Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2019 – 05:53 PM EST

PDB ID	:	5PZX
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-[4-methoxy-3-(2-methylpropyl)phenyl]sulfonylurea
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	:	2.75 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:

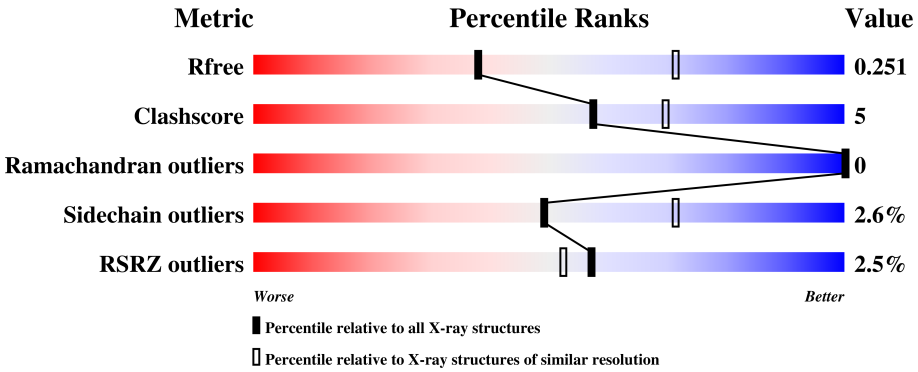
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.75 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	4013 (2.80-2.72)
Clashscore	122126	1029 (2.78-2.74)
Ramachandran outliers	120053	1013 (2.78-2.74)
Sidechain outliers	120020	1013 (2.78-2.74)
RSRZ outliers	108989	3920 (2.80-2.72)

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	338	2% 83% 12% 6%
1	B	338	2% 78% 15% 6%
1	C	338	% 79% 14% 6%
1	D	338	% 80% 13% 6%
1	E	338	3% 84% 10% 6%

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Mol	Chain	Length	Quality of chain
1	F	338	7% 82% 11% • 6%
1	G	338	% 75% 18% • 6%
1	H	338	% 80% 14% 6%

2 Entry composition (i)

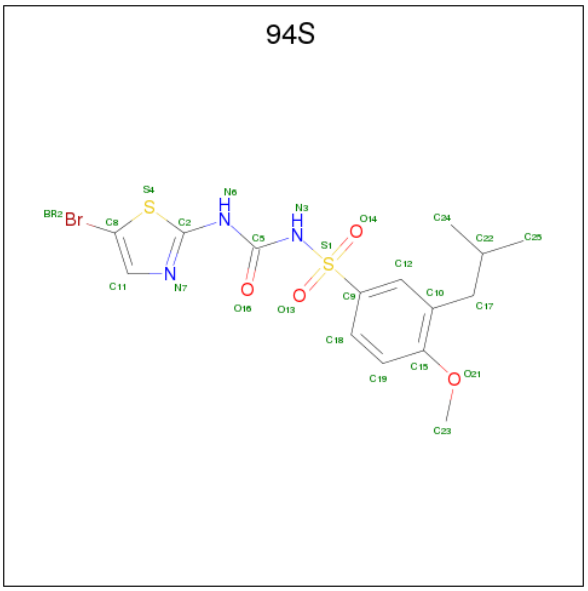
There are 3 unique types of molecules in this entry. The entry contains 19898 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	2	0
			2450	1561	412	459	18			
1	B	317	Total	C	N	O	S	0	1	0
			2431	1548	409	457	17			
1	C	317	Total	C	N	O	S	0	0	0
			2425	1545	406	457	17			
1	D	317	Total	C	N	O	S	0	1	0
			2431	1548	409	457	17			
1	E	319	Total	C	N	O	S	0	1	0
			2447	1559	412	459	17			
1	F	317	Total	C	N	O	S	0	1	0
			2430	1547	409	457	17			
1	G	317	Total	C	N	O	S	0	1	0
			2430	1547	409	457	17			
1	H	317	Total	C	N	O	S	0	0	0
			2425	1545	406	457	17			

- Molecule 2 is N-[(5-bromo-1,3-thiazol-2-yl)carbamoyl]-4-methoxy-3-(2-methylpropyl)benzene-1-sulfonamide (three-letter code: 94S) (formula: $C_{15}H_{18}BrN_3O_4S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Br C N O S 25 1 15 3 4 2	0	0
2	B	1	Total Br C N O S 25 1 15 3 4 2	0	0
2	C	1	Total Br C N O S 25 1 15 3 4 2	0	0
2	D	1	Total Br C N O S 25 1 15 3 4 2	0	0
2	E	1	Total Br C N O S 25 1 15 3 4 2	0	0
2	F	1	Total Br C N O S 25 1 15 3 4 2	0	0
2	G	1	Total Br C N O S 25 1 15 3 4 2	0	0
2	H	1	Total Br C N O S 25 1 15 3 4 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	B	18	Total O 18 18	0	0
3	C	52	Total O 52 52	0	0
3	D	41	Total O 41 41	0	0

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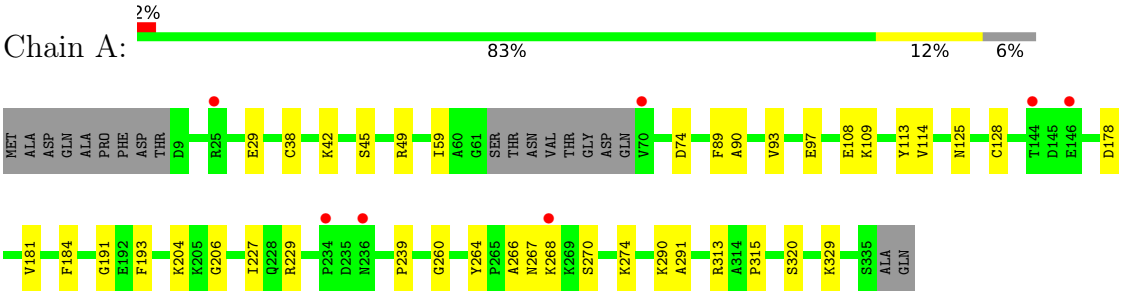
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	19	Total O 19 19	0	0
3	F	10	Total O 10 10	0	0
3	G	28	Total O 28 28	0	0
3	H	34	Total O 34 34	0	0

