	0
			40	10	5	20	5		
2	H	1	Total	C	N	O	P	0	0
			40	10	5	20	5		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

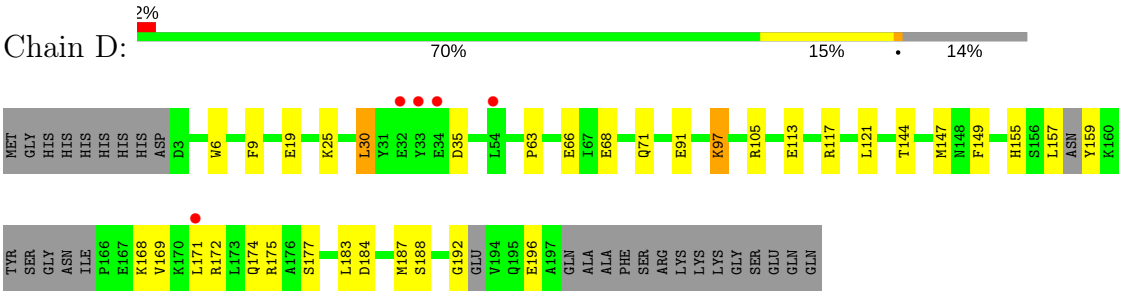
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

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

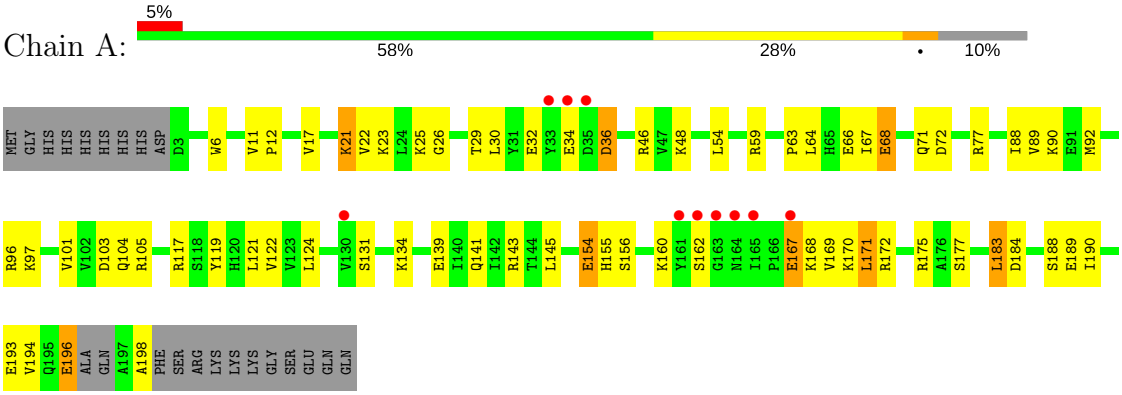
• Molecule 1: GTP pyrophosphokinase YjbM

Chain D:



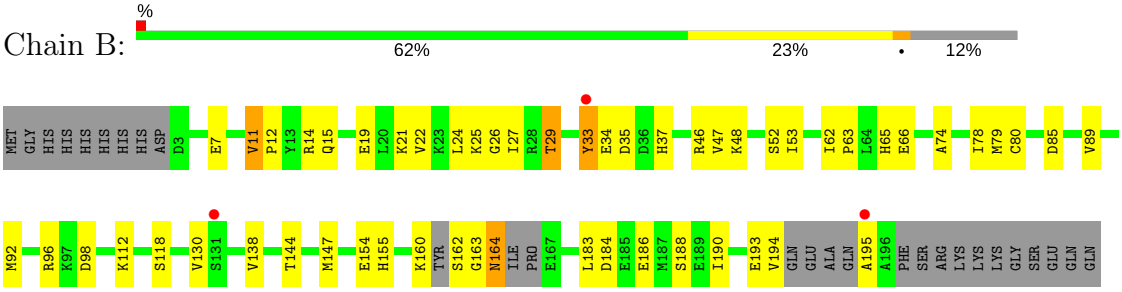
• Molecule 1: GTP pyrophosphokinase YjbM

Chain A:



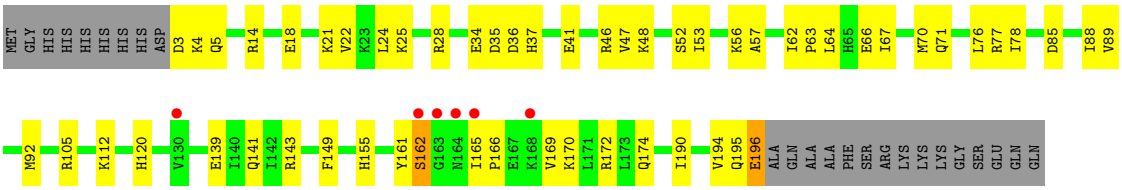
• Molecule 1: GTP pyrophosphokinase YjbM

Chain B:



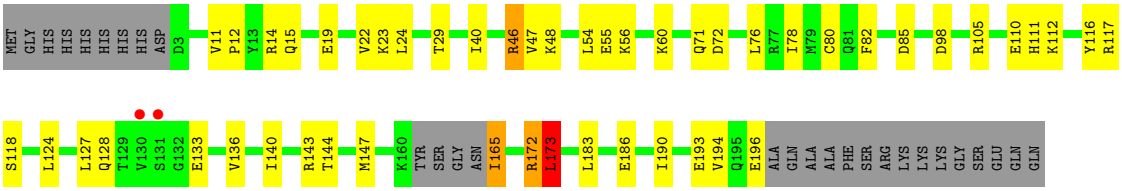
• Molecule 1: GTP pyrophosphokinase YjbM

Chain C:



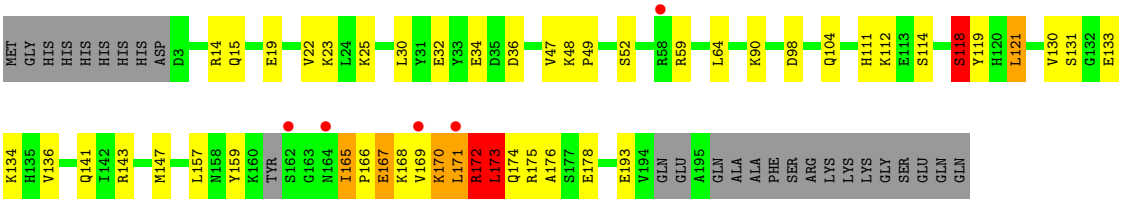
• Molecule 1: GTP pyrophosphokinase YjbM

Chain E:



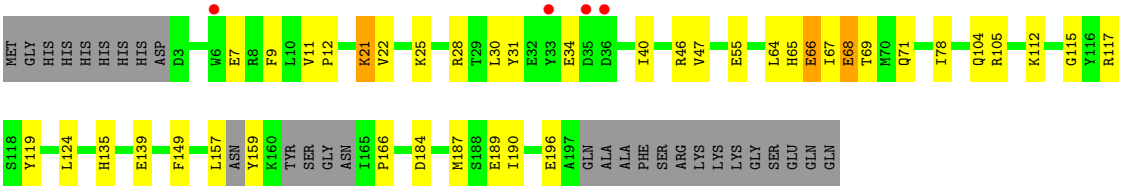
• Molecule 1: GTP pyrophosphokinase YjbM

Chain F:



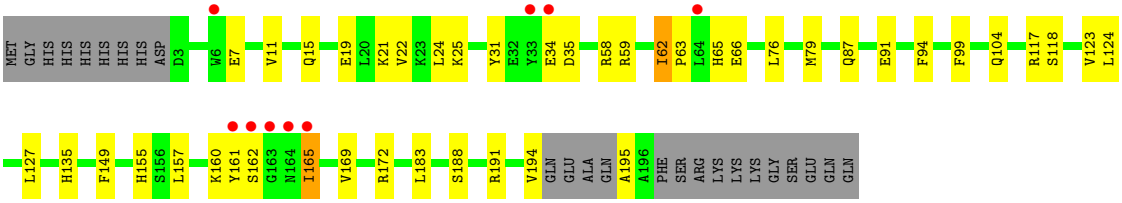
• Molecule 1: GTP pyrophosphokinase YjbM

