Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2019 – 11:56 PM EST

PDB ID	:	5Q0C
Title	:	Human liver fructose-1,6-bisphosphatase 1 (fructose 1,6-bisphosphate 1-phosphatase, E.C.3.1.3.11) complexed with the allosteric inhibitor 1-(5-bromo-1,3-thiazol-2-yl)-3-[5-(4-methoxyphenyl)thiophen-2-yl]sulfonylurea and with fructose-2,6-diphosphate
Authors	:	Ruf, A.; Joseph, C.; Alker, A.; Banner, D.; Tetaz, T.; Benz, J.; Kuhn, B.; Rudolph, M.G.; Yang, H.; Shao, C.; Burley, S.K.
Deposited on	:	2017-04-18
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

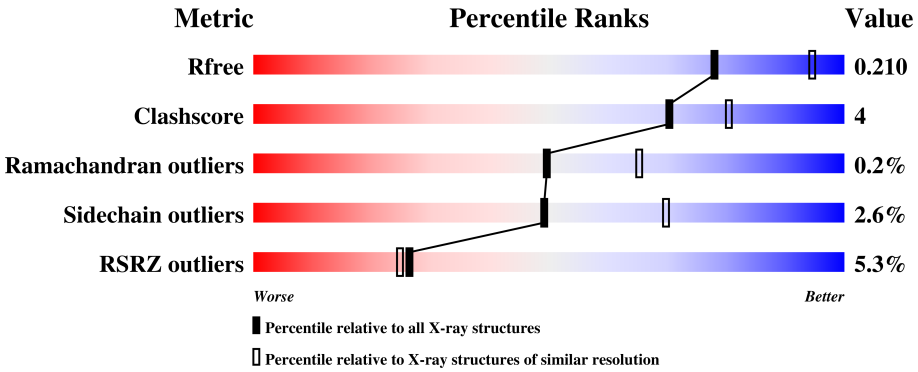
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

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 2.40 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}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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	339	4% 86% 10%
1	B	339	5% 90% 6%
1	C	339	5% 86% 10%
1	D	339	3% 86% 9% 5%
1	E	339	8% 87% 9%

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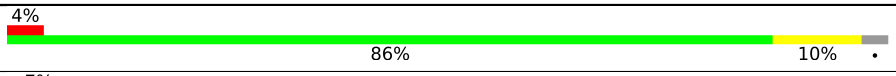
Mol	Chain	Length	Quality of chain
1	F	339	
1	G	339	
1	H	339	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20845 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.

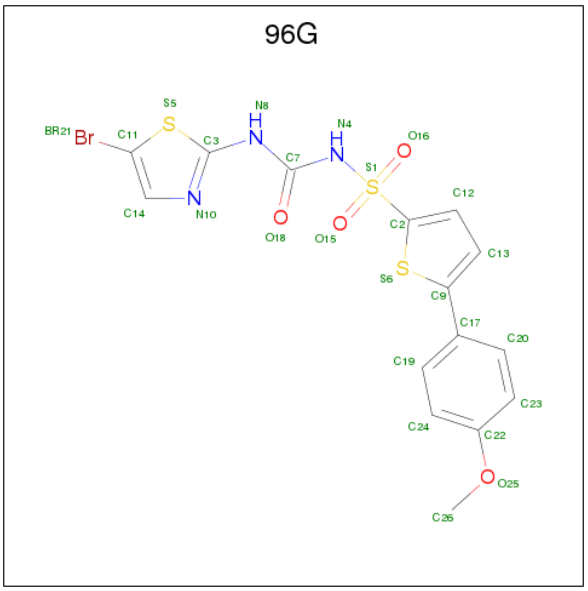
- Molecule 1 is a protein called Fructose-1,6-bisphosphatase isozyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2497	1586	415	484	12			
1	B	328	Total	C	N	O	S	0	0	0
			2497	1586	415	484	12			
1	C	328	Total	C	N	O	S	0	0	0
			2497	1586	415	484	12			
1	D	322	Total	C	N	O	S	0	0	0
			2453	1560	408	473	12			
1	E	328	Total	C	N	O	S	0	0	0
			2497	1586	415	484	12			
1	F	328	Total	C	N	O	S	0	0	0
			2497	1586	415	484	12			
1	G	328	Total	C	N	O	S	0	0	0
			2497	1586	415	484	12			
1	H	328	Total	C	N	O	S	0	0	0
			2497	1586	415	484	12			

There are 8 discrepancies between the modelled and reference sequences:

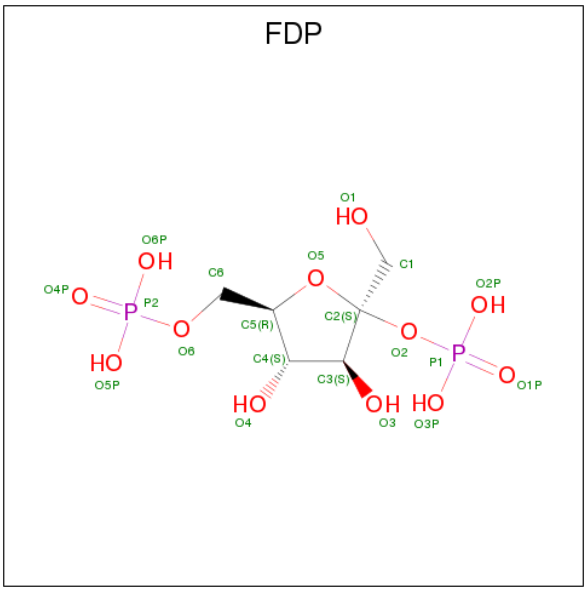
Chain	Residue	Modelled	Actual	Comment	Reference
A	86	LEU	VAL	conflict	UNP O00757
B	86	LEU	VAL	conflict	UNP O00757
C	86	LEU	VAL	conflict	UNP O00757
D	86	LEU	VAL	conflict	UNP O00757
E	86	LEU	VAL	conflict	UNP O00757
F	86	LEU	VAL	conflict	UNP O00757
G	86	LEU	VAL	conflict	UNP O00757
H	86	LEU	VAL	conflict	UNP O00757