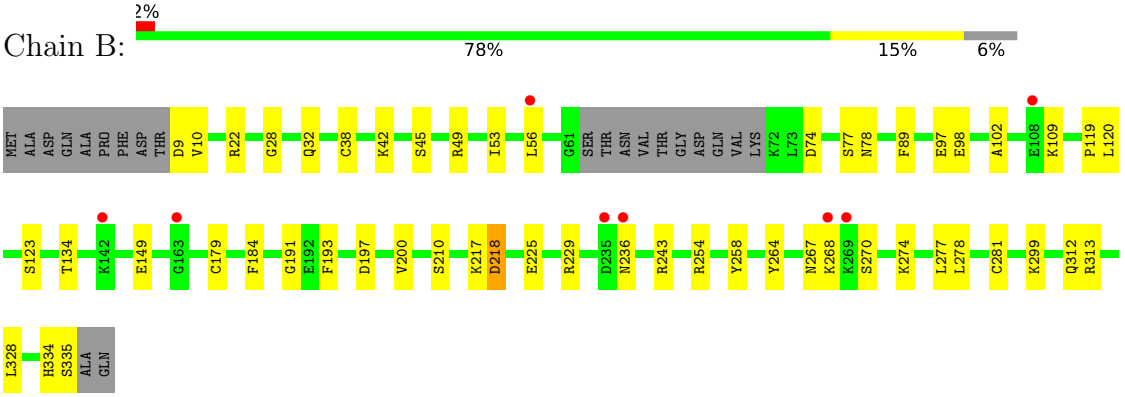
3 Residue-property plots

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 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.

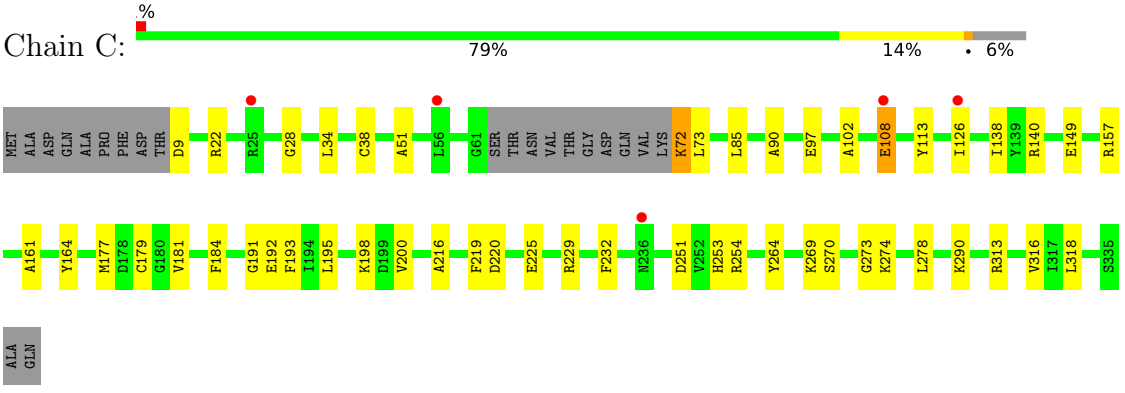
• Molecule 1: Fructose-1,6-bisphosphatase 1



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

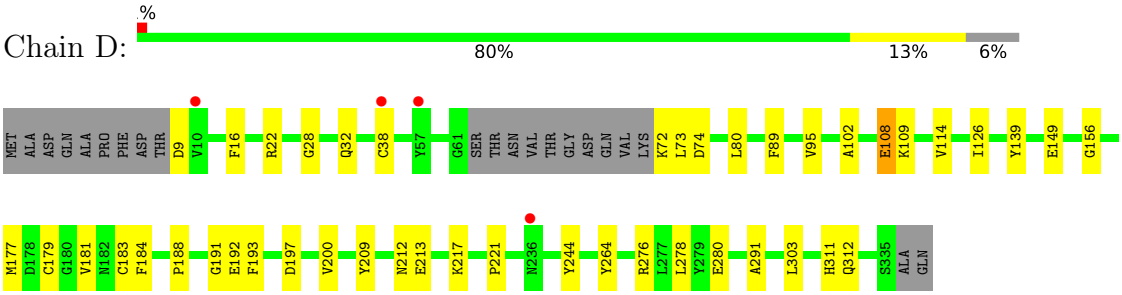


• Molecule 1: Fructose-1,6-bisphosphatase 1



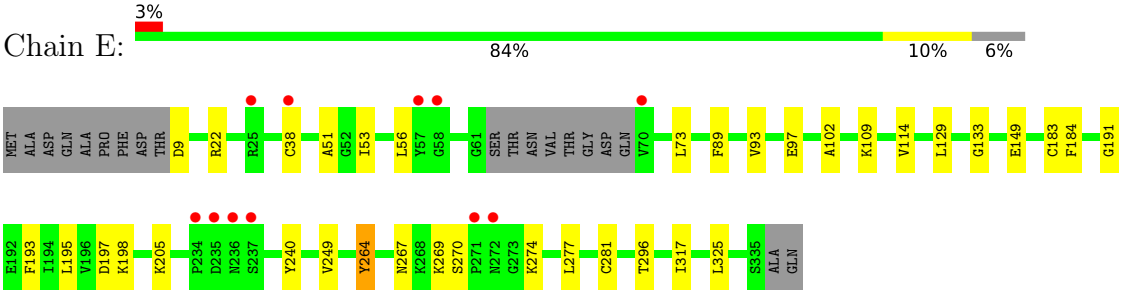
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain D:



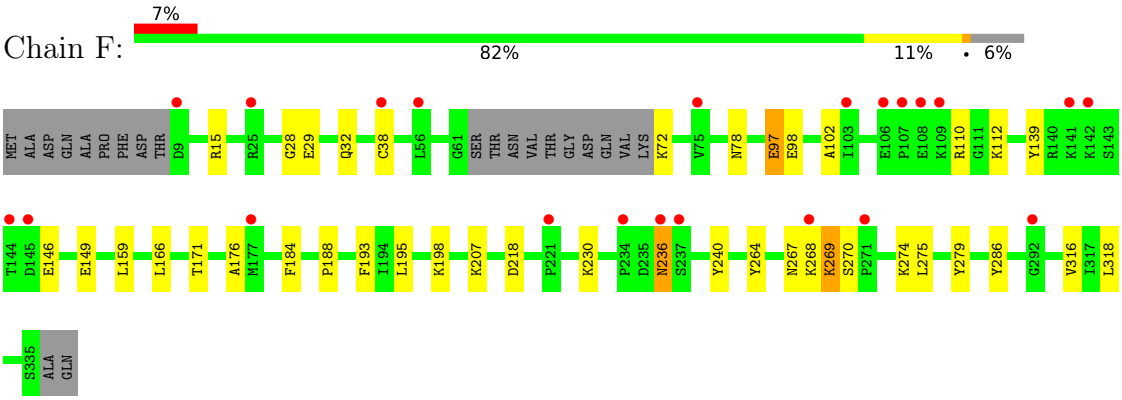
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain E:



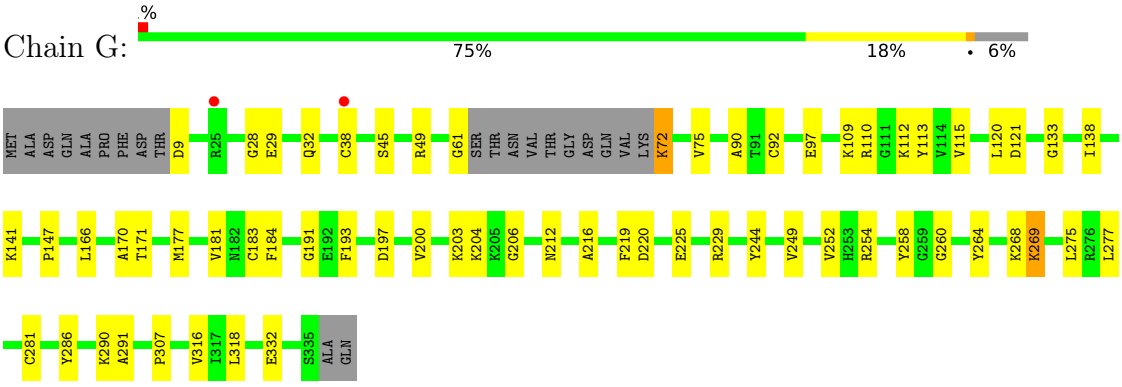
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain F:



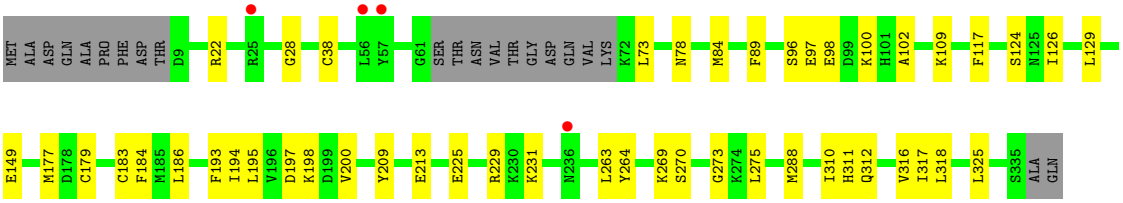
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain G:



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

Chain H:


MET ALA ASP GLN ALA PRO PHE ASP THR D9 R22 R25 G28 C38 L56 Y57 G61 SER THR ASN VAL THR GLY ASP GLN VAL LYS K72 L73 N78 M84 F89 S96 E97 E98 D99 K100 H101 A102 K109 F117 S124 N125 I126 L129
E149 M177 D178 C179 C183 F184 H185 L186 F193 I194 L195 V196 D197 K198 D199 V200 Y209 E213 E225 R229 K230 K231 N236 L263 Y264 K269 S270 G273 K274 L275 M288 I310 H311 Q312 V316 I317 L318 L325 S335 ALA GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.36Å 284.60Å 83.31Å 90.00° 97.71° 90.00°	Depositor
Resolution (Å)	29.90 – 2.75 29.90 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.90-2.75) 99.9 (29.90-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.179 , 0.251 0.179 , 0.251	Depositor DCC
R_{free} test set	3964 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19898	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 94S

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	0/2503	0.63	0/3378
1	B	0.43	0/2479	0.65	0/3347
1	C	0.47	0/2468	0.65	0/3333
1	D	0.47	0/2479	0.68	0/3347
1	E	0.40	0/2495	0.61	0/3368
1	F	0.42	0/2479	0.61	0/3347
1	G	0.48	1/2479 (0.0%)	0.64	0/3347
1	H	0.44	0/2468	0.64	0/3333
All	All	0.44	1/19850 (0.0%)	0.64	0/26800