Chain G:



• Molecule 1: GTP pyrophosphokinase YjbM

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	197.87Å 113.49Å 139.85Å 90.00° 127.17° 90.00°	Depositor
Resolution (Å)	50.57 – 2.94 50.57 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.57-2.94) 98.2 (50.57-2.94)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.85 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.180 , 0.245 0.178 , 0.246	Depositor DCC
R_{free} test set	2634 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13016	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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 50.93 % 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 6.0332e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, 0O2

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	0.47	0/1637	0.59	0/2206
1	B	0.48	0/1585	0.59	0/2133
1	C	0.48	0/1621	0.60	0/2186
1	D	0.45	0/1571	0.58	0/2115
1	E	0.46	0/1579	0.60	1/2130 (0.0%)
1	F	0.47	0/1591	0.68	2/2146 (0.1%)
1	G	0.45	0/1559	0.61	1/2102 (0.0%)
1	H	0.43	0/1611	0.61	0/2170
All	All	0.46	0/12754	0.61	4/17188 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	121	LEU	CA-CB-CG	5.78	128.59	115.30
1	E	173	LEU	N-CA-C	-5.77	95.43	111.00
1	G	166	PRO	N-CA-CB	5.56	109.97	103.30
1	F	173	LEU	CA-CB-CG	5.40	127.73	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	171	LEU	Peptide