- Molecule 2 is N-[(5-bromo-1,3-thiazol-2-yl)carbamoyl]-5-(4-methoxyphenyl)thiophene-2-sulfonamide (three-letter code: 96G) (formula: $C_{15}H_{12}BrN_3O_4S_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	S	0	0
			26	1	15	3	4	3		
2	B	1	Total	Br	C	N	O	S	0	0
			26	1	15	3	4	3		
2	C	1	Total	Br	C	N	O	S	0	0
			26	1	15	3	4	3		
2	D	1	Total	Br	C	N	O	S	0	0
			26	1	15	3	4	3		
2	E	1	Total	Br	C	N	O	S	0	0
			26	1	15	3	4	3		
2	F	1	Total	Br	C	N	O	S	0	0
			26	1	15	3	4	3		
2	G	1	Total	Br	C	N	O	S	0	0
			26	1	15	3	4	3		
2	H	1	Total	Br	C	N	O	S	0	0
			26	1	15	3	4	3		

- Molecule 3 is FRUCTOSE-2,6-DIPHOSPHATE (three-letter code: FDP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 20 6 12 2	0	0
3	B	1	Total C O P 20 6 12 2	0	0
3	C	1	Total C O P 20 6 12 2	0	0
3	D	1	Total C O P 20 6 12 2	0	0
3	E	1	Total C O P 20 6 12 2	0	0
3	F	1	Total C O P 20 6 12 2	0	0
3	G	1	Total C O P 20 6 12 2	0	0
3	H	1	Total C O P 20 6 12 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	85	Total O 85 85	0	0
4	B	82	Total O 82 82	0	0
4	C	65	Total O 65 65	0	0
4	D	83	Total O 83 83	0	0

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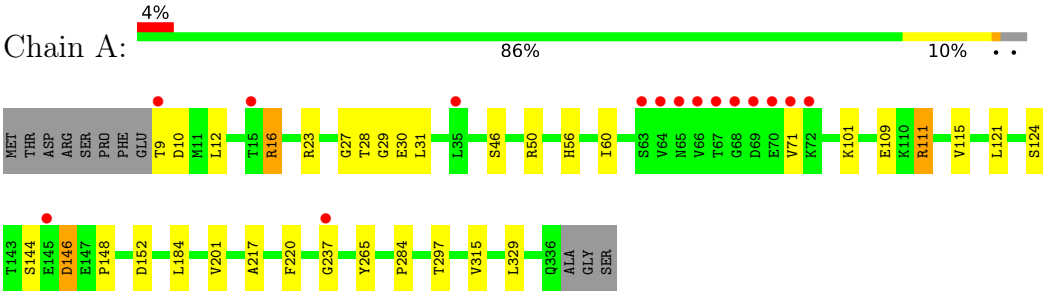
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	36	Total O 36 36	0	0
4	F	72	Total O 72 72	0	0
4	G	45	Total O 45 45	0	0
4	H	77	Total O 77 77	0	0

3 Residue-property plots (i)

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

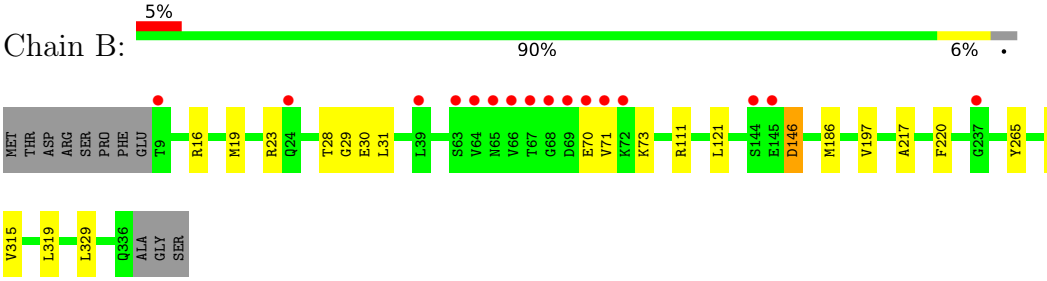
• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

Chain A:



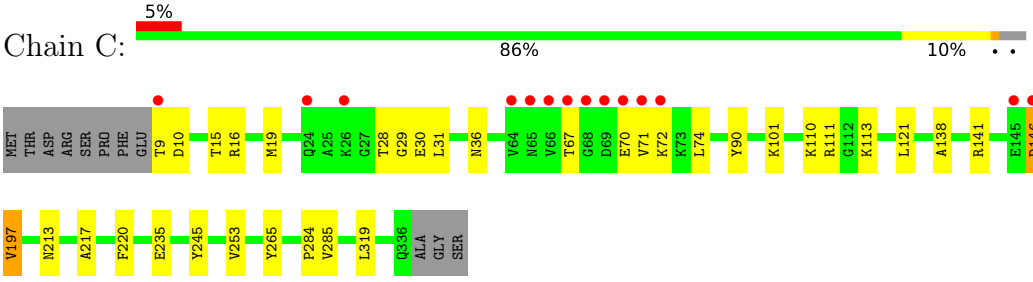
• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

Chain B:



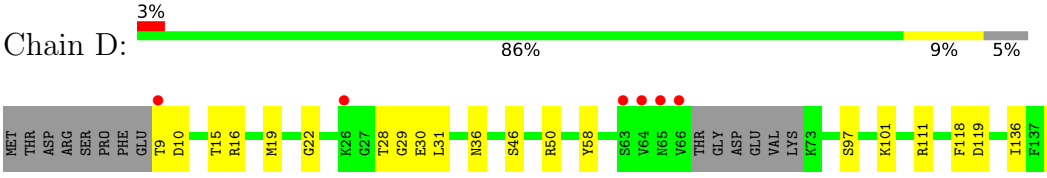
• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

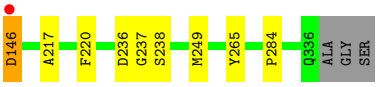
Chain C:



• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

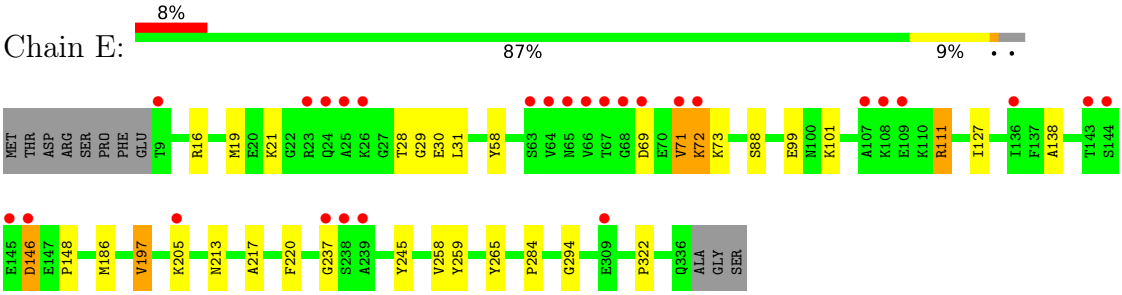
Chain D:





