



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2019 – 08:00 PM EST

PDB ID : 5Q07
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-(4-bromo-6-morpholin-4-ylpyridin-2-yl)-3-[5-(2-methoxyethyl)-4-methylthiophen-2-yl]sulfonyleurea
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 : 2017-04-16
Resolution : 2.42 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

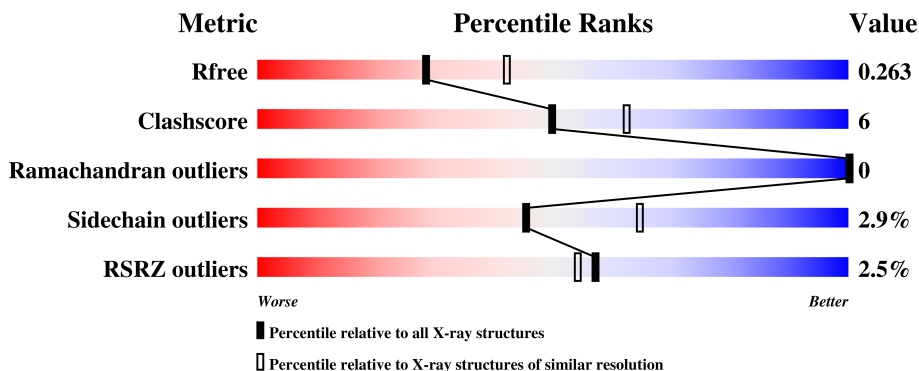
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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.



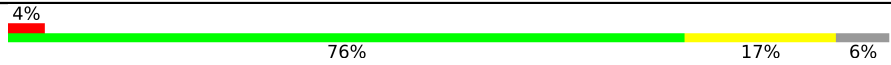


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	4090 (2.44-2.40)
Clashscore	122126	4587 (2.44-2.40)
Ramachandran outliers	120053	4522 (2.44-2.40)
Sidechain outliers	120020	4523 (2.44-2.40)
RSRZ outliers	108989	3987 (2.44-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	
1	B	338	
1	C	338	
1	D	338	
1	E	338	

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Mol	Chain	Length	Quality of chain
1	F	338	 4% 76% 17% 6%
1	G	338	 79% 14% 6%
1	H	338	 2% 80% 14% 6%

2 Entry composition [i](#)

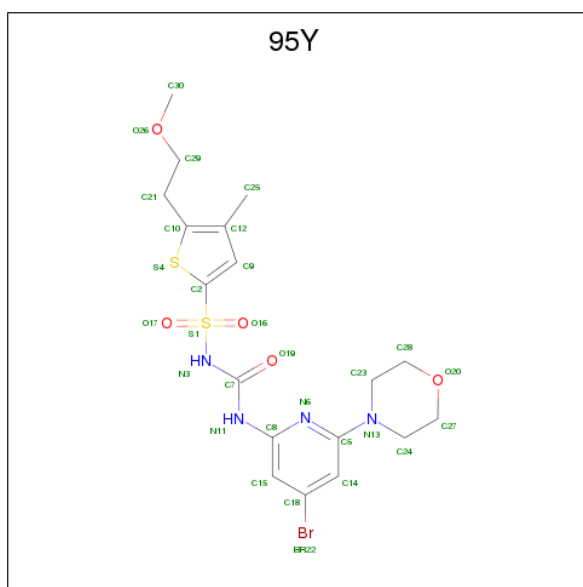
There are 3 unique types of molecules in this entry. The entry contains 20402 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	319	2446	1558	412	459	17	0	1	0
1	B	317	2431	1548	409	457	17	0	1	0
1	C	317	2425	1545	406	457	17	0	0	0
1	D	317	2431	1548	409	457	17	0	1	0
1	E	319	2447	1559	412	459	17	0	1	0
1	F	317	2430	1547	409	457	17	0	1	0
1	G	317	2430	1547	409	457	17	0	1	0
1	H	317	2425	1545	406	457	17	0	0	0

- Molecule 2 is N-{{4-bromo-6-(morpholin-4-yl)pyridin-2-yl}carbonyl}-5-(2-methoxyethyl)-4-methylthiophene-2-sulfonamide (three-letter code: 95Y) (formula: C₁₈H₂₃BrN₄O₅S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	Br	C	N	O			S
2	A	1	Total 30	Br 1	C 18	N 4	O 5	S 2	0	0
2	B	1	Total 30	Br 1	C 18	N 4	O 5	S 2	0	0
2	C	1	Total 30	Br 1	C 18	N 4	O 5	S 2	0	0
2	D	1	Total 30	Br 1	C 18	N 4	O 5	S 2	0	0
2	E	1	Total 30	Br 1	C 18	N 4	O 5	S 2	0	0
2	F	1	Total 30	Br 1	C 18	N 4	O 5	S 2	0	0
2	G	1	Total 30	Br 1	C 18	N 4	O 5	S 2	0	0
2	H	1	Total 30	Br 1	C 18	N 4	O 5	S 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total 92	O 92	0	0
3	B	72	Total 72	O 72	0	0
3	C	93	Total 93	O 93	0	0
3	D	118	Total 118	O 118	0	0