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	281	CYS	CB-SG	-6.35	1.71	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2450	0	2501	23	0
1	B	2431	0	2478	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2425	0	2469	29	0
1	D	2431	0	2478	30	0
1	E	2447	0	2500	24	0
1	F	2430	0	2474	28	0
1	G	2430	0	2474	35	0
1	H	2425	0	2469	32	0
2	A	25	0	0	0	0
2	B	25	0	0	1	0
2	C	25	0	0	1	0
2	D	25	0	0	1	0
2	E	25	0	0	0	0
2	F	25	0	0	1	0
2	G	25	0	0	1	0
2	H	25	0	0	1	0
3	A	27	0	0	0	0
3	B	18	0	0	1	0
3	C	52	0	0	2	0
3	D	41	0	0	1	0
3	E	19	0	0	0	0
3	F	10	0	0	2	0
3	G	28	0	0	3	0
3	H	34	0	0	1	0
All	All	19898	0	19843	211	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 5.

All (211) 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:B:22:ARG:NH1	1:D:32:GLN:OE1	2.16	0.77
1:H:183:CYS:HB2	1:H:197:ASP:HB2	1.69	0.74
1:E:102:ALA:HB3	1:E:149:GLU:HG2	1.70	0.73
1:A:178:ASP:OD1	1:A:290:LYS:NZ	2.19	0.71
1:E:129:LEU:HD12	1:F:166:LEU:HD23	1.74	0.69
1:H:100:LYS:HD2	1:H:311:HIS:HD2	1.57	0.68
1:F:218:ASP:OD2	1:F:269:LYS:HD3	1.94	0.67
1:C:108:GLU:CD	1:C:108:GLU:H	1.98	0.67
1:E:184:PHE:HB3	1:E:193:PHE:HB3	1.76	0.67
1:F:110:ARG:NH1	1:F:146:GLU:OE2	2.28	0.66
1:D:183:CYS:HB2	1:D:197:ASP:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:269:LYS:NZ	3:F:501:HOH:O	2.22	0.66
1:D:102:ALA:HB3	1:D:149:GLU:HG2	1.78	0.65
1:H:225:GLU:OE2	1:H:229:ARG:NH2	2.29	0.65
1:A:274:LYS:HA	1:A:313:ARG:HD3	1.80	0.64
1:C:51:ALA:HA	1:D:188:PRO:HD2	1.78	0.63
1:F:102:ALA:HB3	1:F:149:GLU:HG2	1.81	0.62
1:B:53:ILE:HG13	1:B:56:LEU:HD12	1.80	0.62
1:C:9:ASP:N	3:C:503:HOH:O	2.32	0.61
1:G:275:LEU:HD12	1:G:316:VAL:HG11	1.83	0.61
1:H:184:PHE:HB3	1:H:193:PHE:HB3	1.81	0.61
1:B:78:ASN:HB2	1:B:98:GLU:HG3	1.81	0.60
1:C:274:LYS:O	1:C:313:ARG:NH1	2.34	0.60
1:E:267:ASN:OD1	1:E:270:SER:N	2.34	0.60
1:E:51:ALA:HA	1:F:188:PRO:HD2	1.84	0.59
1:G:204:LYS:NZ	3:G:506:HOH:O	2.35	0.59
1:H:100:LYS:HD2	1:H:311:HIS:CD2	2.36	0.59
1:D:89:PHE:CE1	1:D:109:LYS:HG2	2.37	0.59
1:G:115:VAL:HG22	1:G:138:ILE:HG12	1.85	0.58
1:E:191:GLY:HA3	1:G:191:GLY:HA3	1.85	0.58
1:D:184:PHE:HB3	1:D:193:PHE:HB3	1.85	0.58
1:A:93:VAL:HB	1:A:114:VAL:HG13	1.86	0.57
1:H:195:LEU:HD21	1:H:198:LYS:HG2	1.85	0.57
1:G:183:CYS:HB2	1:G:197:ASP:HB2	1.86	0.57
1:B:109:LYS:NZ	1:D:9:ASP:OD2	2.38	0.56
1:D:156:GLY:HA3	1:D:303:LEU:HD22	1.87	0.56
1:C:232:PHE:CE2	1:D:217:LYS:HA	2.41	0.56
1:C:157:ARG:NH2	3:C:504:HOH:O	2.38	0.56
1:A:42:LYS:NZ	1:C:192:GLU:OE1	2.38	0.55
1:F:139:TYR:HE1	1:F:159:LEU:HG	1.71	0.55
1:C:251:ASP:OD1	1:C:254:ARG:NH2	2.40	0.54
1:B:32:GLN:OE1	1:D:22:ARG:NH1	2.38	0.54
1:B:191:GLY:HA3	1:D:191:GLY:HA3	1.90	0.53
1:E:205:LYS:HE2	1:E:240:TYR:OH	2.08	0.53
1:G:61:GLY:O	3:G:501:HOH:O	2.19	0.53
1:B:184:PHE:HB3	1:B:193:PHE:HB3	1.90	0.53
1:H:28:GLY:HA2	2:H:401:94S:C5	2.38	0.53
1:C:270:SER:HB3	1:C:273:GLY:O	2.09	0.53
1:A:59:ILE:HA	1:B:10:VAL:HG11	1.91	0.53
1:G:277:LEU:HD23	1:G:307:PRO:HB3	1.91	0.53
1:B:28:GLY:HA2	2:B:401:94S:O16	2.08	0.52
1:F:218:ASP:O	1:F:267:ASN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:VAL:HB	1:E:114:VAL:HG13	1.92	0.51
1:D:89:PHE:HE1	1:D:109:LYS:HG2	1.75	0.51
1:H:100:LYS:O	1:H:310:ILE:HD11	2.11	0.51
1:A:239:PRO:HG3	1:B:217:LYS:HE3	1.93	0.51
1:E:133:GLY:HA3	1:E:249:VAL:HG21	1.93	0.51
1:H:275:LEU:HD12	1:H:316:VAL:HG11	1.92	0.51
1:A:181:VAL:HG21	1:A:291:ALA:HB2	1.93	0.50
1:G:29:GLU:OE2	1:G:112:LYS:N	2.40	0.50
1:E:109:LYS:NZ	1:G:9:ASP:OD2	2.44	0.50
1:D:177:MET:HE2	1:D:179:CYS:H	1.77	0.50
1:A:125:ASN:HD22	1:B:258:TYR:HE2	1.59	0.50
1:C:28:GLY:HA2	2:C:401:94S:O16	2.12	0.50
1:G:252:VAL:HG22	1:G:318:LEU:HD11	1.92	0.50
1:H:89:PHE:HE1	1:H:109:LYS:HG2	1.76	0.50