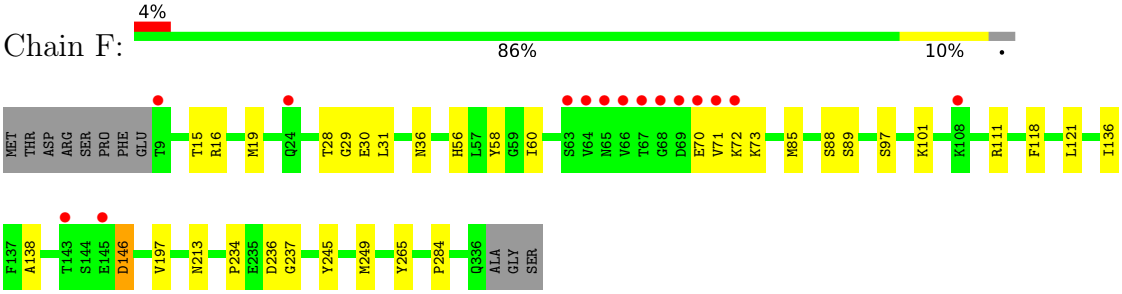
• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

Chain E:



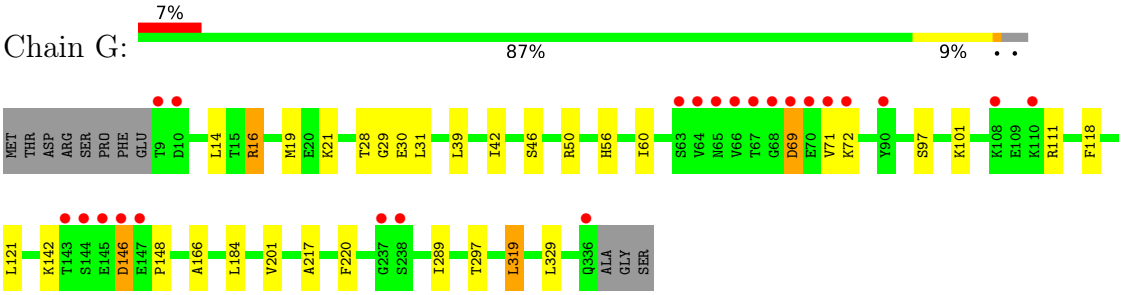
• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

Chain F:



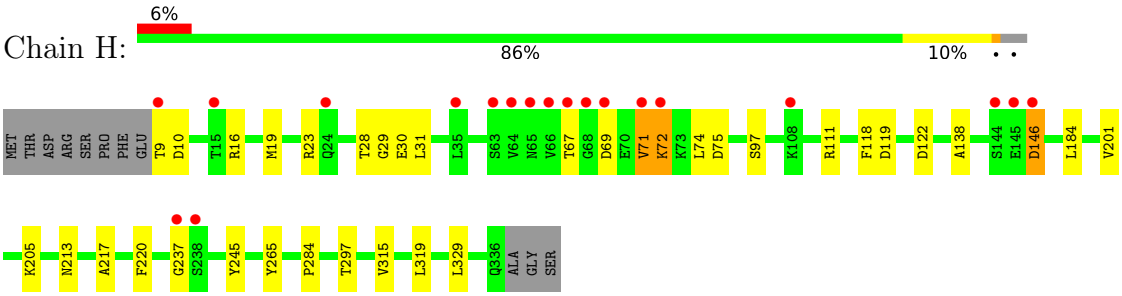
• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

Chain G:



• Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	222.47Å 240.52Å 138.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.40 29.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.79-2.40) 97.5 (29.79-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.81 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.168 , 0.210 0.168 , 0.210	Depositor DCC
R_{free} test set	6943 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20845	wwPDB-VP
Average B, all atoms (Å^2)	57.0	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 29.13 % 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 1.6340e-03. 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: FDP, 96G

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	0.43	0/2536	0.60	0/3430
1	B	0.41	0/2536	0.60	0/3430
1	C	0.42	0/2536	0.60	0/3430
1	D	0.42	0/2491	0.60	0/3368
1	E	0.39	0/2536	0.57	0/3430
1	F	0.40	0/2536	0.58	0/3430
1	G	0.39	0/2536	0.56	0/3430
1	H	0.41	0/2536	0.60	0/3430
All	All	0.41	0/20243	0.59	0/27378

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	235	GLU	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	2497	0	2549	22	0
1	B	2497	0	2549	11	0
1	C	2497	0	2549	18	0
1	D	2453	0	2506	20	0
1	E	2497	0	2549	25	0
1	F	2497	0	2549	25	0
1	G	2497	0	2549	20	0
1	H	2497	0	2549	24	0
2	A	26	0	0	3	0
2	B	26	0	0	2	0
2	C	26	0	0	2	0
2	D	26	0	0	3	0
2	E	26	0	0	3	0
2	F	26	0	0	2	0
2	G	26	0	0	3	0
2	H	26	0	0	3	0
3	A	20	0	10	1	0
3	B	20	0	10	0	0
3	C	20	0	10	0	0
3	D	20	0	10	1	0
3	E	20	0	10	0	0
3	F	20	0	10	0	0
3	G	20	0	10	0	0
3	H	20	0	10	0	0
4	A	85	0	0	0	0
4	B	82	0	0	0	0
4	C	65	0	0	0	0
4	D	83	0	0	3	0
4	E	36	0	0	0	0
4	F	72	0	0	0	0
4	G	45	0	0	0	0
4	H	77	0	0	2	0
All	All	20845	0	20429	157	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 4.