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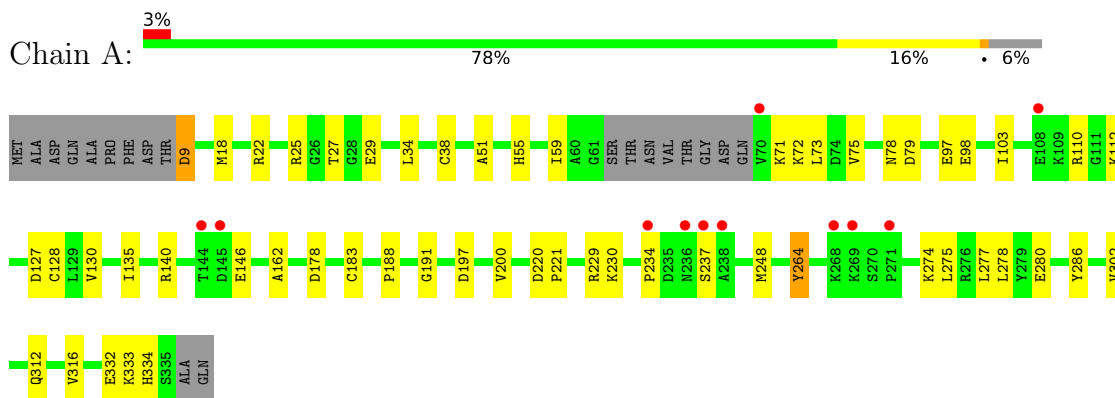
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	79	Total 79	O 79	0	0
3	F	61	Total 61	O 61	0	0
3	G	99	Total 99	O 99	0	0
3	H	83	Total 83	O 83	0	0

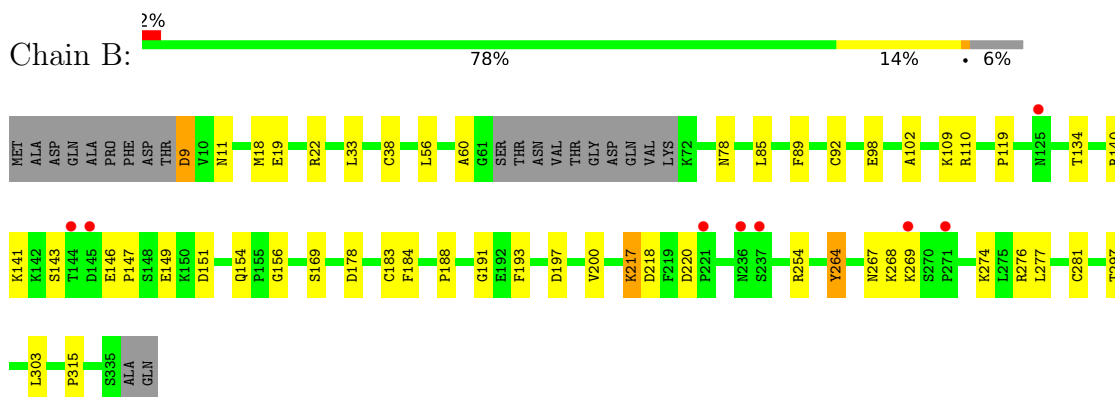
3 Residue-property plots i

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

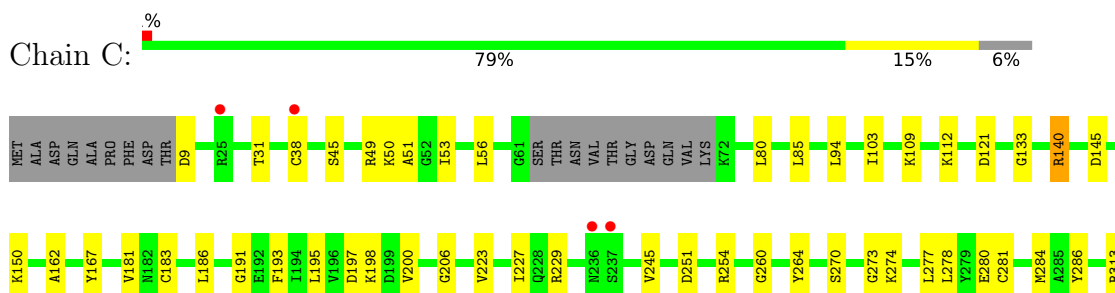
- Molecule 1: Fructose-1,6-bisphosphatase 1

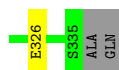


- Molecule 1: Fructose-1,6-bisphosphatase 1

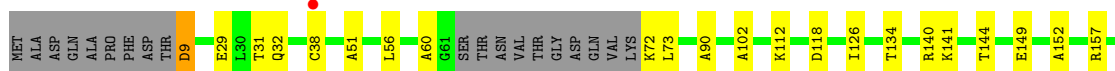
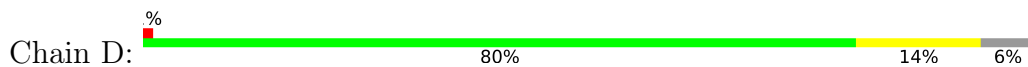


- Molecule 1: Fructose-1,6-bisphosphatase 1

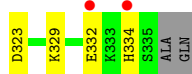
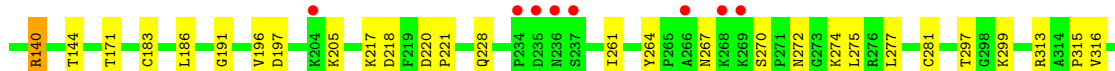
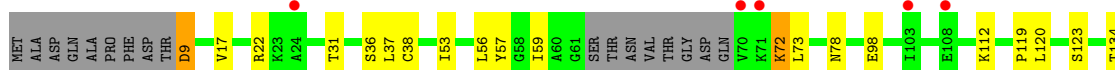
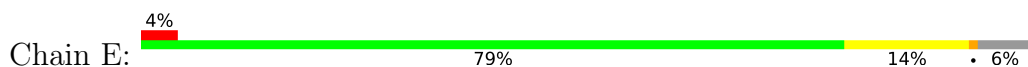




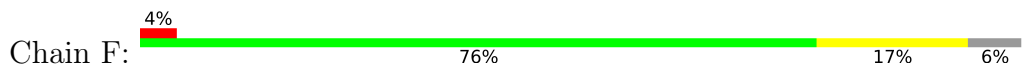
- Molecule 1: Fructose-1,6-bisphosphatase 1