1:F:269:LYS:HB3	3:F:501:HOH:O	2.11	0.50
1:F:78:ASN:HB2	1:F:98:GLU:HG3	1.94	0.49
1:E:9:ASP:OD2	1:G:109:LYS:NZ	2.45	0.49
1:A:229:ARG:HH12	1:A:329:LYS:HE3	1.77	0.49
1:B:119:PRO:HA	1:B:134:THR:HG23	1.94	0.49
1:E:22:ARG:NH1	1:G:32:GLN:OE1	2.37	0.49
1:B:334:HIS:O	1:B:335:SER:HB2	2.13	0.48
1:G:216:ALA:HA	1:G:219:PHE:CD2	2.47	0.48
1:C:184:PHE:HB3	1:C:193:PHE:HB3	1.94	0.48
1:B:45:SER:O	1:B:49:ARG:HD3	2.13	0.48
1:D:73:LEU:HD23	1:D:126:ILE:HD13	1.94	0.48
1:A:90:ALA:O	1:A:113:TYR:HB2	2.14	0.48
1:G:275:LEU:HD12	1:G:316:VAL:CG1	2.44	0.48
1:E:277:LEU:HD12	1:E:281:CYS:HB2	1.96	0.48
1:E:73:LEU:HD23	1:E:73:LEU:HA	1.75	0.48
1:G:183:CYS:SG	1:G:200:VAL:HG21	2.54	0.48
1:A:206:GLY:HA3	1:A:260:GLY:N	2.29	0.47
1:B:89:PHE:CD2	1:B:109:LYS:HA	2.48	0.47
1:H:184:PHE:HA	1:H:194:ILE:O	2.14	0.47
1:H:325:LEU:HD23	1:H:325:LEU:HA	1.75	0.47
1:A:45:SER:O	1:A:49:ARG:HD3	2.13	0.47
1:C:72:LYS:HD3	1:C:72:LYS:N	2.29	0.47
1:F:166:LEU:O	1:F:171:THR:HA	2.14	0.47
1:C:102:ALA:HB3	1:C:149:GLU:HG2	1.97	0.47
1:F:236:ASN:ND2	1:F:236:ASN:O	2.39	0.47
1:G:133:GLY:HA3	1:G:249:VAL:HG21	1.97	0.47
1:H:197:ASP:HB3	1:H:200:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:SER:HB2	1:H:117:PHE:CZ	2.50	0.47
1:C:138:ILE:HD12	1:C:161:ALA:HB3	1.95	0.47
1:D:102:ALA:CB	1:D:149:GLU:HG2	2.45	0.47
1:G:110:ARG:HD3	1:G:147:PRO:HG3	1.97	0.47
1:B:225:GLU:O	1:B:229:ARG:HG3	2.14	0.47
1:G:212:ASN:HB2	1:G:244:TYR:CE2	2.50	0.47
1:G:225:GLU:O	1:G:229:ARG:HG3	2.15	0.47
1:A:267:ASN:OD1	1:A:270:SER:N	2.47	0.46
1:A:184:PHE:HB3	1:A:193:PHE:HB3	1.96	0.46
1:B:236:ASN:O	1:B:236:ASN:ND2	2.48	0.46
1:D:114:VAL:HB	1:D:139:TYR:HB2	1.97	0.46
1:F:316:VAL:CG2	1:F:318:LEU:HD23	2.46	0.46
1:H:213:GLU:OE2	1:H:231:LYS:NZ	2.34	0.46
1:E:89:PHE:HD2	1:E:109:LYS:HA	1.81	0.46
1:C:225:GLU:O	1:C:229:ARG:HG3	2.15	0.46
1:B:42:LYS:NZ	1:D:192:GLU:HG2	2.31	0.46
1:E:277:LEU:HA	1:E:281:CYS:HB2	1.97	0.45
1:C:90:ALA:O	1:C:113:TYR:HB2	2.17	0.45
1:H:102:ALA:HB3	1:H:149:GLU:HG2	1.99	0.45
1:H:288:MET:HG3	1:H:318:LEU:HD13	1.98	0.45
1:B:120:LEU:HG	1:B:123:SER:HB3	1.99	0.45
1:D:108:GLU:H	1:D:108:GLU:CD	2.19	0.45
1:H:149:GLU:OE1	3:H:501:HOH:O	2.21	0.45
1:H:209:TYR:OH	1:H:231:LYS:NZ	2.49	0.45
1:B:267:ASN:OD1	1:B:270:SER:N	2.49	0.45
1:D:212:ASN:HB2	1:D:244:TYR:CE2	2.51	0.45
1:E:183:CYS:HB2	1:E:197:ASP:HB2	1.99	0.45
1:H:73:LEU:HD23	1:H:126:ILE:HD13	1.98	0.45
1:D:276:ARG:NH1	1:D:311:HIS:O	2.50	0.45
1:B:102:ALA:HB3	1:B:149:GLU:HG2	1.99	0.45
1:G:166:LEU:O	1:G:171:THR:HA	2.17	0.45
1:B:274:LYS:HA	1:B:313:ARG:HD3	1.98	0.44
1:B:89:PHE:CE2	1:B:109:LYS:HG2	2.53	0.44
1:F:184:PHE:HB3	1:F:193:PHE:HB3	1.97	0.44
1:C:164:TYR:OH	1:C:253:HIS:ND1	2.39	0.44
1:G:203:LYS:HD2	1:G:258:TYR:O	2.18	0.44
1:G:286:TYR:CZ	1:G:290:LYS:HE3	2.53	0.44
1:B:197:ASP:HB3	1:B:200:VAL:CG1	2.48	0.44
1:B:274:LYS:O	1:B:313:ARG:NH1	2.50	0.44
1:G:90:ALA:O	1:G:113:TYR:HB2	2.17	0.44
1:C:195:LEU:CD2	1:C:198:LYS:HE2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:VAL:HB	1:C:200:VAL:HG22	1.98	0.44
1:D:276:ARG:O	1:D:280:GLU:HB2	2.17	0.44
1:D:74:ASP:OD1	1:D:74:ASP:N	2.51	0.44
1:B:299:LYS:NZ	3:B:508:HOH:O	2.50	0.44
1:D:181:VAL:HG21	1:D:291:ALA:HB2	1.99	0.44
1:H:225:GLU:O	1:H:229:ARG:HG3	2.17	0.44
1:E:195:LEU:HD21	1:E:198:LYS:HG2	1.98	0.44
1:G:181:VAL:HG21	1:G:291:ALA:HB2	2.00	0.44
1:A:266:ALA:HB2	1:A:315:PRO:HG3	2.00	0.44
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.74	0.44
1:C:316:VAL:CG2	1:C:318:LEU:HD23	2.47	0.44
1:B:74:ASP:OD1	1:B:74:ASP:N	2.51	0.43
1:E:325:LEU:HD23	1:E:325:LEU:HA	1.81	0.43
1:H:270:SER:HB3	1:H:273:GLY:O	2.17	0.43
1:E:56:LEU:HA	1:E:56:LEU:HD23	1.87	0.43