All (157) 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:89:SER:HA	1:H:16:ARG:HH12	1.43	0.82
1:H:146:ASP:N	1:H:146:ASP:OD1	2.15	0.79
1:H:119:ASP:OD2	4:H:501:HOH:O	2.03	0.77
1:D:119:ASP:OD2	4:D:501:HOH:O	2.05	0.74
1:G:146:ASP:N	1:G:146:ASP:OD1	2.18	0.74
1:E:146:ASP:OD1	1:E:146:ASP:N	2.23	0.72
1:D:146:ASP:OD1	1:D:146:ASP:N	2.23	0.71
1:A:146:ASP:OD1	1:A:146:ASP:N	2.23	0.70
1:F:146:ASP:OD1	1:F:146:ASP:N	2.25	0.68
1:C:16:ARG:HA	1:C:19:MET:HE2	1.77	0.66
1:H:122:ASP:OD1	4:H:501:HOH:O	2.12	0.66
1:H:28:THR:HG23	1:H:30:GLU:H	1.62	0.65
1:E:88:SER:OG	1:G:16:ARG:NH2	2.30	0.64
1:F:138:ALA:HB2	1:F:284:PRO:HG3	1.80	0.62
1:F:16:ARG:HA	1:F:19:MET:HE2	1.79	0.62
1:H:16:ARG:HA	1:H:19:MET:HE2	1.82	0.62
1:A:12:LEU:HD11	1:A:16:ARG:HH21	1.66	0.61
1:B:146:ASP:OD1	1:B:146:ASP:N	2.34	0.60
1:G:69:ASP:HB3	1:G:72:LYS:HB3	1.84	0.60
1:G:289:ILE:HG13	1:G:319:LEU:HD22	1.83	0.59
1:F:28:THR:HG23	1:F:30:GLU:H	1.67	0.59
1:C:146:ASP:OD1	1:C:146:ASP:N	2.34	0.59
1:B:28:THR:HG23	1:B:30:GLU:H	1.69	0.58
1:D:138:ALA:HB2	1:D:284:PRO:HG3	1.86	0.58
1:B:16:ARG:HA	1:B:19:MET:HE2	1.86	0.58
1:C:15:THR:HG21	1:C:36:ASN:OD1	2.04	0.58
1:F:89:SER:HA	1:H:16:ARG:NH1	2.14	0.58
1:G:217:ALA:HA	1:G:220:PHE:CD2	2.39	0.57
1:G:29:GLY:HA2	2:G:401:96G:O18	2.04	0.57
1:F:85:MET:HE3	1:H:16:ARG:HH21	1.68	0.57
1:B:289:ILE:HG13	1:B:319:LEU:HD22	1.85	0.57
1:C:28:THR:HG23	1:C:30:GLU:H	1.69	0.57
1:C:29:GLY:HA2	2:C:401:96G:C7	2.34	0.56
1:F:29:GLY:HA2	2:F:401:96G:C7	2.36	0.56
1:D:16:ARG:HA	1:D:19:MET:HE2	1.89	0.55
1:D:28:THR:HG23	1:D:30:GLU:H	1.71	0.55
1:G:29:GLY:HA2	2:G:401:96G:C7	2.37	0.55
1:G:16:ARG:HA	1:G:19:MET:HE2	1.89	0.54
1:E:101:LYS:H	1:E:101:LYS:HD3	1.73	0.53
1:D:29:GLY:HA2	2:D:401:96G:C7	2.37	0.53
1:E:111:ARG:HD3	1:E:148:PRO:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:GLY:HA2	2:C:401:96G:O18	2.09	0.53
1:C:217:ALA:HA	1:C:220:PHE:CD2	2.44	0.53
1:E:72:LYS:NZ	1:E:99:GLU:OE1	2.40	0.52
1:H:213:ASN:HB2	1:H:245:TYR:CE2	2.44	0.52
1:B:29:GLY:HA2	2:B:401:96G:C7	2.40	0.52
1:A:297:THR:HG21	1:A:329:LEU:HD21	1.92	0.52
1:C:138:ALA:HB2	1:C:284:PRO:HG3	1.92	0.52
1:E:29:GLY:HA2	2:E:401:96G:O18	2.10	0.51
1:G:142:LYS:HE3	1:G:148:PRO:HG3	1.91	0.51
1:E:16:ARG:HA	1:E:19:MET:HE2	1.92	0.51
1:E:71:VAL:HB	1:E:127:ILE:HD12	1.92	0.51
1:E:101:LYS:N	1:E:101:LYS:HD3	2.25	0.51
1:E:28:THR:HG23	1:E:30:GLU:H	1.75	0.50
1:E:29:GLY:HA2	2:E:401:96G:C7	2.42	0.50
1:F:56:HIS:HA	1:F:60:ILE:HG22	1.93	0.50
1:H:29:GLY:HA2	2:H:401:96G:O18	2.11	0.50
1:G:28:THR:HG23	1:G:30:GLU:H	1.75	0.50
3:D:402:FDP:O1	4:D:501:HOH:O	2.18	0.50
1:E:101:LYS:H	1:E:101:LYS:CD	2.24	0.50
1:D:217:ALA:HA	1:D:220:PHE:CD2	2.47	0.50
1:A:124:SER:N	3:A:402:FDP:O3P	2.42	0.49
1:D:101:LYS:HD3	1:D:101:LYS:H	1.77	0.49
1:H:29:GLY:HA2	2:H:401:96G:C7	2.42	0.49
1:D:236:ASP:O	1:D:238:SER:N	2.46	0.49
1:F:101:LYS:H	1:F:101:LYS:HD3	1.78	0.49
1:A:28:THR:HG23	1:A:30:GLU:H	1.78	0.49
1:E:58:TYR:CZ	1:F:197:VAL:HG22	2.47	0.49
1:F:29:GLY:HA2	2:F:401:96G:O18	2.13	0.49
1:F:88:SER:OG	1:H:16:ARG:NH2	2.47	0.48
1:B:217:ALA:HA	1:B:220:PHE:CD2	2.48	0.48
1:E:21:LYS:HD3	2:E:401:96G:C23	2.44	0.48
1:H:217:ALA:HA	1:H:220:PHE:CD2	2.49	0.48
1:F:234:PRO:C	1:F:236:ASP:H	2.16	0.48
1:D:101:LYS:N	1:D:101:LYS:HD3	2.29	0.48
1:E:138:ALA:HB2	1:E:284:PRO:HG3	1.95	0.48
1:D:101:LYS:CD	1:D:101:LYS:H	2.27	0.47
1:A:184:LEU:HG	1:A:201:VAL:HG21	1.97	0.47
1:B:186:MET:HG3	1:B:197:VAL:HG11	1.96	0.47
1:A:138:ALA:HB2	1:A:284:PRO:HG3	1.95	0.47
1:A:56:HIS:HA	1:A:60:ILE:HG22	1.97	0.47
1:E:217:ALA:HA	1:E:220:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:HG2	2:A:401:96G:C14	2.45	0.46
1:G:46:SER:O	1:G:50:ARG:HD3	2.14	0.46
1:A:29:GLY:HA2	2:A:401:96G:C7	2.46	0.46