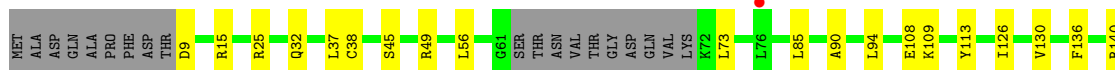
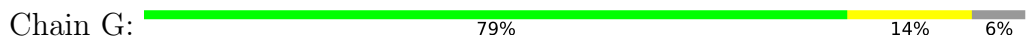
- Molecule 1: Fructose-1,6-bisphosphatase 1



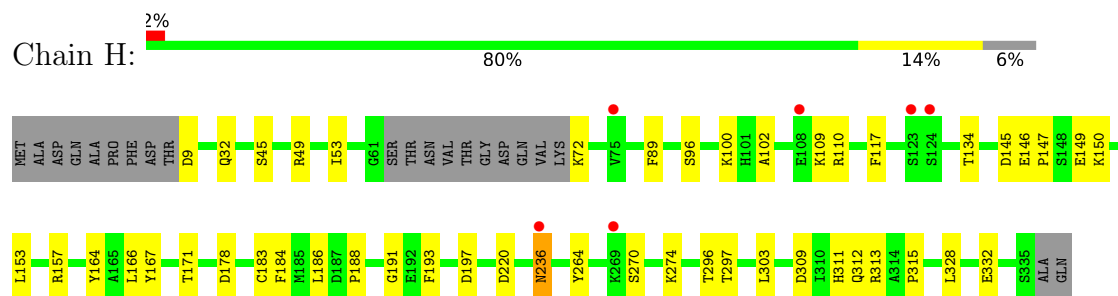
- Molecule 1: Fructose-1,6-bisphosphatase 1



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.19Å 284.51Å 83.23Å 90.00° 97.66° 90.00°	Depositor
Resolution (Å)	29.87 – 2.42 29.87 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.87-2.42) 99.1 (29.87-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.42Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.200 , 0.263 0.200 , 0.263	Depositor DCC
R_{free} test set	5702 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtrriage
Anisotropy	0.436	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20402	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 95Y

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	0.41	0/2495	0.62	0/3368
1	B	0.40	0/2479	0.61	0/3347
1	C	0.44	0/2468	0.64	0/3333
1	D	0.46	0/2479	0.64	0/3347
1	E	0.39	0/2495	0.61	1/3368 (0.0%)
1	F	0.37	0/2479	0.57	0/3347
1	G	0.43	0/2479	0.62	0/3347
1	H	0.42	0/2468	0.64	1/3333 (0.0%)
All	All	0.42	0/19842	0.62	2/26790 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	37	LEU	CA-CB-CG	6.14	129.42	115.30
1	H	220	ASP	CB-CG-OD1	5.72	123.45	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2446	0	2496	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2431	0	2478	35	0
1	C	2425	0	2469	29	0
1	D	2431	0	2478	31	0
1	E	2447	0	2500	30	0
1	F	2430	0	2474	39	0
1	G	2430	0	2474	34	0
1	H	2425	0	2469	31	0
2	A	30	0	0	1	0
2	B	30	0	0	0	0
2	C	30	0	0	0	0
2	D	30	0	0	0	0
2	E	30	0	0	1	0
2	F	30	0	0	0	0
2	G	30	0	0	0	0
2	H	30	0	0	0	0
3	A	92	0	0	14	0
3	B	72	0	0	7	0
3	C	93	0	0	1	0
3	D	118	0	0	10	0
3	E	79	0	0	5	0
3	F	61	0	0	6	0
3	G	99	0	0	6	0
3	H	83	0	0	4	0
All	All	20402	0	19838	248	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 6.