1:B:334:HIS:O	1:F:207:LYS:NZ	2.52	0.43
1:G:269:LYS:HB3	1:G:269:LYS:HE3	1.48	0.43
1:E:264:TYR:CE1	1:E:274:LYS:HB2	2.54	0.43
1:G:121:ASP:N	1:G:133:GLY:O	2.42	0.43
1:H:263:LEU:HD23	1:H:317:ILE:HG12	2.00	0.43
1:A:59:ILE:HG23	1:D:80:LEU:HD21	2.00	0.43
1:C:34:LEU:HA	1:C:34:LEU:HD23	1.84	0.43
1:C:85:LEU:HA	1:C:85:LEU:HD23	1.68	0.43
1:B:278:LEU:HD13	1:B:278:LEU:HA	1.88	0.42
1:F:195:LEU:HD21	1:F:198:LYS:HG2	2.01	0.42
1:H:89:PHE:CE1	1:H:109:LYS:HG2	2.54	0.42
1:F:97:GLU:HG3	1:F:279:TYR:HE1	1.84	0.42
1:B:210:SER:HA	1:B:243:ARG:O	2.19	0.42
1:G:206:GLY:HA3	1:G:260:GLY:N	2.33	0.42
1:D:221:PRO:O	3:D:501:HOH:O	2.22	0.42
1:G:72:LYS:HB3	1:G:75:VAL:HB	2.00	0.42
1:E:53:ILE:HD12	1:E:56:LEU:HD12	2.01	0.42
1:F:15:ARG:NH2	1:H:84:MET:HE3	2.34	0.42
1:B:277:LEU:HA	1:B:281:CYS:HB2	2.01	0.42
1:C:216:ALA:HA	1:C:219:PHE:CD2	2.54	0.42
1:G:184:PHE:HB3	1:G:193:PHE:HB3	2.02	0.42
1:A:204:LYS:O	1:A:320:SER:HB3	2.20	0.42
1:B:218:ASP:HB2	1:B:267:ASN:HB2	2.02	0.42
1:C:316:VAL:HG22	1:C:318:LEU:HD23	2.01	0.42
1:G:120:LEU:HA	1:G:120:LEU:HD12	1.82	0.42
1:A:89:PHE:CD2	1:A:109:LYS:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:HA	1:A:227:ILE:HD13	1.82	0.41
1:H:78:ASN:HB2	1:H:98:GLU:HG3	2.02	0.41
1:F:316:VAL:HG21	1:F:318:LEU:HD23	2.01	0.41
1:H:186:LEU:HB2	1:H:193:PHE:CE1	2.56	0.41
1:A:191:GLY:HA3	1:C:191:GLY:HA3	2.02	0.41
1:F:275:LEU:HD12	1:F:316:VAL:HG11	2.03	0.41
1:A:128:CYS:SG	1:B:254:ARG:HG3	2.61	0.41
1:F:270:SER:CB	1:F:274:LYS:HE3	2.51	0.41
1:G:268:LYS:NZ	3:G:507:HOH:O	2.36	0.41
1:H:177:MET:HE3	1:H:179:CYS:SG	2.61	0.41
1:A:74:ASP:OD1	1:A:74:ASP:N	2.53	0.41
1:F:102:ALA:CB	1:F:149:GLU:HG2	2.48	0.41
1:F:176:ALA:O	1:F:286:TYR:HE1	2.03	0.41
1:B:89:PHE:HD2	1:B:109:LYS:HA	1.85	0.41
1:A:29:GLU:HG3	1:C:22:ARG:HH12	1.86	0.41
1:G:45:SER:O	1:G:49:ARG:HD3	2.21	0.41
1:D:28:GLY:HA2	2:D:401:94S:C5	2.51	0.41
1:E:296:THR:HG23	1:E:317:ILE:HB	2.02	0.41
1:C:73:LEU:HD23	1:C:126:ILE:CD1	2.51	0.41
1:D:16:PHE:CD1	1:D:16:PHE:C	2.94	0.41
1:F:28:GLY:HA2	2:F:401:94S:O16	2.20	0.41
1:B:9:ASP:OD2	1:D:109:LYS:NZ	2.30	0.41
1:F:274:LYS:HA	1:F:274:LYS:HE2	2.02	0.41
1:G:92:CYS:SG	1:G:141:LYS:HD2	2.61	0.41
1:G:170:ALA:HB3	1:H:129:LEU:HD22	2.03	0.41
1:E:89:PHE:CE2	1:E:109:LYS:HG2	2.56	0.40
1:F:32:GLN:OE1	1:H:22:ARG:NH1	2.49	0.40
1:B:77:SER:HB3	1:B:119:PRO:HB2	2.03	0.40
1:C:290:LYS:HA	1:C:290:LYS:HD3	1.91	0.40
1:D:209:TYR:OH	1:D:213:GLU:OE2	2.29	0.40
1:F:230:LYS:HB3	1:F:240:TYR:HB2	2.03	0.40
1:F:29:GLU:HG3	1:H:22:ARG:HH12	1.86	0.40
1:C:269:LYS:HB2	1:C:269:LYS:HE3	1.69	0.40
1:D:95:VAL:HG11	1:D:278:LEU:HD23	2.03	0.40
1:G:28:GLY:HA2	2:G:401:94S:C5	2.52	0.40
1:H:197:ASP:HB3	1:H:200:VAL:HG11	2.03	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	317/338 (94%)	305 (96%)	12 (4%)	0	100	100
1	B	314/338 (93%)	300 (96%)	14 (4%)	0	100	100
1	C	313/338 (93%)	301 (96%)	12 (4%)	0	100	100
1	D	314/338 (93%)	304 (97%)	10 (3%)	0	100	100
1	E	316/338 (94%)	306 (97%)	10 (3%)	0	100	100
1	F	314/338 (93%)	303 (96%)	11 (4%)	0	100	100
1	G	314/338 (93%)	304 (97%)	10 (3%)	0	100	100
1	H	313/338 (93%)	304 (97%)	9 (3%)	0	100	100
All	All	2515/2704 (93%)	2427 (96%)	88 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	268/281 (95%)	263 (98%)	5 (2%)	60	77
1	B	265/281 (94%)	258 (97%)	7 (3%)	49	71
1	C	264/281 (94%)	254 (96%)	10 (4%)	36	60
1	D	265/281 (94%)	259 (98%)	6 (2%)	53	74
1	E	267/281 (95%)	263 (98%)	4 (2%)	67	82
1	F	265/281 (94%)	257 (97%)	8 (3%)	44	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	265/281 (94%)	256 (97%)	9 (3%)	40 64
1	H	264/281 (94%)	258 (98%)	6 (2%)	53 74
All	All	2123/2248 (94%)	2068 (97%)	55 (3%)	49 71