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	1608	0	1612	47	0
1	B	1559	0	1566	34	0
1	C	1591	0	1597	41	0
1	D	1544	0	1550	22	0
1	E	1551	0	1551	33	0
1	F	1563	0	1562	62	0
1	G	1533	0	1512	21	0
1	H	1583	0	1591	26	0
2	A	80	0	25	5	0
2	B	40	0	13	4	0
2	C	40	0	13	4	0
2	D	80	0	24	5	0
2	E	40	0	13	1	0
2	F	40	0	13	4	0
2	G	80	0	24	4	0
2	H	80	0	25	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	13016	0	12691	260	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:GLU:HA	1:F:170:LYS:HB2	1.34	1.08
1:F:172:ARG:HH11	1:F:173:LEU:H	1.12	0.95
2:G:302:0O2:O1D	2:G:302:0O2:O2G	1.88	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:VAL:HG21	1:H:22:VAL:HG21	1.53	0.88
1:F:172:ARG:HG3	1:F:174:GLN:HB2	1.55	0.86
1:F:170:LYS:HA	1:F:170:LYS:NZ	1.91	0.86
1:F:172:ARG:NH1	1:F:173:LEU:H	1.74	0.85
1:E:193:GLU:OE2	1:H:172:ARG:NH1	2.11	0.83
1:A:97:LYS:H	1:E:128:GLN:HE21	1.28	0.81
1:D:157:LEU:O	1:D:159:TYR:N	2.14	0.81
1:C:46:ARG:HH21	1:C:77:ARG:HH22	1.26	0.81
1:F:172:ARG:HE	1:F:174:GLN:CD	1.86	0.79
1:F:170:LYS:HZ3	1:F:172:ARG:NH1	1.82	0.78
1:F:170:LYS:HA	1:F:170:LYS:HZ2	1.49	0.78
2:A:302:0O2:O2B	1:C:25:LYS:NZ	2.19	0.76
1:E:71:GLN:OE1	1:E:105:ARG:NH2	2.22	0.73
1:A:59:ARG:NH2	2:A:301:0O2:O3G	2.21	0.72
1:E:14:ARG:HG2	1:E:47:VAL:HG21	1.72	0.72
1:F:14:ARG:HG2	1:F:47:VAL:HG21	1.72	0.71
1:C:190:ILE:O	1:C:194:VAL:HG23	1.91	0.70
1:F:23:LYS:NZ	1:F:98:ASP:OD2	2.24	0.70
1:F:141:GLN:NE2	2:F:301:0O2:H7	2.06	0.70
1:F:170:LYS:HZ3	1:F:172:ARG:CZ	2.05	0.70
1:A:194:VAL:HG22	1:C:165:ILE:HG21	1.74	0.69
1:A:97:LYS:H	1:E:128:GLN:NE2	1.91	0.69
1:F:90:LYS:HD2	1:F:119:TYR:CZ	2.27	0.69
1:A:71:GLN:OE1	1:A:105:ARG:NH2	2.16	0.68
1:A:193:GLU:OE1	1:C:172:ARG:NH1	2.27	0.67
1:C:46:ARG:NH2	1:C:77:ARG:HH22	1.90	0.67
1:A:90:LYS:HD2	1:A:119:TYR:CZ	2.29	0.67
1:C:46:ARG:NH1	2:C:301:0O2:O1D	2.28	0.66
1:B:194:VAL:O	1:B:195:ALA:N	2.29	0.66
1:B:63:PRO:HG2	1:B:66:GLU:HB2	1.76	0.66
1:B:130:VAL:HG13	1:G:30:LEU:HD13	1.77	0.66
1:C:46:ARG:HH21	1:C:77:ARG:NH2	1.93	0.66
1:F:141:GLN:HE21	2:F:301:0O2:H7	1.60	0.66
1:F:172:ARG:HH21	1:F:174:GLN:HG3	1.62	0.65
1:B:33:TYR:O	1:B:35:ASP:N	2.29	0.65
1:D:113:GLU:O	1:D:174:GLN:NE2	2.31	0.64
1:E:24:LEU:HD12	1:E:76:LEU:HD22	1.80	0.64
1:B:22:VAL:HG21	1:G:22:VAL:HG21	1.80	0.63
1:A:34:GLU:HB2	1:A:36:ASP:HB2	1.80	0.63
2:D:302:0O2:H8	2:D:302:0O2:O1B	1.97	0.63
1:A:167:GLU:HA	1:A:170:LYS:HE2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:VAL:HA	1:A:92:MET:HE2	1.80	0.62
1:C:37:HIS:NE2	1:C:85:ASP:OD2	2.30	0.62
1:F:112:LYS:NZ	2:F:301:0O2:O2B	2.33	0.62
1:F:171:LEU:O	1:F:175:ARG:NH1	2.32	0.61
1:C:48:LYS:HG3	1:C:52:SER:HB2	1.82	0.61
1:A:196:GLU:C	1:A:198:ALA:H	2.03	0.61
1:F:170:LYS:CA	1:F:170:LYS:NZ	2.64	0.60
1:H:63:PRO:HG2	1:H:66:GLU:HB2	1.83	0.60
1:A:101:VAL:HG22	1:A:121:LEU:HD11	1.83	0.60
1:F:171:LEU:O	1:F:172:ARG:HB2	2.02	0.59
1:G:157:LEU:O	1:G:159:TYR:N	2.35	0.59
1:F:170:LYS:HA	1:F:170:LYS:HZ1	1.67	0.59
1:B:89:VAL:HA	1:B:92:MET:HE2	1.86	0.58
1:A:29:THR:HA	1:A:32:GLU:HG2	1.86	0.58
1:H:31:TYR:HA	1:H:34:GLU:OE1	2.04	0.58
1:C:64:LEU:H	1:C:64:LEU:HD12	1.67	0.58
1:H:59:ARG:NH2	2:H:301:0O2:O3G	2.37	0.58
1:F:169:VAL:HG23	1:G:190:ILE:HG23	1.86	0.57
1:D:71:GLN:OE1	1:D:105:ARG:NH2	2.26	0.57
1:C:28:ARG:NH1	1:C:41:GLU:O	2.34	0.57
1:F:173:LEU:HG	1:G:190:ILE:HD13	1.86	0.57
1:F:172:ARG:CG	1:F:174:GLN:HB2	2.32	0.57
1:B:14:ARG:HG2	1:B:47:VAL:HG21	1.87	0.57
1:C:71:GLN:OE1	1:C:105:ARG:NH2	2.20	0.57
1:F:170:LYS:NZ	1:F:172:ARG:NH1	2.52	0.57
1:F:59:ARG:NH2	2:F:301:0O2:O3G	2.37	0.57
1:A:22:VAL:HG21	1:E:22:VAL:HG21	1.88	0.56
1:H:24:LEU:HD12	1:H:76:LEU:HD22	1.87	0.56
1:F:172:ARG:NH1	1:F:173:LEU:N	2.51	0.55
1:A:77:ARG:NH1	1:A:141:GLN:OE1	2.36	0.55
1:C:48:LYS:HG2	1:C:53:ILE:HG12	1.87	0.55
1:D:155:HIS:NE2	2:D:301:0O2:O3D	2.35	0.55
1:C:3:ASP:O	1:C:5:GLN:N	2.40	0.54
1:A:167:GLU:OE1	1:A:167:GLU:N	2.41	0.54
1:G:21:LYS:O	1:G:25:LYS:HG3	2.08	0.54
1:A:6:TRP:CZ2	1:A:54:LEU:HD21	2.43	0.54
1:F:170:LYS:HZ3	1:F:172:ARG:CD	2.21	0.54
1:C:24:LEU:HD13	1:C:78:ILE:HD11	1.90	0.53
1:F:170:LYS:CA	1:F:170:LYS:HZ1	2.20	0.53
1:A:154:GLU:HG3	1:A:155:HIS:N	2.23	0.53
1:D:68:GLU:N	1:D:68:GLU:OE1	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ARG:HH21	2:B:301:0O2:PD	2.31	0.53
1:C:21:LYS:O	1:C:25:LYS:HG3	2.08	0.53
1:A:189:GLU:HB3	1:C:172:ARG:HH22	1.72	0.53
1:A:63:PRO:O	1:A:66:GLU:N	2.37	0.53
1:A:117:ARG:NH1	1:A:177:SER:OG	2.41	0.52
1:F:167:GLU:CA	1:F:170:LYS:HB2	2.24	0.52
1:C:194:VAL:O	1:C:196:GLU:N	2.43	0.52
1:D:183:LEU:O	1:D:187:MET:HG2	2.10	0.52
1:H:15:GLN:O	1:H:19:GLU:HG3	2.10	0.52
1:F:170:LYS:HZ3	1:F:172:ARG:HH11	1.58	0.51
1:B:164:ASN:OD1	1:B:164:ASN:N	2.43	0.51
1:A:122:VAL:HG22	1:A:139:GLU:HG3	1.92	0.51
1:G:71:GLN:OE1	1:G:105:ARG:NH2	2.43	0.51
1:B:21:LYS:O	1:B:25:LYS:HG3	2.10	0.51
1:D:168:LYS:O	1:D:172:ARG:HG3	2.11	0.51
1:D:117:ARG:NH1	1:D:177:SER:OG	2.44	0.51
1:E:183:LEU:HD13	1:H:149:PHE:HE2	1.74	0.51
1:C:161:TYR:O	1:C:162:SER:HB2	2.11	0.50
1:A:90:LYS:HD2	1:A:119:TYR:CE1	2.46	0.50
1:G:104:GLN:OE1	1:G:119:TYR:OH	2.28	0.50
1:G:139:GLU:OE1	2:G:301:0O2:H7	2.10	0.50
1:F:104:GLN:OE1	1:F:119:TYR:OH	2.28	0.50
1:F:174:GLN:O	1:F:178:GLU:HG2	2.12	0.50
1:B:190:ILE:O	1:B:194:VAL:HG23	2.11	0.50
1:B:155:HIS:HB2	2:B:301:0O2:N2	2.27	0.50
1:B:7:GLU:O	1:B:11:VAL:HG12	2.12	0.50
1:F:172:ARG:NE	1:F:174:GLN:H	2.09	0.49
1:B:155:HIS:HB2	2:B:301:0O2:H16	1.77	0.49
1:F:172:ARG:HB3	1:F:175:ARG:HB2	1.93	0.49
1:A:6:TRP:HZ2	1:A:54:LEU:HD21	1.77	0.49
1:E:15:GLN:HG3	1:E:127:LEU:HD11	1.93	0.49
1:F:172:ARG:CZ	1:F:174:GLN:N	2.76	0.49
1:B:15:GLN:O	1:B:19:GLU:HG3	2.12	0.49
1:A:26:GLY:O	1:A:29:THR:HG22	2.13	0.48
1:C:14:ARG:HG2	1:C:47:VAL:HG21	1.94	0.48
1:E:56:LYS:O	1:E:60:LYS:HG2	2.13	0.48
1:F:118:SER:OG	1:F:143:ARG:HG2	2.14	0.48
1:F:114:SER:O	1:F:172:ARG:NH2	2.46	0.48
1:F:172:ARG:HG3	1:F:175:ARG:H	1.78	0.48
1:H:34:GLU:OE1	1:H:34:GLU:N	2.43	0.48
1:E:118:SER:HA	1:E:147:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ARG:HB3	1:B:98:ASP:OD1	2.13	0.48
1:F:25:LYS:NZ	2:G:302:0O2:O2D	2.38	0.47
1:E:111:HIS:ND1	1:E:112:LYS:O	2.40	0.47
1:H:87:GLN:NE2	1:H:91:GLU:OE2	2.46	0.47
1:H:124:LEU:HG	1:H:135:HIS:HB3	1.96	0.47
1:A:77:ARG:HD2	1:A:143:ARG:CZ	2.45	0.47
1:F:169:VAL:CG2	1:G:190:ILE:HG23	2.44	0.47
1:B:27:ILE:HG21	1:B:92:MET:HE1	1.96	0.47
1:H:155:HIS:NE2	2:H:301:0O2:O3D	2.44	0.47
1:A:96:ARG:HG2	1:E:128:GLN:HG2	1.97	0.47
1:C:34:GLU:O	1:C:36:ASP:N	2.43	0.47
1:D:172:ARG:NH1	1:B:193:GLU:OE1	2.48	0.47
1:E:190:ILE:O	1:E:194:VAL:HG23	2.14	0.47
1:A:169:VAL:HG13	1:C:190:ILE:HG23	1.97	0.47
1:E:23:LYS:HD3	1:E:98:ASP:OD2	2.15	0.47
1:F:172:ARG:CZ	1:F:174:GLN:H	2.28	0.47
1:E:196:GLU:N	1:E:196:GLU:OE1	2.48	0.47
1:A:25:LYS:NZ	2:A:302:0O2:O2C	2.46	0.47
1:C:139:GLU:OE1	2:C:301:0O2:H7	2.15	0.47
1:C:63:PRO:HB2	1:C:66:GLU:HG2	1.97	0.47
1:G:196:GLU:N	1:G:196:GLU:OE1	2.48	0.47
1:D:30:LEU:HD23	1:F:130:VAL:HG23	1.96	0.46
1:A:12:PRO:HG3	1:A:134:LYS:HE2	1.98	0.46
1:C:112:LYS:NZ	2:C:301:0O2:O2B	2.32	0.46
1:A:190:ILE:O	1:A:194:VAL:HG23	2.15	0.46
1:A:155:HIS:HB2	2:A:301:0O2:N2	2.30	0.46
1:G:64:LEU:O	1:G:66:GLU:N	2.48	0.46
1:H:87:GLN:O	1:H:91:GLU:HG2	2.15	0.46
1:B:160:LYS:HG3	1:B:160:LYS:O	2.16	0.46
1:D:183:LEU:HD12	1:B:183:LEU:HD12	1.98	0.46
1:B:186:GLU:O	1:B:190:ILE:HG13	2.16	0.46
1:B:24:LEU:HD13	1:B:78:ILE:HD11	1.96	0.46
1:E:183:LEU:HD23	1:E:183:LEU:HA	1.76	0.46
1:G:31:TYR:HA	1:G:34:GLU:CB	2.46	0.46
1:A:171:LEU:HD13	1:A:175:ARG:NH1	2.31	0.46
1:D:155:HIS:HB2	2:D:301:0O2:H16	1.81	0.46
1:G:31:TYR:HA	1:G:34:GLU:HB3	1.97	0.46
1:A:168:LYS:O	1:A:172:ARG:HG3	2.15	0.46
1:G:67:ILE:C	1:G:69:THR:H	2.18	0.46
1:D:97:LYS:HE3	1:F:133:GLU:CD	2.36	0.45
1:H:117:ARG:O	1:H:118:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:302:0O2:PD	2:G:302:0O2:O2G	2.75	0.45
1:A:190:ILE:HG23	1:C:169:VAL:HG13	1.99	0.45
1:D:144:THR:OG1	1:D:147:MET:HG3	2.16	0.45
1:E:116:TYR:HB2	2:E:301:0O2:C6	2.47	0.45
1:A:59:ARG:NH2	2:A:301:0O2:H4	2.13	0.45
1:B:74:ALA:HB3	1:B:138:VAL:HG22	1.99	0.45
1:D:169:VAL:HG12	1:B:193:GLU:OE2	2.16	0.45
1:E:194:VAL:HG22	1:H:169:VAL:HG11	1.99	0.44
1:F:118:SER:HA	1:F:147:MET:HE1	1.99	0.44
1:F:170:LYS:NZ	1:F:170:LYS:CB	2.81	0.44
1:F:168:LYS:C	1:F:170:LYS:N	2.71	0.44
1:G:124:LEU:HG	1:G:135:HIS:HB3	2.00	0.44
1:D:63:PRO:HB2	1:D:66:GLU:HG2	1.99	0.44
1:F:15:GLN:NE2	1:F:19:GLU:OE2	2.33	0.44
1:C:88:ILE:O	1:C:92:MET:HG3	2.17	0.44
1:E:48:LYS:NZ	1:E:72:ASP:OD2	2.48	0.44
1:E:40:ILE:HG23	1:E:78:ILE:HG23	1.98	0.44
1:F:170:LYS:HZ3	1:F:172:ARG:NE	2.16	0.44
1:F:49:PRO:HD2	1:F:52:SER:HB2	2.00	0.44
1:H:194:VAL:O	1:H:195:ALA:N	2.51	0.44
1:F:111:HIS:ND1	1:F:112:LYS:O	2.36	0.43
1:A:171:LEU:HD13	1:A:175:ARG:HH12	1.83	0.43
1:D:25:LYS:NZ	2:D:302:0O2:O1C	2.45	0.43
1:F:90:LYS:HD2	1:F:119:TYR:CE1	2.53	0.43
1:E:46:ARG:HG2	1:E:46:ARG:O	2.16	0.43
1:E:82:PHE:O	1:E:85:ASP:HB2	2.19	0.43
1:C:170:LYS:O	1:C:174:GLN:HG3	2.19	0.43
1:F:173:LEU:O	1:F:176:ALA:HB3	2.18	0.43
1:F:34:GLU:OE1	1:F:36:ASP:HB2	2.19	0.43
1:A:124:LEU:HD12	1:A:124:LEU:HA	1.70	0.43
1:B:80:CYS:O	1:B:144:THR:HA	2.18	0.43
1:E:124:LEU:HA	1:E:124:LEU:HD12	1.87	0.43
1:E:15:GLN:NE2	1:E:19:GLU:OE2	2.30	0.43
1:G:7:GLU:O	1:G:11:VAL:HG23	2.19	0.43
1:B:80:CYS:HB3	1:B:85:ASP:HB2	2.01	0.43
1:A:189:GLU:HB3	1:C:172:ARG:NH2	2.33	0.43
1:B:11:VAL:N	1:B:12:PRO:HD2	2.34	0.43
1:C:18:GLU:O	1:C:22:VAL:HG23	2.18	0.43
1:H:15:GLN:HG3	1:H:127:LEU:HD11	2.01	0.43
1:C:120:HIS:CD2	1:C:141:GLN:HG2	2.54	0.42
1:F:172:ARG:NH2	1:F:174:GLN:HG3	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:GLU:OE2	1:H:172:ARG:NH2	2.49	0.42
1:F:170:LYS:HZ3	1:F:172:ARG:HD2	1.84	0.42
1:H:160:LYS:HE3	1:H:161:TYR:OH	2.19	0.42
1:G:40:ILE:HG23	1:G:78:ILE:HG23	2.01	0.42
1:H:62:ILE:HA	1:H:63:PRO:HD2	1.86	0.42
1:B:112:LYS:NZ	2:B:301:0O2:O2B	2.47	0.42
1:D:6:TRP:O	1:D:9:PHE:HB3	2.19	0.42
1:C:77:ARG:HD2	1:C:143:ARG:CZ	2.50	0.42
1:F:172:ARG:HA	1:F:172:ARG:HD2	1.20	0.42
1:C:57:ALA:HB1	1:C:62:ILE:HB	2.02	0.42
1:C:56:LYS:HD3	1:C:70:MET:SD	2.60	0.42
1:B:48:LYS:HG2	1:B:53:ILE:HG12	2.02	0.42
1:C:77:ARG:NH1	1:C:141:GLN:OE1	2.46	0.42
1:D:155:HIS:HB2	2:D:301:0O2:N2	2.35	0.42
1:F:157:LEU:C	1:F:159:TYR:H	2.24	0.42
1:F:168:LYS:C	1:F:171:LEU:H	2.23	0.42
1:H:157:LEU:HD23	1:H:157:LEU:HA	1.93	0.42
1:H:99:PHE:CE1	1:H:123:VAL:HG11	2.55	0.41
1:A:103:ASP:OD1	1:A:104:GLN:N	2.48	0.41
1:B:98:ASP:OD1	1:B:98:ASP:N	2.51	0.41
1:E:80:CYS:O	1:E:144:THR:HA	2.20	0.41
1:A:90:LYS:HD2	1:A:119:TYR:CE2	2.55	0.41
1:D:19:GLU:HG2	1:F:22:VAL:HG12	2.02	0.41
1:H:21:LYS:O	1:H:25:LYS:HG3	2.19	0.41
1:E:172:ARG:HG3	1:E:172:ARG:H	1.53	0.41
1:A:68:GLU:CD	1:A:68:GLU:H	2.23	0.41
1:C:155:HIS:HB2	2:C:301:0O2:H16	1.86	0.41
1:A:11:VAL:N	1:A:12:PRO:HD2	2.36	0.41
1:A:17:VAL:O	1:A:21:LYS:HB2	2.21	0.41
1:H:165:ILE:HG12	1:H:165:ILE:H	1.55	0.41
1:A:48:LYS:NZ	1:A:72:ASP:OD2	2.43	0.41
1:G:9:PHE:O	1:G:12:PRO:HD2	2.21	0.41
1:H:94:PHE:HZ	1:H:104:GLN:OE1	2.04	0.41
1:D:172:ARG:HH21	1:B:186:GLU:CD	2.24	0.41
1:F:172:ARG:HE	1:F:174:GLN:CG	2.33	0.41
1:G:64:LEU:C	1:G:66:GLU:H	2.24	0.41
1:A:183:LEU:HG	1:C:149:PHE:CE2	2.56	0.41
1:E:143:ARG:CB	1:E:147:MET:HE2	2.51	0.41
1:H:7:GLU:O	1:H:11:VAL:HG23	2.21	0.41
1:D:171:LEU:O	1:D:175:ARG:HG2	2.21	0.40
1:F:165:ILE:HG12	1:F:166:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:GLY:O	1:G:117:ARG:HG3	2.21	0.40
1:B:26:GLY:O	1:B:29:THR:HG22	2.21	0.40
1:C:89:VAL:HA	1:C:92:MET:HE2	2.03	0.40
1:E:117:ARG:O	1:E:118:SER:OG	2.36	0.40
1:E:165:ILE:HG13	1:E:165:ILE:O	2.21	0.40
1:A:183:LEU:HG	1:C:149:PHE:HE2	1.86	0.40
1:E:11:VAL:HB	1:E:12:PRO:HD3	2.03	0.40
1:F:48:LYS:HA	1:F:49:PRO:HD3	1.96	0.40
1:B:144:THR:OG1	1:B:147:MET:HG3	2.21	0.40
1:B:63:PRO:HB2	1:B:65:HIS:CD2	2.56	0.40
1:E:54:LEU:HA	1:E:54:LEU:HD23	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	192/218 (88%)	181 (94%)	9 (5%)	2 (1%)	18 50
1	B	185/218 (85%)	169 (91%)	11 (6%)	5 (3%)	6 22
1	C	192/218 (88%)	181 (94%)	7 (4%)	4 (2%)	8 29
1	D	182/218 (84%)	169 (93%)	10 (6%)	3 (2%)	11 36
1	E	186/218 (85%)	171 (92%)	14 (8%)	1 (0%)	32 67
1	F	189/218 (87%)	172 (91%)	12 (6%)	5 (3%)	6 23
1	G	184/218 (84%)	171 (93%)	10 (5%)	3 (2%)	11 36
1	H	190/218 (87%)	180 (95%)	8 (4%)	2 (1%)	17 47
All	All	1500/1744 (86%)	1394 (93%)	81 (5%)	25 (2%)	11 35