All (248) 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:E:191:GLY:HA3	1:G:191:GLY:HA3	1.55	0.89
1:G:130:VAL:O	3:G:501:HOH:O	1.92	0.86
1:E:205:LYS:NZ	3:E:501:HOH:O	2.09	0.85
1:C:251:ASP:OD1	1:C:254:ARG:NH2	2.13	0.81
1:A:191:GLY:HA3	1:C:191:GLY:HA3	1.64	0.79
1:B:102:ALA:HB3	1:B:149:GLU:HG2	1.66	0.76
1:D:102:ALA:HB3	1:D:149:GLU:HG2	1.67	0.75
1:F:296:THR:HG21	1:F:328:LEU:HD21	1.68	0.74
1:E:297:THR:HB	1:E:315:PRO:HG2	1.69	0.73
1:D:118:ASP:OD2	3:D:501:HOH:O	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLN:O	3:A:501:HOH:O	2.07	0.72
1:F:110:ARG:NH1	1:F:146:GLU:OE2	2.22	0.71
1:A:9:ASP:OD2	1:C:109:LYS:NZ	2.23	0.71
1:F:19:GLU:HG3	1:H:32:GLN:HE22	1.56	0.70
1:B:141:LYS:HE3	1:B:143:SER:O	1.93	0.69
1:G:183:CYS:HB2	1:G:197:ASP:HB2	1.74	0.69
1:E:217:LYS:NZ	3:E:505:HOH:O	2.27	0.68
1:B:9:ASP:N	3:B:501:HOH:O	2.28	0.67
1:B:191:GLY:HA3	1:D:191:GLY:HA3	1.75	0.67
1:E:299:LYS:O	3:E:502:HOH:O	2.11	0.67
1:F:61:GLY:O	3:F:501:HOH:O	2.12	0.67
1:E:53:ILE:HG13	1:E:56:LEU:HD12	1.76	0.67
1:E:228:GLN:NE2	3:E:506:HOH:O	2.27	0.66
1:B:156:GLY:HA3	1:B:303:LEU:HD22	1.78	0.66
1:A:127:ASP:OD2	3:A:502:HOH:O	2.14	0.65
1:D:51:ALA:O	3:D:502:HOH:O	2.14	0.65
1:B:119:PRO:HA	1:B:134:THR:HG23	1.78	0.65
1:H:183:CYS:HB2	1:H:197:ASP:HB2	1.78	0.65
1:D:152:ALA:O	3:D:503:HOH:O	2.15	0.64
1:A:230:LYS:NZ	3:A:512:HOH:O	2.30	0.64
1:F:183:CYS:HB2	1:F:197:ASP:HB2	1.79	0.64
1:B:109:LYS:NZ	1:D:9:ASP:OD2	2.27	0.63
1:F:191:GLY:HA3	1:H:191:GLY:HA3	1.80	0.63
1:G:113:TYR:OH	1:G:140[B]:ARG:NH2	2.32	0.63
1:A:280:GLU:OE2	3:A:503:HOH:O	2.15	0.63
1:A:302:VAL:O	3:A:504:HOH:O	2.15	0.63
1:G:251:ASP:OD1	1:G:254:ARG:NH2	2.32	0.63
1:H:236:ASN:OD1	1:H:236:ASN:N	2.33	0.62
1:F:157:ARG:NH2	3:F:505:HOH:O	2.26	0.62
1:F:29:GLU:OE2	3:F:502:HOH:O	2.16	0.61
1:B:183:CYS:HB2	1:B:197:ASP:HB2	1.83	0.61
1:F:119:PRO:HA	1:F:134:THR:HG23	1.83	0.61
1:E:72:LYS:HE2	1:E:72:LYS:HA	1.83	0.60
1:F:156:GLY:HA3	1:F:303:LEU:HD22	1.83	0.60
1:H:89:PHE:HE1	1:H:109:LYS:HG2	1.66	0.60
1:F:113:TYR:OH	1:F:140[B]:ARG:NH1	2.34	0.60
1:A:237:SER:O	3:A:505:HOH:O	2.16	0.60
1:H:89:PHE:CE1	1:H:109:LYS:HG2	2.36	0.60
1:B:110:ARG:NH1	1:B:146:GLU:OE2	2.27	0.59
1:H:100:LYS:O	1:H:311:HIS:NE2	2.35	0.59
1:G:229:ARG:NH1	3:G:503:HOH:O	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLU:OE1	3:A:506:HOH:O	2.17	0.58
1:E:9:ASP:OD2	1:G:109:LYS:NZ	2.36	0.58
1:E:218:ASP:O	1:E:267:ASN:HB2	2.04	0.58
1:E:274:LYS:O	1:E:313:ARG:NH1	2.36	0.58
1:H:150:LYS:NZ	3:H:502:HOH:O	2.22	0.58
1:H:178:ASP:O	3:H:501:HOH:O	2.17	0.57
1:C:245:VAL:HG23	1:C:254:ARG:HH21	1.68	0.57
1:A:178:ASP:O	3:A:507:HOH:O	2.17	0.57
1:F:33:LEU:HD11	1:F:85:LEU:HD22	1.84	0.57
1:B:267:ASN:ND2	3:B:502:HOH:O	2.30	0.57
1:E:22:ARG:NH1	1:G:32:GLN:OE1	2.37	0.57
1:F:13:LEU:HD22	1:F:173:LEU:HD13	1.86	0.56
1:A:71:LYS:HD3	1:A:75:VAL:HG12	1.88	0.56
1:H:186:LEU:HB2	1:H:193:PHE:CE1	2.40	0.56
1:D:277:LEU:HA	1:D:281:CYS:HB2	1.88	0.56
1:C:195:LEU:HD21	1:C:198:LYS:HG2	1.88	0.55
1:B:92:CYS:SG	1:B:141:LYS:HD2	2.47	0.55
1:G:277:LEU:HA	1:G:281:CYS:HB2	1.89	0.55
1:B:277:LEU:HA	1:B:281:CYS:HB2	1.88	0.55
1:F:277:LEU:HA	1:F:281:CYS:HB2	1.89	0.54
1:C:186:LEU:HB2	1:C:193:PHE:CE1	2.43	0.54
1:B:11:ASN:ND2	3:B:508:HOH:O	2.37	0.54
1:D:183:CYS:HB2	1:D:197:ASP:HB2	1.90	0.54
1:E:119:PRO:HA	1:E:134:THR:HG23	1.90	0.54
1:F:184:PHE:HB3	1:F:193:PHE:HB3	1.90	0.53
1:H:297:THR:HB	1:H:315:PRO:HG2	1.91	0.53
1:H:134:THR:HG1	1:H:167:TYR:HH	1.57	0.53
1:C:229:ARG:NH2	1:C:326:GLU:OE2	2.33	0.53
1:G:201:LYS:N	3:G:512:HOH:O	2.36	0.52
1:C:50:LYS:HD2	1:C:53:ILE:HD12	1.92	0.52
1:G:276:ARG:HG3	1:G:279:TYR:CE1	2.45	0.52
1:H:150:LYS:HE2	1:H:153:LEU:HD12	1.91	0.52
1:F:146:GLU:OE1	3:F:503:HOH:O	2.19	0.52
1:A:110:ARG:NH1	1:A:146:GLU:OE2	2.36	0.51
1:G:183:CYS:SG	1:G:200:VAL:HG21	2.51	0.51
1:A:229:ARG:NH1	1:A:234:PRO:HG3	2.25	0.51
1:B:33:LEU:HD11	1:B:85:LEU:HD22	1.93	0.51
1:D:280:GLU:OE2	3:D:501:HOH:O	2.18	0.51
1:F:233:PRO:HG2	1:F:237:SER:O	2.10	0.51
1:E:22:ARG:HG2	2:E:401:95Y:C14	2.40	0.51
1:A:27:THR:HG23	3:A:555:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:THR:HB	1:D:315:PRO:HG2	1.92	0.51
1:G:126:ILE:HG13	3:G:501:HOH:O	2.09	0.51
1:B:141:LYS:HZ1	1:B:147:PRO:HA	1.75	0.50
1:D:140[B]:ARG:HD3	1:D:141:LYS:O	2.11	0.50
1:D:72:LYS:NZ	3:D:505:HOH:O	2.27	0.50
1:A:112:LYS:HB2	3:A:546:HOH:O	2.12	0.50
1:D:134:THR:O	1:D:164:TYR:HA	2.11	0.50
1:F:309:ASP:HB3	1:F:312:GLN:HB3	1.93	0.50
1:C:112:LYS:HB2	1:C:140:ARG:NH1	2.26	0.50
1:H:145:ASP:HA	3:H:573:HOH:O	2.11	0.50
1:F:157:ARG:NH1	3:F:510:HOH:O	2.45	0.50
1:B:78:ASN:HB2	1:B:98:GLU:HG3	1.94	0.50
1:E:57:TYR:CZ	1:F:196:VAL:HG12	2.47	0.50
1:D:157:ARG:HG2	1:D:303:LEU:O	2.12	0.49
1:C:45:SER:O	1:C:49:ARG:HD3	2.12	0.49
1:A:221:PRO:HB2	1:A:334:HIS:CD2	2.47	0.49
1:C:274:LYS:O	1:C:313:ARG:NH1	2.46	0.49
1:H:96:SER:HB2	1:H:117:PHE:CZ	2.46	0.49
1:A:29:GLU:OE1	1:A:112:LYS:HG2	2.13	0.49
1:E:272:ASN:HA	3:E:509:HOH:O	2.13	0.49
1:H:72:LYS:NZ	3:H:516:HOH:O	2.46	0.48
1:D:184:PHE:HB3	1:D:193:PHE:HB3	1.95	0.48
1:G:181:VAL:HG21	1:G:291:ALA:HB2	1.94	0.48
1:E:277:LEU:HA	1:E:281:CYS:HB2	1.96	0.48
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.74	0.48
1:C:162:ALA:HB3	1:C:286:TYR:CD1	2.49	0.48
1:G:146:GLU:CD	1:G:147:PRO:HD2	2.34	0.48
1:A:221:PRO:HB2	1:A:334:HIS:HD2	1.79	0.48
1:B:151:ASP:O	1:B:154:GLN:NE2	2.42	0.48
1:H:270:SER:OG	1:H:274:LYS:HE3	2.15	0.47
1:A:22:ARG:NE	3:A:523:HOH:O	2.46	0.47
1:B:264:TYR:CZ	1:B:274:LYS:HD3	2.49	0.47
1:G:108:GLU:N	1:G:108:GLU:OE1	2.41	0.47
1:H:184:PHE:HB3	1:H:193:PHE:HB3	1.97	0.47
1:B:218:ASP:O	1:B:267:ASN:HB2	2.15	0.47
1:E:112:LYS:HD2	1:E:140[B]:ARG:NE	2.30	0.47
1:C:133:GLY:HA2	1:C:167:TYR:CD2	2.50	0.47
1:F:140[B]:ARG:NH2	3:F:511:HOH:O	2.48	0.47
1:G:45:SER:O	1:G:49:ARG:HD3	2.14	0.47
1:B:141:LYS:NZ	1:B:151:ASP:OD2	2.48	0.46
1:A:183:CYS:HB2	1:A:197:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:PHE:HB3	1:B:193:PHE:HB3	1.98	0.46