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	CYS
1	A	97	GLU
1	A	108	GLU
1	A	264	TYR
1	A	268	LYS
1	B	38	CYS
1	B	97	GLU
1	B	179	CYS
1	B	218	ASP
1	B	264	TYR
1	B	268	LYS
1	B	312	GLN
1	C	38	CYS
1	C	72	LYS
1	C	97	GLU
1	C	108	GLU
1	C	140	ARG
1	C	177	MET
1	C	179	CYS
1	C	220	ASP
1	C	264	TYR
1	C	278	LEU
1	D	38	CYS
1	D	72	LYS
1	D	108	GLU
1	D	200	VAL
1	D	264	TYR
1	D	312	GLN
1	E	38	CYS
1	E	97	GLU
1	E	264	TYR
1	E	269	LYS
1	F	38	CYS
1	F	72	LYS

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Mol	Chain	Res	Type
1	F	97	GLU
1	F	112	LYS
1	F	236	ASN
1	F	264	TYR
1	F	268	LYS
1	F	269	LYS
1	G	38	CYS
1	G	72	LYS
1	G	97	GLU
1	G	177	MET
1	G	220	ASP
1	G	254	ARG
1	G	264	TYR
1	G	269	LYS
1	G	332	GLU
1	H	38	CYS
1	H	97	GLU
1	H	124	SER
1	H	264	TYR
1	H	269	LYS
1	H	312	GLN

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)

8 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	94S	A	401	-	23,26,26	0.86	1 (4%)	28,37,37	0.70	1 (3%)
2	94S	B	401	-	23,26,26	0.60	0	28,37,37	0.77	1 (3%)
2	94S	C	401	-	23,26,26	1.00	1 (4%)	28,37,37	0.85	2 (7%)
2	94S	D	401	-	23,26,26	0.87	1 (4%)	28,37,37	0.71	1 (3%)
2	94S	E	401	-	23,26,26	1.19	2 (8%)	28,37,37	0.72	1 (3%)
2	94S	F	401	-	23,26,26	0.59	0	28,37,37	0.66	1 (3%)
2	94S	G	401	-	23,26,26	0.59	0	28,37,37	0.76	1 (3%)
2	94S	H	401	-	23,26,26	0.93	2 (8%)	28,37,37	0.64	1 (3%)