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	196	GLU
1	B	34	GLU
1	C	4	LYS
1	C	162	SER
1	E	173	LEU
1	H	162	SER
1	D	192	GLY
1	A	36	ASP
1	B	162	SER
1	F	172	ARG
1	A	162	SER
1	C	195	GLN
1	G	112	LYS
1	B	33	TYR
1	B	62	ILE
1	F	118	SER
1	G	68	GLU
1	H	35	ASP
1	F	30	LEU
1	F	134	LYS
1	G	65	HIS
1	D	35	ASP
1	F	193	GLU
1	B	163	GLY
1	C	166	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	174/195 (89%)	155 (89%)	19 (11%)	7 22
1	B	168/195 (86%)	158 (94%)	10 (6%)	22 53
1	C	172/195 (88%)	168 (98%)	4 (2%)	56 84
1	D	167/195 (86%)	160 (96%)	7 (4%)	34 68
1	E	167/195 (86%)	157 (94%)	10 (6%)	22 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	169/195 (87%)	158 (94%)	11 (6%)	20 49
1	G	161/195 (83%)	150 (93%)	11 (7%)	18 46
1	H	170/195 (87%)	162 (95%)	8 (5%)	30 64
All	All	1348/1560 (86%)	1268 (94%)	80 (6%)	23 54