1:A:135:ILE:HD12	1:A:280:GLU:HG2	1.98	0.46
1:E:196:VAL:HG12	1:F:57:TYR:CZ	2.50	0.46
1:G:225:GLU:O	1:G:229:ARG:HG3	2.16	0.46
1:D:112:LYS:HB2	1:D:140[B]:ARG:NH2	2.30	0.46
1:G:278:LEU:HD12	1:G:310:ILE:HA	1.98	0.46
1:D:73:LEU:HD23	1:D:126:ILE:HD13	1.98	0.46
1:E:36:SER:OG	1:G:15:ARG:NH2	2.42	0.46
1:B:60:ALA:HB2	1:C:80:LEU:HD23	1.97	0.46
1:D:172:MET:SD	1:D:183:CYS:HB3	2.55	0.46
1:G:73:LEU:HD23	1:G:126:ILE:HD13	1.96	0.46
1:G:146:GLU:HG3	1:G:147:PRO:HD2	1.97	0.46
1:B:140[A]:ARG:HD3	3:B:509:HOH:O	2.16	0.46
1:A:55:HIS:HA	1:A:59:ILE:HG22	1.98	0.45
1:D:102:ALA:CB	1:D:149:GLU:HG2	2.39	0.45
1:D:186:LEU:HB2	1:D:193:PHE:CE1	2.51	0.45
1:H:102:ALA:HB3	1:H:149:GLU:HG2	1.98	0.45
1:C:112:LYS:HD2	1:C:140:ARG:CZ	2.46	0.45
1:C:270:SER:HB3	1:C:273:GLY:O	2.17	0.45
1:A:112:LYS:HD2	3:A:519:HOH:O	2.16	0.45
1:D:32:GLN:HG2	3:D:530:HOH:O	2.16	0.45
1:G:146:GLU:CG	1:G:147:PRO:HD2	2.45	0.45
1:G:276:ARG:O	1:G:280:GLU:HB2	2.16	0.45
1:A:277:LEU:N	3:A:501:HOH:O	2.42	0.45
1:A:333:LYS:NZ	3:A:525:HOH:O	2.50	0.45
1:F:55:HIS:HA	1:F:59:ILE:HG22	1.98	0.45
1:A:22:ARG:HG2	2:A:401:95Y:C14	2.47	0.45
1:B:218:ASP:OD2	1:B:269:LYS:HD2	2.15	0.45
1:B:217:LYS:HE3	1:B:217:LYS:HB3	1.54	0.45
1:G:275:LEU:HD12	1:G:316:VAL:HG11	1.97	0.45
1:C:183:CYS:HB2	1:C:197:ASP:HB2	1.99	0.45
1:F:112:LYS:HE3	1:F:113:TYR:CZ	2.52	0.45
1:B:18:MET:SD	1:D:31:THR:HG22	2.56	0.44
1:D:140[B]:ARG:NH1	1:D:141:LYS:O	2.47	0.44
1:F:209:TYR:CD2	1:F:227:ILE:HD12	2.53	0.44
1:A:264:TYR:OH	1:A:274:LYS:HD3	2.17	0.44
1:C:85:LEU:HA	1:C:85:LEU:HD23	1.80	0.44
1:D:9:ASP:N	3:D:516:HOH:O	2.50	0.44
1:H:274:LYS:HA	1:H:313:ARG:HD3	1.98	0.44
1:E:17:VAL:HG12	1:E:31:THR:HG23	1.99	0.44
1:B:19:GLU:HG3	3:D:594:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ARG:NE	3:B:515:HOH:O	2.50	0.44
1:E:78:ASN:HB2	1:E:98:GLU:HG3	1.99	0.44
1:F:186:LEU:HB2	1:F:193:PHE:CE1	2.53	0.44
1:A:130:VAL:O	1:B:169:SER:HB3	2.18	0.44
1:G:185:MET:HG2	1:H:53:ILE:HD13	1.99	0.43
1:G:186:LEU:HB2	1:G:193:PHE:CE1	2.53	0.43
1:A:18:MET:SD	1:C:31:THR:HG22	2.58	0.43
1:C:223:VAL:O	1:C:227:ILE:HG12	2.18	0.43
1:G:25:ARG:HB3	3:G:508:HOH:O	2.19	0.43
1:G:37:LEU:HD21	1:G:136:PHE:CG	2.54	0.43
1:E:275:LEU:HD12	1:E:316:VAL:HG11	2.01	0.43
1:H:110:ARG:NH1	1:H:146:GLU:OE2	2.45	0.43
1:C:277:LEU:HA	1:C:281:CYS:HB2	2.01	0.43
1:F:274:LYS:HA	1:F:274:LYS:HE2	2.00	0.43
1:A:275:LEU:HD12	1:A:316:VAL:HG11	2.00	0.43
1:C:181:VAL:HB	1:C:200:VAL:HG22	2.00	0.43
1:F:330:VAL:O	1:F:334:HIS:HD2	2.01	0.43
1:C:206:GLY:HA3	1:C:260:GLY:N	2.33	0.42
1:H:157:ARG:HG2	1:H:303:LEU:O	2.19	0.42
1:F:197:ASP:HB3	1:F:200:VAL:CG2	2.49	0.42
1:F:78:ASN:HB2	1:F:98:GLU:HG3	2.01	0.42
1:A:71:LYS:HD3	1:A:75:VAL:CG1	2.48	0.42
1:E:171:THR:HB	1:E:186:LEU:HB3	2.00	0.42
1:F:225:GLU:OE1	1:F:334:HIS:NE2	2.48	0.42
1:E:120:LEU:HG	1:E:123:SER:HB3	2.00	0.42
1:E:270:SER:OG	1:E:274:LYS:HE3	2.19	0.42
1:A:103:ILE:N	1:A:103:ILE:HD12	2.35	0.42
1:A:78:ASN:HB2	1:A:98:GLU:HG3	2.02	0.42
1:C:94:LEU:HB2	1:C:103:ILE:HB	2.02	0.42
1:H:296:THR:HG21	1:H:328:LEU:HD21	2.00	0.42
1:C:145:ASP:HB2	3:C:551:HOH:O	2.19	0.42
1:E:183:CYS:HB2	1:E:197:ASP:HB2	2.01	0.42
1:D:229:ARG:HD3	3:D:515:HOH:O	2.19	0.42
1:G:90:ALA:O	1:G:113:TYR:HB2	2.19	0.42
1:H:134:THR:O	1:H:164:TYR:HA	2.19	0.42
1:A:51:ALA:HA	1:B:188:PRO:HD2	2.02	0.41
1:A:72:LYS:HB2	1:A:72:LYS:HE2	1.68	0.41
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.85	0.41
1:D:206:GLY:HA3	1:D:260:GLY:N	2.36	0.41
1:D:29:GLU:HG2	1:D:90:ALA:HA	2.02	0.41
1:F:197:ASP:HB3	1:F:200:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:VAL:HG12	1:G:258:TYR:CD1	2.55	0.41
1:A:79:ASP:HB3	1:D:60:ALA:O	2.21	0.41
1:F:120:LEU:HG	1:F:123:SER:HB3	2.01	0.41
1:G:85:LEU:HD13	1:G:94:LEU:HD22	2.02	0.41
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.75	0.41
1:B:22:ARG:NH1	3:B:517:HOH:O	2.53	0.41
1:B:297:THR:HB	1:B:315:PRO:HG2	2.01	0.41
1:G:275:LEU:HD12	1:G:316:VAL:CG1	2.51	0.41
1:H:166:LEU:O	1:H:171:THR:HA	2.20	0.41
1:B:254:ARG:HD3	3:B:555:HOH:O	2.20	0.41
1:E:261:ILE:HB	1:E:323:ASP:HB3	2.03	0.41
1:E:221:PRO:HB2	1:E:334:HIS:CD2	2.56	0.41
1:H:146:GLU:CD	1:H:147:PRO:HD2	2.40	0.41
1:H:45:SER:O	1:H:49:ARG:HD3	2.21	0.41
1:C:51:ALA:HA	1:D:188:PRO:HD2	2.03	0.41
1:H:309:ASP:HB3	1:H:312:GLN:HB3	2.02	0.41
1:F:133:GLY:HA2	1:F:167:TYR:CD2	2.55	0.41
1:A:128:CYS:SG	1:A:130:VAL:HB	2.61	0.41
1:B:89:PHE:HA	1:B:109:LYS:O	2.21	0.41
1:F:212:ASN:ND2	1:F:215:TYR:HE2	2.18	0.41
1:F:18:MET:SD	1:H:32:GLN:HG2	2.61	0.41
1:C:280:GLU:O	1:C:284:MET:HG2	2.21	0.41
1:D:290:LYS:NZ	3:D:521:HOH:O	2.54	0.41
1:F:183:CYS:CB	1:F:197:ASP:HB2	2.50	0.41
1:F:257:VAL:HG12	1:F:258:TYR:CD1	2.55	0.41
1:G:140[A]:ARG:NE	3:G:522:HOH:O	2.53	0.40
1:C:121:ASP:N	1:C:133:GLY:O	2.53	0.40
1:C:150:LYS:HB2	1:C:150:LYS:HE2	1.61	0.40
1:H:186:LEU:O	1:H:188:PRO:HD3	2.21	0.40
1:D:182:ASN:OD1	1:D:198:LYS:HA	2.21	0.40
1:E:59:ILE:HA	1:F:10:VAL:HG11	2.03	0.40
1:A:162:ALA:HB3	1:A:286:TYR:CD1	2.56	0.40
1:B:141:LYS:NZ	1:B:147:PRO:HA	2.36	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	316/338 (94%)	310 (98%)	6 (2%)	0	100	100
1	B	314/338 (93%)	308 (98%)	6 (2%)	0	100	100
1	C	313/338 (93%)	305 (97%)	8 (3%)	0	100	100
1	D	314/338 (93%)	306 (98%)	8 (2%)	0	100	100
1	E	316/338 (94%)	310 (98%)	6 (2%)	0	100	100
1	F	314/338 (93%)	307 (98%)	7 (2%)	0	100	100
1	G	314/338 (93%)	308 (98%)	6 (2%)	0	100	100
1	H	313/338 (93%)	304 (97%)	9 (3%)	0	100	100
All	All	2514/2704 (93%)	2458 (98%)	56 (2%)	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	267/281 (95%)	256 (96%)	11 (4%)	33	50
1	B	265/281 (94%)	256 (97%)	9 (3%)	40	58
1	C	264/281 (94%)	258 (98%)	6 (2%)	53	72
1	D	265/281 (94%)	257 (97%)	8 (3%)	44	63
1	E	267/281 (95%)	256 (96%)	11 (4%)	33	50
1	F	265/281 (94%)	258 (97%)	7 (3%)	49	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	265/281 (94%)	258 (97%)	7 (3%)	49	68
1	H	264/281 (94%)	260 (98%)	4 (2%)	67	82
All	All	2122/2248 (94%)	2059 (97%)	63 (3%)	45	63