1:E:205:LYS:HA	1:E:205:LYS:HD3	1.78	0.46
1:G:97:SER:HB2	1:G:118:PHE:CZ	2.50	0.46
1:G:56:HIS:HA	1:G:60:ILE:HG22	1.98	0.46
1:H:69:ASP:OD2	1:H:72:LYS:HB2	2.15	0.46
1:F:121:LEU:HA	1:F:121:LEU:HD12	1.81	0.46
1:F:97:SER:HB2	1:F:118:PHE:CZ	2.51	0.46
1:A:16:ARG:O	1:A:16:ARG:HD2	2.17	0.45
1:C:101:LYS:HD3	1:C:101:LYS:H	1.82	0.45
1:G:184:LEU:HG	1:G:201:VAL:HG21	1.99	0.45
1:F:136:ILE:HD13	1:F:249:MET:HE2	1.99	0.45
1:F:72:LYS:HE2	1:F:72:LYS:HB2	1.84	0.45
1:H:23:ARG:HG2	2:H:401:96G:C14	2.47	0.45
1:E:258:VAL:HG23	1:E:259:TYR:CD1	2.52	0.45
1:H:184:LEU:HG	1:H:201:VAL:HG21	1.98	0.45
1:A:217:ALA:HA	1:A:220:PHE:CD2	2.52	0.45
1:F:85:MET:CE	1:H:16:ARG:HH21	2.30	0.45
1:D:97:SER:HB2	1:D:118:PHE:CZ	2.52	0.44
1:H:138:ALA:HB2	1:H:284:PRO:HG3	2.00	0.44
1:H:297:THR:HG21	1:H:329:LEU:HD21	1.99	0.44
1:B:23:ARG:HG2	2:B:401:96G:C14	2.47	0.44
1:A:109:GLU:OE1	1:A:109:GLU:N	2.43	0.44
1:D:46:SER:O	1:D:50:ARG:HD3	2.18	0.44
1:F:236:ASP:OD1	1:F:237:GLY:N	2.47	0.44
1:E:186:MET:HG3	1:E:197:VAL:HG21	1.99	0.44
1:D:22:GLY:HA2	2:D:401:96G:S6	2.58	0.44
1:A:121:LEU:HA	1:A:121:LEU:HD12	1.71	0.43
1:D:29:GLY:HA2	2:D:401:96G:O18	2.18	0.43
1:D:28:THR:HG22	4:D:546:HOH:O	2.18	0.43
1:A:101:LYS:HD3	1:A:101:LYS:H	1.82	0.43
1:C:197:VAL:HG22	1:D:58:TYR:CZ	2.54	0.43
1:F:213:ASN:HB2	1:F:245:TYR:CE2	2.53	0.43
1:C:90:TYR:HE1	1:C:110:LYS:HG2	1.84	0.43
1:A:142:LYS:NZ	1:A:144:SER:OG	2.46	0.43
1:C:213:ASN:HB2	1:C:245:TYR:CE2	2.53	0.43
1:G:121:LEU:HD12	1:G:121:LEU:HA	1.74	0.43
1:H:9:THR:HB	1:H:10:ASP:H	1.64	0.43
1:H:97:SER:HB2	1:H:118:PHE:CZ	2.55	0.42
1:C:121:LEU:HD12	1:C:121:LEU:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:LYS:HA	1:C:72:LYS:HD2	1.82	0.42
1:G:21:LYS:HB3	2:G:401:96G:C20	2.49	0.42
1:F:73:LYS:HD3	1:F:73:LYS:HA	1.81	0.42
1:D:15:THR:HG21	1:D:36:ASN:OD1	2.19	0.42
1:B:121:LEU:HA	1:B:121:LEU:HD12	1.84	0.42
1:A:16:ARG:HD2	1:A:16:ARG:C	2.40	0.42
1:E:197:VAL:HG22	1:F:58:TYR:CZ	2.54	0.42
1:H:205:LYS:HA	1:H:205:LYS:HD3	1.80	0.42
1:D:136:ILE:HD13	1:D:249:MET:HE2	2.02	0.42
1:A:9:THR:HB	1:A:10:ASP:H	1.75	0.41
1:B:73:LYS:HA	1:B:73:LYS:HD3	1.86	0.41
1:C:9:THR:HB	1:C:10:ASP:H	1.66	0.41
1:C:74:LEU:HD12	1:C:74:LEU:HA	1.89	0.41
1:E:73:LYS:HA	1:E:73:LYS:HD3	1.91	0.41
1:D:9:THR:HB	1:D:10:ASP:H	1.76	0.41
1:E:69:ASP:OD2	1:E:72:LYS:HB2	2.20	0.41
1:A:27:GLY:HA3	2:A:401:96G:N4	2.36	0.41
1:H:71:VAL:HG23	1:H:75:ASP:OD1	2.21	0.41
1:H:74:LEU:HD12	1:H:74:LEU:HA	1.93	0.41
1:A:115:VAL:HG21	1:A:152:ASP:HB3	2.02	0.41
1:C:113:LYS:HD2	1:C:141:ARG:HE	1.84	0.41
1:G:101:LYS:H	1:G:101:LYS:HD3	1.86	0.41
1:A:46:SER:O	1:A:50:ARG:HD3	2.20	0.41
1:E:213:ASN:HB2	1:E:245:TYR:CE2	2.56	0.41
1:C:253:VAL:HG11	1:C:285:VAL:HB	2.02	0.40
1:E:294:GLY:HA2	1:E:322:PRO:HD3	2.03	0.40
1:G:297:THR:HG21	1:G:329:LEU:HD21	2.02	0.40
1:E:72:LYS:HD2	1:E:72:LYS:HA	1.42	0.40
1:G:42:ILE:HD13	1:G:166:ALA:HB2	2.02	0.40
1:A:111:ARG:HD3	1:A:148:PRO:HG2	2.03	0.40
1:F:101:LYS:N	1:F:101:LYS:HD3	2.36	0.40
1:F:15:THR:HG21	1:F:36:ASN:OD1	2.22	0.40
1:B:297:THR:HG21	1:B:329:LEU:HD21	2.04	0.40
1:G:14:LEU:HD22	1:G:39:LEU:HG	2.02	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	326/339 (96%)	317 (97%)	8 (2%)	1 (0%)	43 58
1	B	326/339 (96%)	320 (98%)	6 (2%)	0	100 100
1	C	326/339 (96%)	317 (97%)	9 (3%)	0	100 100
1	D	318/339 (94%)	310 (98%)	7 (2%)	1 (0%)	43 58
1	E	326/339 (96%)	318 (98%)	7 (2%)	1 (0%)	43 58
1	F	326/339 (96%)	317 (97%)	9 (3%)	0	100 100
1	G	326/339 (96%)	319 (98%)	7 (2%)	0	100 100
1	H	326/339 (96%)	318 (98%)	7 (2%)	1 (0%)	43 58
All	All	2600/2712 (96%)	2536 (98%)	60 (2%)	4 (0%)	49 65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	237	GLY
1	A	237	GLY
1	E	237	GLY
1	H	237	GLY

