



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2019 – 05:31 PM EST

PDB ID : 5PZT
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-(3-ethyl-4-phenylphenyl)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 : 2.80 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

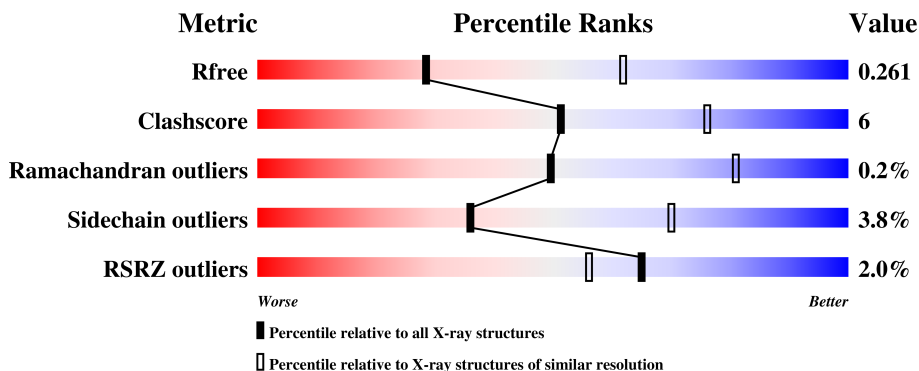
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



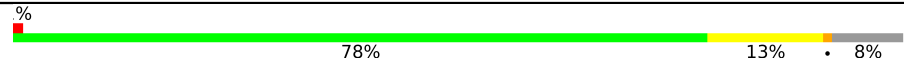

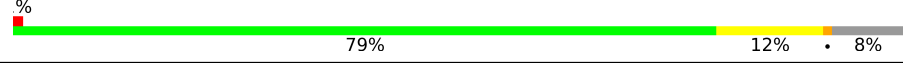
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 76% 15% • 8%</p>
1	B	338	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 78% 13% • 8%</p>
1	C	338	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 74% 17% • 8%</p>
1	D	338	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 78% 13% 8%</p>
1	E	338	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 77% 14% • 8%</p>

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Mol	Chain	Length	Quality of chain
1	F	338	 <p>% 78% 13% 8%</p>
1	G	338	 <p>% 73% 18% 8%</p>
1	H	338	 <p>% 79% 12% 8%</p>

2 Entry composition

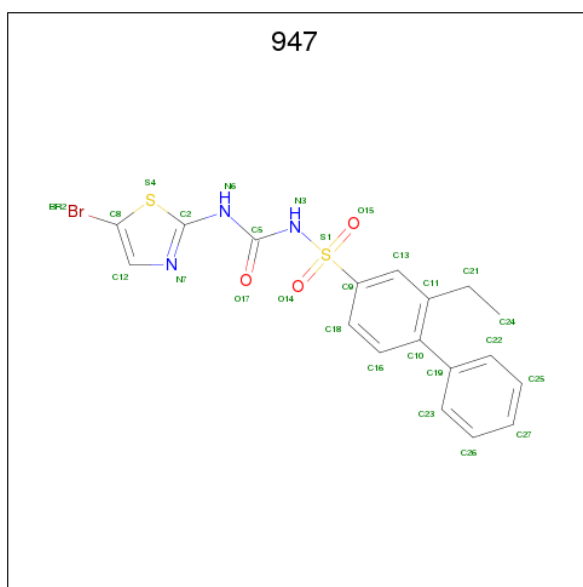
There are 3 unique types of molecules in this entry. The entry contains 19352 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	312	Total 2395	C 1524	N 403	O 451	S 17	0	1	0
1	B	310	Total 2380	C 1514	N 400	O 449	S 17	0	1	0
1	C	310	Total 2374	C 1511	N 397	O 449	S 17	0	0	0
1	D	310	Total 2380	C 1514	N 400	O 449	S 17	0	1	0
1	E	312	Total 2396	C 1525	N 403	O 451	S 17	0	1	0
1	F	310	Total 2379	C 1513	N 400	O 449	S 17	0	1	0
1	G	310	Total 2379	C 1513	N 400	O 449	S 17	0	1	0
1	H	310	Total 2374	C 1511	N 397	O 449	S 17	0	0	0