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	25	ARG
1	A	38	CYS
1	A	140[A]	ARG
1	A	140[B]	ARG
1	A	188	PRO
1	A	200	VAL
1	A	220	ASP
1	A	248	MET
1	A	264	TYR
1	A	332	GLU
1	B	9	ASP
1	B	38	CYS
1	B	56	LEU
1	B	178	ASP
1	B	200	VAL
1	B	217	LYS
1	B	220	ASP
1	B	264	TYR
1	B	268	LYS
1	C	9	ASP
1	C	38	CYS
1	C	56	LEU
1	C	140	ARG
1	C	264	TYR
1	C	278	LEU
1	D	9	ASP
1	D	38	CYS
1	D	56	LEU
1	D	144	THR
1	D	200	VAL
1	D	228	GLN
1	D	264	TYR
1	D	312	GLN

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Mol	Chain	Res	Type
1	E	9	ASP
1	E	38	CYS
1	E	72	LYS
1	E	73	LEU
1	E	140[A]	ARG
1	E	140[B]	ARG
1	E	144	THR
1	E	220	ASP
1	E	264	TYR
1	E	329	LYS
1	E	332	GLU
1	F	9	ASP
1	F	38	CYS
1	F	56	LEU
1	F	144	THR
1	F	200	VAL
1	F	264	TYR
1	F	268	LYS
1	G	9	ASP
1	G	38	CYS
1	G	56	LEU
1	G	150	LYS
1	G	254	ARG
1	G	264	TYR
1	G	332	GLU
1	H	9	ASP
1	H	236	ASN
1	H	264	TYR
1	H	332	GLU