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	30	LEU
1	D	91	GLU
1	D	97	LYS
1	D	121	LEU
1	D	149	PHE
1	D	184	ASP
1	D	188	SER
1	A	21	LYS
1	A	23	LYS
1	A	30	LEU
1	A	46	ARG
1	A	64	LEU
1	A	67	ILE
1	A	68	GLU
1	A	88	ILE
1	A	131	SER
1	A	145	LEU
1	A	154	GLU
1	A	156	SER
1	A	160	LYS
1	A	167	GLU
1	A	171	LEU
1	A	183	LEU
1	A	184	ASP
1	A	188	SER
1	A	196	GLU
1	B	11	VAL
1	B	29	THR
1	B	37	HIS
1	B	52	SER
1	B	79	MET
1	B	118	SER
1	B	154	GLU

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Mol	Chain	Res	Type
1	B	164	ASN
1	B	184	ASP
1	B	188	SER
1	C	35	ASP
1	C	67	ILE
1	C	76	LEU
1	C	196	GLU
1	E	29	THR
1	E	46	ARG
1	E	55	GLU
1	E	110	GLU
1	E	133	GLU
1	E	136	VAL
1	E	140	ILE
1	E	165	ILE
1	E	172	ARG
1	E	173	LEU
1	F	32	GLU
1	F	64	LEU
1	F	118	SER
1	F	121	LEU
1	F	131	SER
1	F	136	VAL
1	F	165	ILE
1	F	167	GLU
1	F	170	LYS
1	F	172	ARG
1	F	173	LEU
1	G	21	LYS
1	G	28	ARG
1	G	46	ARG
1	G	47	VAL
1	G	55	GLU
1	G	66	GLU
1	G	68	GLU
1	G	149	PHE
1	G	184	ASP
1	G	187	MET
1	G	189	GLU
1	H	58	ARG
1	H	62	ILE
1	H	65	HIS

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Mol	Chain	Res	Type
1	H	79	MET
1	H	165	ILE
1	H	183	LEU
1	H	188	SER
1	H	191	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	128	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
2	0O2	A	301	-	34,42,42	3.13	10 (29%)	36,68,68	2.51	12 (33%)
2	0O2	A	302	3	34,42,42	3.12	9 (26%)	36,68,68	2.68	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	0O2	B	301	-	34,42,42	3.14	9 (26%)	36,68,68	2.54	12 (33%)
2	0O2	C	301	-	34,42,42	3.07	9 (26%)	36,68,68	2.51	13 (36%)
2	0O2	D	301	-	34,42,42	2.93	9 (26%)	36,68,68	2.49	13 (36%)
2	0O2	D	302	3	34,42,42	3.18	10 (29%)	36,68,68	2.55	8 (22%)
2	0O2	E	301	-	34,42,42	3.00	9 (26%)	36,68,68	2.39	15 (41%)
2	0O2	F	301	-	34,42,42	2.93	8 (23%)	36,68,68	2.34	13 (36%)
2	0O2	G	301	-	34,42,42	3.12	9 (26%)	36,68,68	2.51	14 (38%)
2	0O2	G	302	3	34,42,42	2.62	9 (26%)	36,68,68	2.82	17 (47%)
2	0O2	H	301	-	34,42,42	3.12	10 (29%)	36,68,68	2.47	12 (33%)
2	0O2	H	302	3	34,42,42	2.91	11 (32%)	36,68,68	2.62	14 (38%)

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	0O2	A	301	-	4/4/9/9	0/29/49/49	0/3/3/3
2	0O2	A	302	3	4/4/9/9	1/29/49/49	0/3/3/3
2	0O2	B	301	-	3/3/9/9	0/29/49/49	0/3/3/3
2	0O2	C	301	-	4/4/9/9	0/29/49/49	0/3/3/3
2	0O2	D	301	-	4/4/9/9	0/29/49/49	0/3/3/3
2	0O2	D	302	3	4/4/9/9	1/29/49/49	0/3/3/3
2	0O2	E	301	-	4/4/9/9	0/29/49/49	0/3/3/3
2	0O2	F	301	-	4/4/9/9	0/29/49/49	0/3/3/3
2	0O2	G	301	-	4/4/9/9	0/29/49/49	0/3/3/3
2	0O2	G	302	3	4/4/9/9	0/29/49/49	0/3/3/3
2	0O2	H	301	-	4/4/9/9	0/29/49/49	0/3/3/3
2	0O2	H	302	3	4/4/9/9	0/29/49/49	0/3/3/3