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	271/280 (97%)	264 (97%)	7 (3%)	49 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	271/280 (97%)	264 (97%)	7 (3%)	49 70
1	C	271/280 (97%)	262 (97%)	9 (3%)	41 61
1	D	266/280 (95%)	262 (98%)	4 (2%)	67 83
1	E	271/280 (97%)	264 (97%)	7 (3%)	49 70
1	F	271/280 (97%)	265 (98%)	6 (2%)	55 74
1	G	271/280 (97%)	264 (97%)	7 (3%)	49 70
1	H	271/280 (97%)	262 (97%)	9 (3%)	41 61
All	All	2163/2240 (97%)	2107 (97%)	56 (3%)	49 70

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	31	LEU
1	A	71	VAL
1	A	111	ARG
1	A	146	ASP
1	A	265	TYR
1	A	315	VAL
1	B	31	LEU
1	B	70	GLU
1	B	71	VAL
1	B	111	ARG
1	B	146	ASP
1	B	265	TYR
1	B	315	VAL
1	C	31	LEU
1	C	67	THR
1	C	70	GLU
1	C	71	VAL
1	C	111	ARG
1	C	146	ASP
1	C	197	VAL
1	C	265	TYR
1	C	319	LEU
1	D	31	LEU
1	D	111	ARG
1	D	146	ASP
1	D	265	TYR
1	E	31	LEU

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Mol	Chain	Res	Type
1	E	71	VAL
1	E	72	LYS
1	E	111	ARG
1	E	146	ASP
1	E	197	VAL
1	E	265	TYR
1	F	31	LEU
1	F	70	GLU
1	F	71	VAL
1	F	111	ARG
1	F	146	ASP
1	F	265	TYR
1	G	16	ARG
1	G	31	LEU
1	G	69	ASP
1	G	71	VAL
1	G	111	ARG
1	G	146	ASP
1	G	319	LEU
1	H	31	LEU
1	H	67	THR
1	H	71	VAL
1	H	72	LYS
1	H	111	ARG
1	H	146	ASP
1	H	265	TYR
1	H	315	VAL
1	H	319	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

16 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	96G	A	401	-	22,28,28	1.03	1 (4%)	22,40,40	1.62	2 (9%)
3	FDP	A	402	-	19,20,20	1.35	3 (15%)	30,32,32	1.41	6 (20%)
2	96G	B	401	-	22,28,28	1.15	2 (9%)	22,40,40	1.10	2 (9%)
3	FDP	B	402	-	19,20,20	1.15	2 (10%)	30,32,32	1.26	1 (3%)
2	96G	C	401	-	22,28,28	0.98	1 (4%)	22,40,40	0.95	2 (9%)
3	FDP	C	402	-	19,20,20	1.01	0	30,32,32	1.39	3 (10%)
2	96G	D	401	-	22,28,28	1.19	2 (9%)	22,40,40	0.89	1 (4%)
3	FDP	D	402	-	19,20,20	1.18	1 (5%)	30,32,32	1.26	2 (6%)
2	96G	E	401	-	22,28,28	0.91	1 (4%)	22,40,40	0.99	2 (9%)
3	FDP	E	402	-	19,20,20	1.24	3 (15%)	30,32,32	1.26	2 (6%)
2	96G	F	401	-	22,28,28	1.16	2 (9%)	22,40,40	1.08	2 (9%)
3	FDP	F	402	-	19,20,20	1.20	2 (10%)	30,32,32	1.30	3 (10%)
2	96G	G	401	-	22,28,28	0.99	2 (9%)	22,40,40	1.01	2 (9%)
3	FDP	G	402	-	19,20,20	1.44	4 (21%)	30,32,32	1.53	6 (20%)
2	96G	H	401	-	22,28,28	0.95	1 (4%)	22,40,40	1.00	2 (9%)
3	FDP	H	402	-	19,20,20	1.04	1 (5%)	30,32,32	1.37	4 (13%)