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

Mol	Chain	Res	Type
1	H	32	GLN

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	95Y	A	401	-	29,32,32	0.80	1 (3%)	34,45,45	1.25	3 (8%)
2	95Y	B	401	-	29,32,32	0.68	1 (3%)	34,45,45	1.13	3 (8%)
2	95Y	C	401	-	29,32,32	0.59	0	34,45,45	0.76	2 (5%)
2	95Y	D	401	-	29,32,32	0.66	0	34,45,45	1.03	2 (5%)
2	95Y	E	401	-	29,32,32	0.84	2 (6%)	34,45,45	0.95	2 (5%)
2	95Y	F	401	-	29,32,32	0.55	0	34,45,45	0.90	2 (5%)
2	95Y	G	401	-	29,32,32	0.63	0	34,45,45	0.96	4 (11%)
2	95Y	H	401	-	29,32,32	1.05	1 (3%)	34,45,45	1.17	2 (5%)

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	95Y	A	401	-	-	0/16/31/31	0/3/3/3
2	95Y	B	401	-	-	0/16/31/31	0/3/3/3
2	95Y	C	401	-	-	0/16/31/31	0/3/3/3
2	95Y	D	401	-	-	0/16/31/31	0/3/3/3
2	95Y	E	401	-	-	0/16/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	95Y	F	401	-	-	0/16/31/31	0/3/3/3
2	95Y	G	401	-	-	0/16/31/31	0/3/3/3
2	95Y	H	401	-	-	0/16/31/31	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	95Y	C2-S1	-4.72	1.69	1.76
2	E	401	95Y	C2-S1	-2.87	1.72	1.76
2	A	401	95Y	C2-S1	-2.79	1.72	1.76
2	B	401	95Y	C2-S1	-2.50	1.72	1.76
2	E	401	95Y	C2-S4	-2.33	1.68	1.72