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	0O2	C2'-C1'	-9.63	1.38	1.53
2	G	301	0O2	C2'-C1'	-9.56	1.38	1.53
2	A	301	0O2	C2'-C1'	-9.41	1.38	1.53
2	D	302	0O2	C2'-C1'	-9.32	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	0O2	C2'-C1'	-9.10	1.39	1.53
2	H	301	0O2	C2'-C1'	-9.07	1.39	1.53
2	B	301	0O2	C2'-C1'	-8.96	1.39	1.53
2	B	301	0O2	O4'-C1'	-8.85	1.29	1.41
2	A	302	0O2	C2'-C1'	-8.84	1.39	1.53
2	D	301	0O2	C2'-C1'	-8.76	1.39	1.53
2	A	302	0O2	O4'-C1'	-8.72	1.29	1.41
2	A	301	0O2	O4'-C1'	-8.45	1.29	1.41
2	G	301	0O2	O4'-C1'	-8.42	1.29	1.41
2	F	301	0O2	C2'-C1'	-8.35	1.40	1.53
2	C	301	0O2	O4'-C1'	-8.26	1.29	1.41
2	D	302	0O2	O4'-C1'	-8.21	1.29	1.41
2	H	301	0O2	O4'-C1'	-8.17	1.30	1.41
2	E	301	0O2	O4'-C1'	-7.84	1.30	1.41
2	D	301	0O2	O4'-C1'	-7.84	1.30	1.41
2	F	301	0O2	O4'-C1'	-7.70	1.30	1.41
2	H	302	0O2	O4'-C1'	-7.48	1.30	1.41
2	D	302	0O2	O4'-C4'	-7.26	1.28	1.45
2	H	302	0O2	O4'-C4'	-7.26	1.28	1.45
2	H	302	0O2	C2'-C1'	-7.19	1.42	1.53
2	A	302	0O2	O4'-C4'	-7.17	1.28	1.45
2	G	302	0O2	C2'-C1'	-7.06	1.42	1.53
2	B	301	0O2	O4'-C4'	-6.69	1.29	1.45
2	H	301	0O2	O4'-C4'	-6.66	1.29	1.45
2	E	301	0O2	O4'-C4'	-6.64	1.30	1.45
2	A	301	0O2	C2'-C3'	-6.50	1.38	1.53
2	A	301	0O2	O4'-C4'	-6.42	1.30	1.45
2	G	301	0O2	O4'-C4'	-6.40	1.30	1.45
2	C	301	0O2	O4'-C4'	-6.33	1.30	1.45
2	G	302	0O2	O4'-C4'	-6.26	1.30	1.45
2	F	301	0O2	O4'-C4'	-6.22	1.30	1.45
2	B	301	0O2	C2'-C3'	-6.11	1.39	1.53
2	D	301	0O2	O4'-C4'	-6.04	1.31	1.45
2	G	301	0O2	C2'-C3'	-6.01	1.39	1.53
2	H	301	0O2	C2'-C3'	-5.96	1.39	1.53
2	F	301	0O2	C2'-C3'	-5.65	1.40	1.53
2	G	302	0O2	O4'-C1'	-5.59	1.33	1.41
2	E	301	0O2	C2'-C3'	-5.58	1.40	1.53
2	C	301	0O2	C2'-C3'	-5.43	1.40	1.53
2	D	301	0O2	C2'-C3'	-5.32	1.41	1.53
2	A	302	0O2	C2'-C3'	-5.31	1.41	1.53
2	D	302	0O2	C2'-C3'	-5.23	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	0O2	C3'-C4'	-4.57	1.40	1.52
2	H	302	0O2	C3'-C4'	-4.53	1.40	1.52
2	H	301	0O2	C3'-C4'	-4.39	1.40	1.52
2	E	301	0O2	C3'-C4'	-4.30	1.40	1.52
2	B	301	0O2	C3'-C4'	-4.29	1.40	1.52
2	D	302	0O2	C3'-C4'	-4.02	1.41	1.52
2	C	301	0O2	C3'-C4'	-3.92	1.42	1.52
2	G	302	0O2	C3'-C4'	-3.89	1.42	1.52
2	A	301	0O2	C3'-C4'	-3.83	1.42	1.52
2	G	301	0O2	C3'-C4'	-3.82	1.42	1.52
2	A	302	0O2	C3'-C4'	-3.72	1.42	1.52
2	H	302	0O2	C2'-C3'	-3.64	1.44	1.53
2	D	301	0O2	C3'-C4'	-3.61	1.42	1.52
2	D	302	0O2	PG-O3B	-3.13	1.55	1.60
2	H	302	0O2	O2'-C2'	-2.95	1.36	1.43
2	D	301	0O2	PG-O3B	-2.84	1.55	1.60
2	G	301	0O2	O2'-C2'	-2.72	1.36	1.43
2	H	301	0O2	PG-O3B	-2.68	1.55	1.60
2	A	301	0O2	O2'-C2'	-2.63	1.36	1.43
2	A	301	0O2	PG-O3B	-2.58	1.55	1.60
2	B	301	0O2	PG-O3B	-2.53	1.56	1.60
2	G	302	0O2	C2'-C3'	-2.45	1.47	1.53
2	G	301	0O2	PG-O3B	-2.45	1.56	1.60
2	D	302	0O2	PC-O3'	-2.41	1.54	1.60
2	C	301	0O2	O2'-C2'	-2.41	1.37	1.43
2	D	302	0O2	O2'-C2'	-2.38	1.37	1.43
2	B	301	0O2	O2'-C2'	-2.36	1.37	1.43
2	H	301	0O2	O2'-C2'	-2.32	1.37	1.43
2	H	302	0O2	PC-O3'	-2.30	1.54	1.60
2	A	302	0O2	O2'-C2'	-2.30	1.37	1.43
2	D	301	0O2	O2'-C2'	-2.28	1.37	1.43
2	E	301	0O2	O2'-C2'	-2.28	1.37	1.43
2	A	302	0O2	PC-O3'	-2.26	1.55	1.60
2	H	302	0O2	PG-O3B	-2.22	1.56	1.60
2	H	302	0O2	PD-O3C	-2.20	1.56	1.60
2	G	302	0O2	O5'-C5'	-2.18	1.36	1.44
2	E	301	0O2	O3'-C3'	-2.17	1.35	1.44
2	F	301	0O2	PG-O3B	-2.11	1.56	1.60
2	C	301	0O2	PG-O3B	-2.08	1.56	1.60
2	A	301	0O2	O3'-C3'	-2.04	1.36	1.44
2	H	301	0O2	O3'-C3'	-2.01	1.36	1.44
2	G	302	0O2	C6-N1	2.34	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	0O2	C2-N2	4.18	1.42	1.34
2	A	301	0O2	C2-N2	4.19	1.42	1.34
2	D	301	0O2	C2-N2	4.29	1.42	1.34
2	F	301	0O2	C2-N2	4.36	1.43	1.34
2	C	301	0O2	C2-N2	4.37	1.43	1.34
2	E	301	0O2	C2-N2	4.44	1.43	1.34
2	B	301	0O2	C2-N2	4.47	1.43	1.34
2	H	301	0O2	C2-N2	4.47	1.43	1.34
2	D	302	0O2	C2-N2	4.53	1.43	1.34
2	A	302	0O2	C2-N2	4.62	1.43	1.34
2	A	301	0O2	O6-C6	4.78	1.36	1.24
2	E	301	0O2	O6-C6	4.80	1.36	1.24
2	H	302	0O2	C2-N2	4.95	1.44	1.34
2	B	301	0O2	O6-C6	5.10	1.37	1.24
2	G	301	0O2	O6-C6	5.12	1.37	1.24
2	F	301	0O2	O6-C6	5.13	1.37	1.24
2	H	301	0O2	O6-C6	5.17	1.37	1.24
2	D	301	0O2	O6-C6	5.17	1.37	1.24
2	G	302	0O2	C2-N2	5.26	1.44	1.34
2	C	301	0O2	O6-C6	5.28	1.37	1.24
2	H	302	0O2	O6-C6	5.47	1.38	1.24
2	A	302	0O2	O6-C6	5.47	1.38	1.24
2	D	302	0O2	O6-C6	5.72	1.38	1.24
2	G	302	0O2	O6-C6	6.33	1.40	1.24