- Molecule 2 is N-[(5-bromo-1,3-thiazol-2-yl)carbamoyl]-2-ethyl[1,1'-biphenyl]-4-sulfonamide (three-letter code: 947) (formula: C₁₈H₁₆BrN₃O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	Br	C	N	O			S
2	A	1	Total	Br	C	N	O	S	0	0
			27	1	18	3	3	2		
2	B	1	Total	Br	C	N	O	S	0	0
			27	1	18	3	3	2		
2	C	1	Total	Br	C	N	O	S	0	0
			27	1	18	3	3	2		
2	D	1	Total	Br	C	N	O	S	0	0
			27	1	18	3	3	2		
2	E	1	Total	Br	C	N	O	S	0	0
			27	1	18	3	3	2		
2	F	1	Total	Br	C	N	O	S	0	0
			27	1	18	3	3	2		
2	G	1	Total	Br	C	N	O	S	0	0
			27	1	18	3	3	2		
2	H	1	Total	Br	C	N	O	S	0	0
			27	1	18	3	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	6	Total	O	0	0
			6	6		
3	C	10	Total	O	0	0
			10	10		
3	D	11	Total	O	0	0
			11	11		

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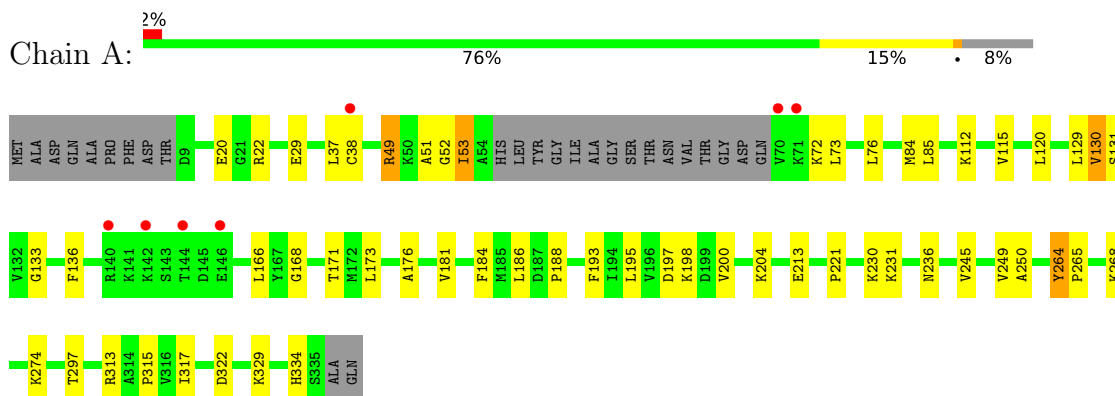
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	8	Total O 8 8	0	0
3	F	3	Total O 3 3	0	0
3	G	10	Total O 10 10	0	0
3	H	18	Total O 18 18	0	0

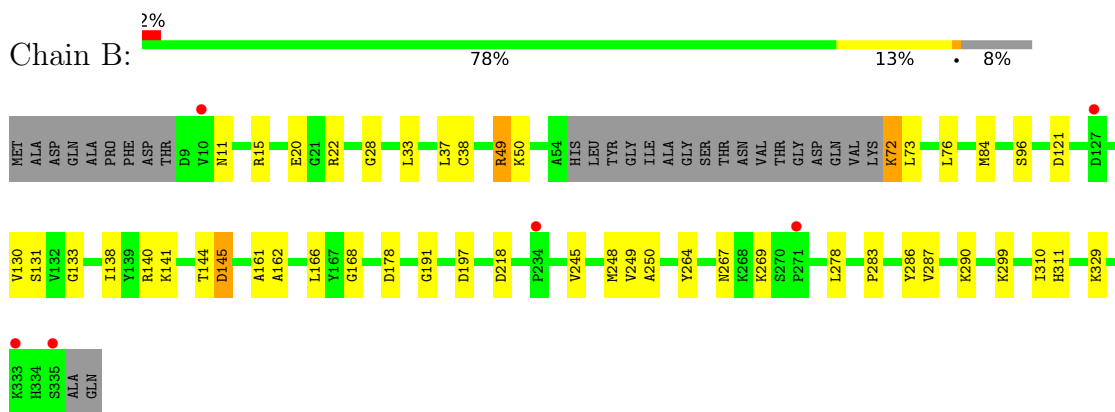
3 Residue-property plots [i](#)

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.