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	96G	A	401	-	-	0/13/21/21	0/3/3/3
3	FDP	A	402	-	-	0/12/34/34	0/1/1/1
2	96G	B	401	-	-	0/13/21/21	0/3/3/3
3	FDP	B	402	-	-	0/12/34/34	0/1/1/1
2	96G	C	401	-	-	0/13/21/21	0/3/3/3
3	FDP	C	402	-	-	0/12/34/34	0/1/1/1
2	96G	D	401	-	-	0/13/21/21	0/3/3/3
3	FDP	D	402	-	-	0/12/34/34	0/1/1/1
2	96G	E	401	-	-	0/13/21/21	0/3/3/3
3	FDP	E	402	-	-	0/12/34/34	0/1/1/1
2	96G	F	401	-	-	0/13/21/21	0/3/3/3
3	FDP	F	402	-	-	0/12/34/34	0/1/1/1
2	96G	G	401	-	-	0/13/21/21	0/3/3/3
3	FDP	G	402	-	-	0/12/34/34	0/1/1/1
2	96G	H	401	-	-	0/13/21/21	0/3/3/3
3	FDP	H	402	-	-	0/12/34/34	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	96G	C2-S6	-3.72	1.65	1.72
2	B	401	96G	C2-S6	-3.64	1.66	1.72
2	D	401	96G	C2-S6	-3.49	1.66	1.72
3	D	402	FDP	O6-C6	-2.88	1.33	1.44
2	G	401	96G	C2-S6	-2.78	1.67	1.72
2	C	401	96G	C2-S1	-2.74	1.72	1.76
2	A	401	96G	C2-S6	-2.61	1.67	1.72
3	G	402	FDP	O6-C6	-2.56	1.34	1.44
3	H	402	FDP	O6-C6	-2.43	1.35	1.44
2	D	401	96G	C2-S1	-2.41	1.72	1.76
3	A	402	FDP	O6-C6	-2.32	1.35	1.44
2	E	401	96G	C2-S6	-2.25	1.68	1.72
3	G	402	FDP	O3-C3	-2.23	1.38	1.42
3	F	402	FDP	O6-C6	-2.23	1.36	1.44
2	F	401	96G	C2-S1	-2.22	1.73	1.76
3	E	402	FDP	O6-C6	-2.12	1.36	1.44
2	G	401	96G	C2-S1	-2.09	1.73	1.76
3	B	402	FDP	C6-C5	2.14	1.58	1.51
2	B	401	96G	C3-N8	2.18	1.40	1.36
3	A	402	FDP	C6-C5	2.20	1.58	1.51
3	E	402	FDP	C6-C5	2.32	1.59	1.51
3	F	402	FDP	P1-O2	2.40	1.63	1.59
3	G	402	FDP	C6-C5	2.57	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	96G	C12-C13	2.65	1.52	1.39
3	E	402	FDP	P1-O2	2.83	1.64	1.59
3	B	402	FDP	P1-O2	2.90	1.64	1.59
3	G	402	FDP	P1-O2	3.19	1.65	1.59
3	A	402	FDP	P1-O2	3.66	1.66	1.59