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	302	0O2	N3-C2-N1	-4.48	120.92	127.46
2	D	302	0O2	C5-C6-N1	-3.96	117.84	123.48
2	G	302	0O2	C5-C6-N1	-3.57	118.40	123.48
2	H	302	0O2	N3-C2-N1	-3.41	122.48	127.46
2	G	302	0O2	C4-C5-N7	-3.39	106.13	109.41
2	D	302	0O2	N3-C2-N1	-3.33	122.59	127.46
2	G	302	0O2	C6-C5-C4	-3.32	117.54	120.84
2	H	302	0O2	C5-C6-N1	-3.18	118.95	123.48
2	H	301	0O2	C5-C6-N1	-3.18	118.95	123.48
2	C	301	0O2	C5-C6-N1	-3.17	118.97	123.48
2	B	301	0O2	C5-C6-N1	-3.13	119.02	123.48
2	A	302	0O2	C5-C6-N1	-3.08	119.10	123.48
2	F	301	0O2	N3-C2-N1	-3.03	123.03	127.46
2	G	301	0O2	C5-C6-N1	-3.02	119.18	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	0O2	N3-C2-N1	-3.02	123.04	127.46
2	F	301	0O2	C5-C6-N1	-3.00	119.22	123.48
2	H	301	0O2	N3-C2-N1	-3.00	123.08	127.46
2	C	301	0O2	N3-C2-N1	-2.99	123.09	127.46
2	B	301	0O2	N3-C2-N1	-2.94	123.17	127.46
2	E	301	0O2	C5-C6-N1	-2.92	119.32	123.48
2	A	302	0O2	N3-C2-N1	-2.87	123.27	127.46
2	A	301	0O2	N3-C2-N1	-2.86	123.28	127.46
2	D	301	0O2	N3-C2-N1	-2.84	123.32	127.46
2	D	301	0O2	C5-C6-N1	-2.63	119.74	123.48
2	A	302	0O2	O3C-PC-O3'	-2.60	97.41	102.05
2	G	301	0O2	N3-C2-N1	-2.52	123.78	127.46
2	A	302	0O2	C6-C5-C4	-2.42	118.44	120.84
2	F	301	0O2	C6-C5-C4	-2.40	118.46	120.84
2	D	302	0O2	C6-C5-C4	-2.25	118.61	120.84
2	A	301	0O2	C5-C6-N1	-2.05	120.57	123.48
2	E	301	0O2	C6-C5-C4	-2.05	118.81	120.84
2	B	301	0O2	O3'-C3'-C2'	2.03	119.14	111.63
2	E	301	0O2	C3'-C2'-C1'	2.03	104.51	99.95
2	E	301	0O2	O1C-PC-O3'	2.05	114.73	106.49
2	E	301	0O2	O4'-C4'-C3'	2.05	109.34	104.81
2	C	301	0O2	O3C-PC-O3'	2.08	105.76	102.05
2	A	301	0O2	O3'-PC-O2C	2.13	117.84	109.46
2	F	301	0O2	C3'-C2'-C1'	2.15	104.78	99.95
2	D	301	0O2	O3'-C3'-C2'	2.18	119.72	111.63
2	G	301	0O2	C2-N3-C4	2.21	117.74	115.16
2	C	301	0O2	O3'-C3'-C2'	2.22	119.85	111.63
2	E	301	0O2	C2-N3-C4	2.23	117.77	115.16
2	G	301	0O2	O4'-C4'-C3'	2.25	109.78	104.81
2	H	302	0O2	O4'-C4'-C3'	2.25	109.79	104.81
2	G	301	0O2	O4'-C4'-C5'	2.26	117.04	109.40
2	G	301	0O2	O3C-PC-O3'	2.28	106.12	102.05
2	A	302	0O2	C3'-C2'-C1'	2.29	105.09	99.95
2	B	301	0O2	O4'-C4'-C5'	2.30	117.16	109.40
2	H	301	0O2	O3'-C3'-C2'	2.30	120.14	111.63
2	H	301	0O2	C3'-C2'-C1'	2.34	105.19	99.95
2	G	301	0O2	C6-N1-C2	2.35	119.45	116.06
2	E	301	0O2	C1'-N9-C4	2.36	130.72	126.64
2	G	301	0O2	O3'-C3'-C2'	2.37	120.39	111.63
2	A	301	0O2	O4'-C4'-C5'	2.38	117.43	109.40
2	H	302	0O2	C4'-O4'-C1'	2.38	112.30	109.77
2	C	301	0O2	O4'-C4'-C5'	2.47	117.74	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	0O2	C3'-C2'-C1'	2.48	105.51	99.95
2	E	301	0O2	O3'-C3'-C2'	2.48	120.82	111.63
2	H	301	0O2	C2-N3-C4	2.49	118.06	115.16
2	F	301	0O2	C2-N3-C4	2.51	118.09	115.16
2	A	301	0O2	C3'-C2'-C1'	2.51	105.59	99.95
2	C	301	0O2	C3'-C2'-C1'	2.51	105.59	99.95
2	D	301	0O2	C6-N1-C2	2.53	119.70	116.06
2	G	302	0O2	N2-C2-N1	2.60	121.40	117.24
2	D	301	0O2	C2-N3-C4	2.63	118.23	115.16
2	F	301	0O2	O4'-C4'-C3'	2.63	110.62	104.81
2	D	301	0O2	O4'-C4'-C5'	2.65	118.36	109.40
2	B	301	0O2	C6-N1-C2	2.65	119.88	116.06
2	C	301	0O2	C2-N3-C4	2.65	118.26	115.16
2	H	301	0O2	O4'-C4'-C5'	2.67	118.41	109.40
2	D	301	0O2	C3'-C2'-C1'	2.71	106.04	99.95
2	A	302	0O2	C6-N1-C2	2.72	119.97	116.06
2	H	301	0O2	C6-N1-C2	2.73	119.98	116.06
2	F	301	0O2	C6-N1-C2	2.76	120.03	116.06
2	G	302	0O2	O1C-PC-O3'	2.79	117.69	106.49
2	D	301	0O2	O3C-PC-O3'	2.79	107.03	102.05
2	C	301	0O2	C6-N1-C2	2.81	120.10	116.06
2	E	301	0O2	O4'-C4'-C5'	2.81	118.91	109.40
2	A	301	0O2	O3C-PC-O3'	2.82	107.09	102.05
2	H	302	0O2	O3'-C3'-C4'	2.85	120.72	110.04
2	B	301	0O2	C2-N3-C4	2.90	118.54	115.16
2	G	302	0O2	C3'-C2'-C1'	2.98	106.64	99.95
2	F	301	0O2	O3'-C3'-C2'	3.00	122.73	111.63
2	H	302	0O2	C6-N1-C2	3.02	120.40	116.06
2	G	301	0O2	C3'-C2'-C1'	3.02	106.74	99.95
2	E	301	0O2	C6-N1-C2	3.08	120.49	116.06
2	A	301	0O2	C2-N3-C4	3.17	118.86	115.16
2	H	302	0O2	C2-N3-C4	3.25	118.95	115.16
2	G	302	0O2	O4'-C4'-C3'	3.40	112.31	104.81
2	H	302	0O2	O4'-C4'-C5'	3.45	121.05	109.40
2	G	302	0O2	C5'-C4'-C3'	3.54	126.29	114.30
2	G	302	0O2	O4'-C4'-C5'	3.55	121.38	109.40
2	G	302	0O2	O3C-PC-O3'	3.58	108.44	102.05
2	D	302	0O2	C6-N1-C2	3.74	121.44	116.06
2	F	301	0O2	O4'-C4'-C5'	3.77	122.12	109.40
2	F	301	0O2	C5'-C4'-C3'	3.82	127.25	114.30
2	A	301	0O2	C1'-N9-C4	3.84	133.28	126.64
2	G	302	0O2	C6-N1-C2	3.85	121.60	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	302	0O2	O3'-C3'-C4'	3.90	124.67	110.04
2	G	302	0O2	O2'-C2'-C1'	3.91	123.86	111.61
2	H	302	0O2	C1'-N9-C4	3.99	133.53	126.64
2	D	301	0O2	C1'-N9-C4	4.24	133.96	126.64
2	H	302	0O2	C5'-C4'-C3'	4.38	129.16	114.30
2	C	301	0O2	C1'-N9-C4	4.41	134.26	126.64
2	A	302	0O2	O2'-C2'-C3'	4.46	123.86	111.18
2	B	301	0O2	O2'-C2'-C3'	4.65	124.40	111.18
2	H	301	0O2	C1'-N9-C4	4.71	134.77	126.64
2	A	301	0O2	O2'-C2'-C3'	4.78	124.77	111.18
2	G	301	0O2	O2'-C2'-C1'	4.79	126.62	111.61
2	G	302	0O2	C2-N3-C4	4.86	120.83	115.16
2	H	302	0O2	O3C-PC-O3'	4.89	110.79	102.05
2	D	301	0O2	O2'-C2'-C3'	5.02	125.47	111.18
2	C	301	0O2	O2'-C2'-C1'	5.03	127.36	111.61
2	H	301	0O2	O2'-C2'-C3'	5.07	125.59	111.18
2	F	301	0O2	O2'-C2'-C3'	5.08	125.61	111.18
2	G	301	0O2	C1'-N9-C4	5.10	135.44	126.64
2	E	301	0O2	C5'-C4'-C3'	5.14	131.73	114.30
2	B	301	0O2	C1'-N9-C4	5.19	135.59	126.64
2	D	302	0O2	O2'-C2'-C3'	5.28	126.20	111.18
2	D	301	0O2	O2'-C2'-C1'	5.36	128.40	111.61
2	H	301	0O2	C5'-C4'-C3'	5.37	132.50	114.30
2	E	301	0O2	O2'-C2'-C3'	5.37	126.46	111.18
2	G	301	0O2	O2'-C2'-C3'	5.41	126.56	111.18
2	D	301	0O2	C5'-C4'-C3'	5.48	132.87	114.30
2	H	302	0O2	O2'-C2'-C1'	5.49	128.79	111.61
2	C	301	0O2	O2'-C2'-C3'	5.54	126.93	111.18
2	E	301	0O2	O2'-C2'-C1'	5.54	128.94	111.61
2	G	301	0O2	C5'-C4'-C3'	5.57	133.18	114.30
2	H	301	0O2	O2'-C2'-C1'	5.58	129.08	111.61
2	C	301	0O2	C5'-C4'-C3'	5.64	133.40	114.30
2	H	302	0O2	O2'-C2'-C3'	5.70	127.39	111.18
2	A	301	0O2	O2'-C2'-C1'	5.72	129.53	111.61
2	B	301	0O2	C5'-C4'-C3'	5.73	133.71	114.30
2	F	301	0O2	O2'-C2'-C1'	5.74	129.57	111.61
2	D	302	0O2	O2'-C2'-C1'	5.75	129.59	111.61
2	B	301	0O2	O2'-C2'-C1'	5.86	129.93	111.61
2	G	302	0O2	O3'-C3'-C2'	5.86	133.31	111.63
2	A	301	0O2	C5'-C4'-C3'	5.89	134.27	114.30
2	F	301	0O2	O3'-C3'-C4'	5.92	132.27	110.04
2	H	302	0O2	O3'-C3'-C2'	6.08	134.14	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	302	0O2	O2'-C2'-C1'	6.20	131.01	111.61
2	D	302	0O2	C5'-C4'-C3'	6.26	135.51	114.30
2	E	301	0O2	O3'-C3'-C4'	6.31	133.73	110.04
2	G	302	0O2	O2'-C2'-C3'	6.44	129.48	111.18
2	H	301	0O2	O3'-C3'-C4'	6.54	134.59	110.04
2	C	301	0O2	O3'-C3'-C4'	6.81	135.59	110.04
2	D	301	0O2	O3'-C3'-C4'	6.86	135.78	110.04
2	B	301	0O2	O3'-C3'-C4'	6.94	136.10	110.04
2	G	301	0O2	O3'-C3'-C4'	6.96	136.17	110.04
2	D	302	0O2	O3'-C3'-C4'	7.37	137.71	110.04
2	A	301	0O2	O3'-C3'-C4'	7.52	138.25	110.04
2	A	302	0O2	C5'-C4'-C3'	7.61	140.10	114.30
2	A	302	0O2	O3'-C3'-C4'	8.66	142.54	110.04