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	95Y	C5-C14-C18	-2.95	117.07	119.28
2	D	401	95Y	C5-C14-C18	-2.89	117.12	119.28
2	A	401	95Y	O16-S1-N3	-2.72	99.01	106.75
2	C	401	95Y	C5-C14-C18	-2.65	117.29	119.28
2	E	401	95Y	C5-C14-C18	-2.58	117.35	119.28
2	H	401	95Y	C5-C14-C18	-2.52	117.39	119.28
2	G	401	95Y	C5-C14-C18	-2.38	117.49	119.28
2	F	401	95Y	C5-C14-C18	-2.37	117.50	119.28
2	A	401	95Y	C5-C14-C18	-2.28	117.58	119.28
2	B	401	95Y	O16-S1-N3	-2.07	100.85	106.75
2	G	401	95Y	O16-S1-N3	-2.03	100.98	106.75
2	C	401	95Y	O17-S1-N3	2.11	112.73	106.75
2	G	401	95Y	C2-S1-N3	2.16	109.72	107.18
2	G	401	95Y	O17-S1-N3	2.52	113.92	106.75
2	F	401	95Y	C2-S1-N3	3.50	111.31	107.18
2	E	401	95Y	C2-S1-N3	3.54	111.35	107.18
2	D	401	95Y	C2-S1-N3	4.02	111.91	107.18
2	B	401	95Y	C2-S1-N3	4.52	112.50	107.18
2	A	401	95Y	C2-S1-N3	5.67	113.86	107.18
2	H	401	95Y	C2-S1-N3	5.88	114.10	107.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	95Y	1	0
2	E	401	95Y	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, 95th 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%)	-0.05	11 (3%) 45 42	18, 39, 76, 118	0
1	B	317/338 (93%)	0.11	8 (2%) 57 54	21, 42, 77, 118	0
1	C	317/338 (93%)	-0.16	4 (1%) 77 75	18, 34, 60, 85	0
1	D	317/338 (93%)	-0.20	4 (1%) 77 75	17, 31, 61, 90	0
1	E	319/338 (94%)	0.25	15 (4%) 31 29	27, 48, 81, 133	0
1	F	317/338 (93%)	0.19	15 (4%) 31 29	24, 47, 84, 114	0
1	G	317/338 (93%)	-0.14	1 (0%) 93 93	22, 36, 64, 89	0
1	H	317/338 (93%)	-0.06	6 (1%) 66 63	23, 38, 69, 109	0
All	All	2540/2704 (93%)	-0.01	64 (2%) 57 54	17, 39, 74, 133	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	235	ASP	5.8
1	E	70	VAL	5.4
1	E	234	PRO	5.2
1	A	144	THR	4.6
1	A	70	VAL	4.1
1	E	269	LYS	4.0
1	H	236	ASN	3.9
1	F	124	SER	3.8
1	F	144	THR	3.8
1	A	145	ASP	3.6
1	F	109	LYS	3.4
1	B	144	THR	3.4
1	E	268	LYS	3.3
1	E	236	ASN	3.2
1	F	268	LYS	3.2
1	B	269	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	268	LYS	3.1
1	F	237	SER	3.1
1	F	269	LYS	3.0
1	F	234	PRO	3.0
1	F	271	PRO	3.0
1	D	236	ASN	2.9
1	F	145	ASP	2.9
1	C	38	CYS	2.8
1	H	269	LYS	2.8
1	E	24	ALA	2.8
1	F	236	ASN	2.8
1	E	108	GLU	2.8
1	D	38	CYS	2.8
1	B	145	ASP	2.7
1	D	268	LYS	2.7
1	A	234	PRO	2.7
1	F	108	GLU	2.7
1	C	236	ASN	2.6
1	E	266	ALA	2.6
1	A	237	SER	2.6
1	E	237	SER	2.6
1	A	269	LYS	2.5
1	G	76	LEU	2.5
1	B	125	ASN	2.5
1	E	334	HIS	2.5
1	C	25	ARG	2.5
1	B	236	ASN	2.5
1	F	308	THR	2.5
1	E	332	GLU	2.5
1	H	108	GLU	2.4
1	B	221	PRO	2.4
1	E	71	LYS	2.4
1	F	270	SER	2.4
1	H	124	SER	2.4
1	A	236	ASN	2.3
1	A	271	PRO	2.3
1	H	123	SER	2.2
1	A	108	GLU	2.2
1	F	75	VAL	2.2
1	E	103	ILE	2.2
1	E	204	LYS	2.2
1	H	75	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	237	SER	2.1
1	B	271	PRO	2.1
1	B	237	SER	2.1
1	F	272	ASN	2.1
1	D	237	SER	2.1
1	A	238	ALA	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, 95th 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	95Y	D	401	30/30	0.94	0.16	22,57,72,74	1
2	95Y	F	401	30/30	0.95	0.16	42,66,89,91	1
2	95Y	H	401	30/30	0.95	0.18	37,56,85,87	1
2	95Y	B	401	30/30	0.95	0.12	28,56,81,83	1
2	95Y	G	401	30/30	0.95	0.15	35,65,75,83	1
2	95Y	C	401	30/30	0.95	0.16	27,59,80,81	1
2	95Y	E	401	30/30	0.96	0.14	28,58,75,79	1
2	95Y	A	401	30/30	0.96	0.13	23,51,67,69	1

6.5 Other polymers [i](#)

There are no such residues in this entry.