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	402	FDP	O2-P1-O1P	-3.61	95.46	109.39
3	A	402	FDP	O2-P1-O1P	-3.38	96.34	109.39
3	C	402	FDP	O2-P1-O1P	-3.06	97.60	109.39
3	C	402	FDP	O6P-P2-O6	-3.04	98.65	106.73
2	E	401	96G	C2-S1-N4	-2.52	104.22	107.18
2	G	401	96G	C2-S1-N4	-2.47	104.28	107.18
3	G	402	FDP	C1-C2-C3	-2.44	106.89	114.52
3	F	402	FDP	O5P-P2-O6	-2.44	100.25	106.73
3	G	402	FDP	O6P-P2-O6	-2.17	100.95	106.73
3	E	402	FDP	O5-C2-C3	-2.16	100.95	105.57
3	G	402	FDP	C6-C5-C4	-2.13	107.28	115.29
3	A	402	FDP	O4-C4-C3	-2.10	105.64	112.15
3	H	402	FDP	O3-C3-C4	-2.05	106.24	113.39
3	A	402	FDP	O3-C3-C4	-2.04	106.29	113.39
3	A	402	FDP	O5-C5-C6	2.02	113.99	109.52
3	A	402	FDP	O6P-P2-O5P	2.03	115.60	107.59
3	D	402	FDP	O6P-P2-O5P	2.04	115.66	107.59
3	E	402	FDP	O5-C5-C6	2.09	114.14	109.52
3	F	402	FDP	O5-C5-C6	2.09	114.14	109.52
3	F	402	FDP	O6P-P2-O5P	2.10	115.91	107.59
3	D	402	FDP	O2P-P1-O1P	2.14	118.96	110.60
2	E	401	96G	BR21-C11-C14	2.27	127.85	124.38
3	C	402	FDP	O3P-P1-O2P	2.36	116.91	107.59
2	H	401	96G	BR21-C11-C14	2.37	128.01	124.38
2	C	401	96G	BR21-C11-C14	2.38	128.03	124.38
2	G	401	96G	BR21-C11-C14	2.38	128.03	124.38
2	D	401	96G	BR21-C11-C14	2.38	128.03	124.38
2	F	401	96G	O16-S1-N4	2.38	113.52	106.75
3	B	402	FDP	O5-C5-C6	2.40	114.83	109.52
2	F	401	96G	BR21-C11-C14	2.41	128.07	124.38
2	B	401	96G	BR21-C11-C14	2.41	128.07	124.38
2	C	401	96G	C2-S1-N4	2.45	110.06	107.18
2	A	401	96G	BR21-C11-C14	2.45	128.14	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	401	96G	O16-S1-N4	2.48	113.79	106.75
3	H	402	FDP	O5-C5-C6	2.55	115.17	109.52
3	G	402	FDP	O5-C2-C1	2.58	114.59	108.03
3	A	402	FDP	O3P-P1-O2P	2.58	117.79	107.59
3	G	402	FDP	O2-C2-C3	2.66	117.07	108.18
3	H	402	FDP	O3P-P1-O2P	2.66	118.13	107.59
3	G	402	FDP	O5-C5-C6	3.75	117.81	109.52
2	B	401	96G	C2-S1-N4	3.80	111.65	107.18
2	A	401	96G	C2-S1-N4	6.60	114.95	107.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	96G	3	0
3	A	402	FDP	1	0
2	B	401	96G	2	0
2	C	401	96G	2	0
2	D	401	96G	3	0
3	D	402	FDP	1	0
2	E	401	96G	3	0
2	F	401	96G	2	0
2	G	401	96G	3	0
2	H	401	96G	3	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^{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	328/339 (96%)	-0.12	15 (4%)	32	30	32, 46, 94, 140	0
1	B	328/339 (96%)	-0.09	16 (4%)	29	28	34, 47, 92, 159	0
1	C	328/339 (96%)	-0.15	16 (4%)	29	28	35, 50, 91, 127	0
1	D	322/339 (94%)	-0.29	9 (2%)	53	50	35, 49, 81, 127	0
1	E	328/339 (96%)	-0.02	27 (8%)	11	10	37, 61, 103, 152	0
1	F	328/339 (96%)	-0.19	15 (4%)	32	30	35, 50, 100, 168	0
1	G	328/339 (96%)	0.08	23 (7%)	16	14	38, 58, 106, 178	0
1	H	328/339 (96%)	-0.07	19 (5%)	23	21	33, 48, 91, 138	0
All	All	2618/2712 (96%)	-0.11	140 (5%)	26	25	32, 51, 98, 178	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	65	ASN	8.0
1	B	67	THR	7.9
1	G	66	VAL	7.4
1	G	65	ASN	7.2
1	G	64	VAL	6.1
1	F	67	THR	6.1
1	H	63	SER	6.0
1	A	71	VAL	6.0
1	C	67	THR	6.0
1	F	72	LYS	5.8
1	G	68	GLY	5.8
1	E	23	ARG	5.7
1	C	65	ASN	5.6
1	G	72	LYS	5.6
1	F	68	GLY	5.6
1	A	64	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	65	ASN	5.4
1	F	65	ASN	5.4
1	B	65	ASN	5.3
1	H	145	GLU	5.3
1	F	64	VAL	5.3
1	H	65	ASN	5.2
1	C	66	VAL	5.2
1	G	67	THR	5.1
1	A	72	LYS	5.0
1	B	69	ASP	4.9
1	G	144	SER	4.9
1	E	69	ASP	4.9
1	C	72	LYS	4.9
1	C	69	ASP	4.8
1	A	68	GLY	4.7
1	H	71	VAL	4.7
1	B	71	VAL	4.6
1	C	71	VAL	4.6
1	A	67	THR	4.6
1	H	69	ASP	4.6
1	C	64	VAL	4.6
1	G	69	ASP	4.5
1	B	68	GLY	4.5
1	D	64	VAL	4.4
1	A	66	VAL	4.4
1	A	69	ASP	4.3
1	E	143	THR	4.3
1	F	69	ASP	4.2
1	E	64	VAL	4.2
1	H	66	VAL	4.2
1	C	68	GLY	4.1
1	B	64	VAL	4.1
1	E	68	GLY	4.0
1	D	66	VAL	4.0
1	E	65	ASN	3.9
1	G	145	GLU	3.9
1	F	71	VAL	3.9
1	B	66	VAL	3.9
1	A	237	GLY	3.8
1	E	145	GLU	3.8
1	A	9	THR	3.8
1	H	64	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	145	GLU	3.6
1	B	72	LYS	3.6
1	H	67	THR	3.5
1	D	9	THR	3.5
1	E	71	VAL	3.4
1	G	71	VAL	3.4
1	H	237	GLY	3.4
1	G	146	ASP	3.4
1	F	63	SER	3.4
1	G	237	GLY	3.3
1	E	9	THR	3.3
1	E	237	GLY	3.2
1	E	67	THR	3.1
1	H	72	LYS	3.1
1	A	145	GLU	3.1
1	C	9	THR	3.1
1	F	145	GLU	3.0
1	B	70	GLU	3.0
1	H	68	GLY	3.0
1	G	63	SER	2.9
1	E	25	ALA	2.9
1	E	107	ALA	2.9
1	E	72	LYS	2.9
1	F	66	VAL	2.9
1	F	108	LYS	2.9
1	G	143	THR	2.9
1	E	144	SER	2.8
1	B	39	LEU	2.8
1	H	144	SER	2.8
1	D	145	GLU	2.7
1	A	15	THR	2.7
1	C	147	GLU	2.7
1	B	237	GLY	2.7
1	C	24	GLN	2.7
1	B	9	THR	2.6
1	D	63	SER	2.6
1	E	24	GLN	2.6
1	H	35	LEU	2.6
1	G	108	LYS	2.6
1	A	63	SER	2.5
1	H	15	THR	2.5
1	A	35	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	26	LYS	2.5
1	B	63	SER	2.5
1	F	143	THR	2.5
1	E	66	VAL	2.5
1	D	146	ASP	2.5
1	E	238	SER	2.4
1	G	9	THR	2.4
1	H	9	THR	2.4
1	G	90	TYR	2.4
1	H	24	GLN	2.4
1	F	24	GLN	2.4
1	H	146	ASP	2.3
1	A	70	GLU	2.3
1	F	70	GLU	2.3
1	H	108	LYS	2.3
1	G	110	LYS	2.3
1	D	26	LYS	2.3
1	G	10	ASP	2.3
1	G	70	GLU	2.3
1	G	147	GLU	2.3
1	D	144	SER	2.2
1	E	239	ALA	2.2
1	C	145	GLU	2.2
1	E	108	LYS	2.2
1	G	336	GLN	2.2
1	G	238	SER	2.2
1	E	309	GLU	2.2
1	E	146	ASP	2.2
1	B	24	GLN	2.1
1	B	144	SER	2.1
1	E	26	LYS	2.1
1	F	9	THR	2.1
1	E	136	ILE	2.1
1	E	109	GLU	2.1
1	E	63	SER	2.1
1	C	70	GLU	2.1
1	C	164	GLY	2.0
1	E	205	LYS	2.0
1	H	238	SER	2.0
1	C	146	ASP	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. 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	B-factors(Å^2)	Q<0.9
2	96G	G	401	26/26	0.93	0.17	67,93,115,118	0
2	96G	E	401	26/26	0.94	0.19	63,109,118,122	0
2	96G	A	401	26/26	0.94	0.14	36,76,89,91	0
2	96G	C	401	26/26	0.95	0.17	36,77,89,92	0
2	96G	D	401	26/26	0.95	0.17	36,67,83,88	0
2	96G	B	401	26/26	0.96	0.14	32,69,81,90	0
2	96G	F	401	26/26	0.96	0.17	38,78,88,90	0
2	96G	H	401	26/26	0.96	0.14	39,75,86,91	0
3	FDP	H	402	20/20	0.97	0.09	42,46,68,77	0
3	FDP	G	402	20/20	0.97	0.10	41,50,69,75	0
3	FDP	D	402	20/20	0.98	0.09	41,49,67,69	0
3	FDP	C	402	20/20	0.98	0.08	37,44,67,72	0
3	FDP	F	402	20/20	0.98	0.10	43,54,72,77	0
3	FDP	B	402	20/20	0.98	0.10	37,45,59,65	0
3	FDP	A	402	20/20	0.98	0.10	37,46,60,67	0
3	FDP	E	402	20/20	0.98	0.10	44,53,74,78	0

6.5 Other polymers (i)

There are no such residues in this entry.