All (47) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	301	0O2	C2'
2	H	301	0O2	C4'
2	H	301	0O2	C1'
2	H	301	0O2	C3'
2	G	302	0O2	C2'
2	G	302	0O2	C4'
2	G	302	0O2	C1'
2	G	302	0O2	C3'
2	B	301	0O2	C2'
2	B	301	0O2	C4'
2	B	301	0O2	C3'
2	H	302	0O2	C2'
2	H	302	0O2	C4'
2	H	302	0O2	C1'
2	H	302	0O2	C3'
2	D	302	0O2	C2'
2	D	302	0O2	C4'
2	D	302	0O2	C1'
2	D	302	0O2	C3'
2	F	301	0O2	C2'
2	F	301	0O2	C4'
2	F	301	0O2	C1'
2	F	301	0O2	C3'
2	A	301	0O2	C2'
2	A	301	0O2	C4'

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Mol	Chain	Res	Type	Atom
2	A	301	0O2	C1’
2	A	301	0O2	C3’
2	C	301	0O2	C2’
2	C	301	0O2	C4’
2	C	301	0O2	C1’
2	C	301	0O2	C3’
2	A	302	0O2	C2’
2	A	302	0O2	C4’
2	A	302	0O2	C1’
2	A	302	0O2	C3’
2	E	301	0O2	C2’
2	E	301	0O2	C4’
2	E	301	0O2	C1’
2	E	301	0O2	C3’
2	D	301	0O2	C2’
2	D	301	0O2	C4’
2	D	301	0O2	C1’
2	D	301	0O2	C3’
2	G	301	0O2	C2’
2	G	301	0O2	C4’
2	G	301	0O2	C1’
2	G	301	0O2	C3’

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	302	0O2	PC-O3’-C3’-C4’
2	A	302	0O2	PC-O3’-C3’-C4’

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	0O2	3	0
2	A	302	0O2	2	0
2	B	301	0O2	4	0
2	C	301	0O2	4	0
2	D	301	0O2	3	0
2	D	302	0O2	2	0
2	E	301	0O2	1	0
2	F	301	0O2	4	0
2	G	301	0O2	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	302	0O2	3	0
2	H	301	0O2	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	195:ALA	C	196:ALA	N	4.14

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^{th} 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	196/218 (89%)	-0.13	10 (5%)	29	27	16, 31, 75, 106	0
1	B	191/218 (87%)	-0.32	3 (1%)	72	72	14, 31, 71, 84	0
1	C	194/218 (88%)	-0.19	6 (3%)	49	46	16, 34, 70, 101	0
1	D	188/218 (86%)	-0.23	5 (2%)	55	53	15, 33, 65, 95	0
1	E	190/218 (87%)	-0.39	2 (1%)	80	81	18, 33, 62, 107	0
1	F	192/218 (88%)	-0.15	5 (2%)	56	55	18, 37, 85, 103	0
1	G	190/218 (87%)	-0.35	4 (2%)	64	63	18, 33, 75, 110	0
1	H	194/218 (88%)	-0.12	9 (4%)	33	31	20, 34, 79, 99	0
All	All	1535/1744 (88%)	-0.23	44 (2%)	52	49	14, 33, 74, 110	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	ASN	8.7
1	H	164	ASN	7.8
1	C	164	ASN	6.3
1	A	33	TYR	6.3
1	A	163	GLY	6.1
1	C	163	GLY	5.5
1	H	163	GLY	5.4
1	H	162	SER	5.3
1	F	164	ASN	4.9
1	D	33	TYR	4.9
1	C	162	SER	4.7
1	F	171	LEU	4.4
1	A	35	ASP	4.2
1	A	161	TYR	3.7
1	A	162	SER	3.6
1	H	161	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	131	SER	2.9
1	A	130	VAL	2.7
1	C	165	ILE	2.7
1	G	35	ASP	2.7
1	F	162	SER	2.6
1	G	33	TYR	2.6
1	H	34	GLU	2.6
1	H	6	TRP	2.5
1	G	6	TRP	2.5
1	E	130	VAL	2.5
1	H	33	TYR	2.5
1	D	34	GLU	2.5
1	B	195	ALA	2.4
1	A	167	GLU	2.3
1	C	168	LYS	2.3
1	B	33	TYR	2.3
1	A	165	ILE	2.3
1	C	130	VAL	2.3
1	H	165	ILE	2.3
1	D	54	LEU	2.2
1	F	169	VAL	2.2
1	B	131	SER	2.2
1	D	171	LEU	2.1
1	G	36	ASP	2.1
1	F	58	ARG	2.1
1	D	32	GLU	2.0
1	A	34	GLU	2.0
1	H	64	LEU	2.0

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. 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	0O2	G	302	40/40	0.91	0.21	2.17	23,37,50,55	0
2	0O2	E	301	40/40	0.91	0.16	0.39	29,53,76,90	0
2	0O2	H	302	40/40	0.97	0.16	-0.18	21,31,42,44	0
2	0O2	F	301	40/40	0.91	0.15	-0.33	37,53,80,100	0
2	0O2	G	301	40/40	0.94	0.13	-0.53	19,40,55,62	0
2	0O2	B	301	40/40	0.95	0.13	-0.77	24,39,54,65	0
2	0O2	D	302	40/40	0.98	0.15	-0.99	13,23,32,35	0
2	0O2	C	301	40/40	0.93	0.13	-0.99	33,47,65,70	0
2	0O2	D	301	40/40	0.94	0.13	-1.15	26,40,61,73	0
2	0O2	H	301	40/40	0.95	0.12	-1.26	25,40,60,63	0
2	0O2	A	302	40/40	0.98	0.14	-1.45	12,20,30,38	0
2	0O2	A	301	40/40	0.96	0.12	-1.49	21,34,45,53	0
3	MG	E	302	1/1	0.88	0.28	-	26,26,26,26	0
3	MG	B	302	1/1	0.97	0.27	-	21,21,21,21	0
3	MG	A	303	1/1	0.98	0.41	-	18,18,18,18	0
3	MG	G	303	1/1	0.97	0.34	-	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.