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	94S	A	401	-	-	0/19/21/21	0/2/2/2
2	94S	B	401	-	-	0/19/21/21	0/2/2/2
2	94S	C	401	-	-	0/19/21/21	0/2/2/2
2	94S	D	401	-	-	0/19/21/21	0/2/2/2
2	94S	E	401	-	-	0/19/21/21	0/2/2/2
2	94S	F	401	-	-	0/19/21/21	0/2/2/2
2	94S	G	401	-	-	0/19/21/21	0/2/2/2
2	94S	H	401	-	-	0/19/21/21	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	94S	C12-C9	-2.91	1.33	1.39
2	H	401	94S	C12-C9	-2.76	1.34	1.39
2	H	401	94S	C2-N6	2.09	1.40	1.36
2	A	401	94S	C2-N6	2.79	1.41	1.36
2	D	401	94S	C2-N6	3.18	1.42	1.36
2	C	401	94S	C2-N6	3.38	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	94S	C2-N6	3.97	1.43	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	94S	N3-C5-N6	2.19	117.91	114.74
2	G	401	94S	BR2-C8-C11	2.19	127.73	124.38
2	H	401	94S	BR2-C8-C11	2.19	127.73	124.38
2	F	401	94S	BR2-C8-C11	2.26	127.85	124.38
2	B	401	94S	BR2-C8-C11	2.29	127.89	124.38
2	A	401	94S	BR2-C8-C11	2.39	128.04	124.38
2	E	401	94S	BR2-C8-C11	2.51	128.22	124.38
2	C	401	94S	BR2-C8-C11	2.51	128.23	124.38
2	D	401	94S	BR2-C8-C11	2.56	128.31	124.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	94S	1	0
2	C	401	94S	1	0
2	D	401	94S	1	0
2	F	401	94S	1	0
2	G	401	94S	1	0
2	H	401	94S	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	319/338 (94%)	-0.17	7 (2%)	62	58	28, 50, 88, 124	0
1	B	317/338 (93%)	-0.06	8 (2%)	57	52	28, 55, 98, 158	0
1	C	317/338 (93%)	-0.28	5 (1%)	72	69	24, 45, 80, 143	0
1	D	317/338 (93%)	-0.30	4 (1%)	77	74	26, 41, 74, 121	0
1	E	319/338 (94%)	0.08	11 (3%)	45	40	38, 63, 101, 151	0
1	F	317/338 (93%)	0.19	22 (6%)	17	13	37, 65, 109, 146	0
1	G	317/338 (93%)	-0.22	2 (0%)	89	88	25, 48, 81, 118	0
1	H	317/338 (93%)	-0.15	4 (1%)	77	74	34, 52, 90, 114	0
All	All	2540/2704 (93%)	-0.11	63 (2%)	57	52	24, 53, 93, 158	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	70	VAL	10.2
1	A	70	VAL	5.8
1	F	107	PRO	5.0
1	F	237	SER	4.9
1	F	236	ASN	4.5
1	A	268	LYS	4.3
1	E	271	PRO	4.1
1	E	236	ASN	3.9
1	D	236	ASN	3.9
1	E	234	PRO	3.8
1	F	106	GLU	3.7
1	F	56	LEU	3.5
1	F	271	PRO	3.5
1	B	268	LYS	3.4
1	H	25	ARG	3.3
1	F	109	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	38	CYS	3.3
1	F	25	ARG	3.3
1	C	236	ASN	3.2
1	F	234	PRO	3.2
1	G	38	CYS	3.2
1	E	235	ASP	3.1
1	C	25	ARG	3.1
1	F	268	LYS	3.1
1	H	236	ASN	3.0
1	A	234	PRO	3.0
1	C	126	ILE	2.9
1	B	108	GLU	2.8
1	F	9	ASP	2.8
1	A	25	ARG	2.8
1	B	56	LEU	2.7
1	H	57	TYR	2.7
1	C	108	GLU	2.7
1	B	269	LYS	2.7
1	E	25	ARG	2.6
1	E	272	ASN	2.6
1	C	56	LEU	2.6
1	F	145	ASP	2.5
1	E	237	SER	2.5
1	B	142	LYS	2.5
1	A	236	ASN	2.5
1	A	144	THR	2.4
1	H	56	LEU	2.4
1	E	57	TYR	2.4
1	F	221	PRO	2.4
1	G	25	ARG	2.4
1	D	10	VAL	2.4
1	F	108	GLU	2.4
1	F	75	VAL	2.3
1	F	177	MET	2.2
1	F	144	THR	2.2
1	E	58	GLY	2.2
1	F	141	LYS	2.2
1	F	292	GLY	2.2
1	A	146	GLU	2.1
1	B	163	GLY	2.1
1	F	103	ILE	2.1
1	F	142	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	236	ASN	2.1
1	B	235	ASP	2.1
1	D	57	TYR	2.0
1	D	38	CYS	2.0
1	E	38	CYS	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	94S	F	401	25/25	0.95	0.16	58,75,92,95	1
2	94S	H	401	25/25	0.95	0.18	61,80,95,100	1
2	94S	B	401	25/25	0.96	0.14	51,65,79,81	1
2	94S	D	401	25/25	0.96	0.14	46,63,76,83	1
2	94S	C	401	25/25	0.97	0.14	40,60,76,78	1
2	94S	A	401	25/25	0.97	0.13	25,52,68,76	1
2	94S	G	401	25/25	0.97	0.14	49,72,87,94	1
2	94S	E	401	25/25	0.97	0.14	48,67,86,93	1

6.5 Other polymers (i)

There are no such residues in this entry.