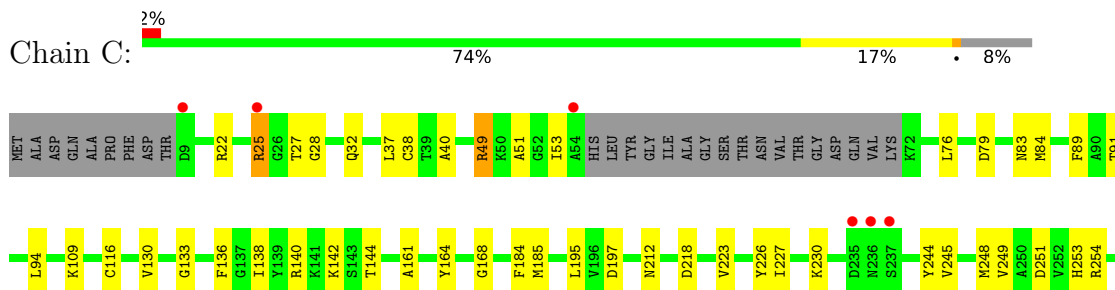
• Molecule 1: Fructose-1,6-bisphosphatase 1



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

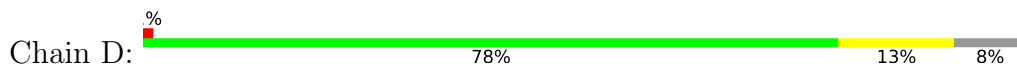


• Molecule 1: Fructose-1,6-bisphosphatase 1

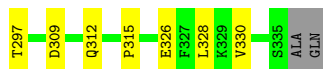
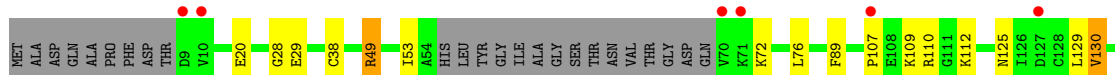
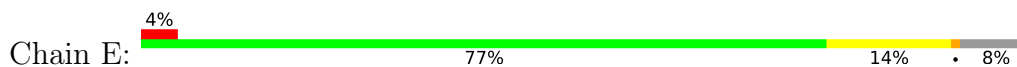




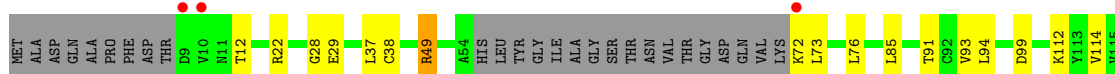
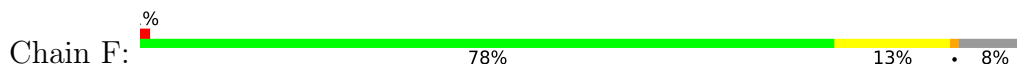
- Molecule 1: Fructose-1,6-bisphosphatase 1



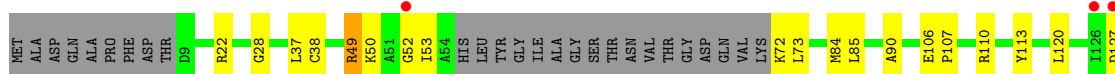
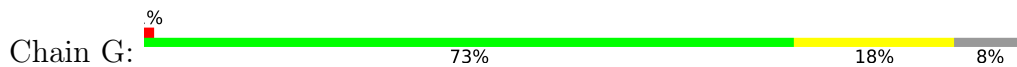
- Molecule 1: Fructose-1,6-bisphosphatase 1



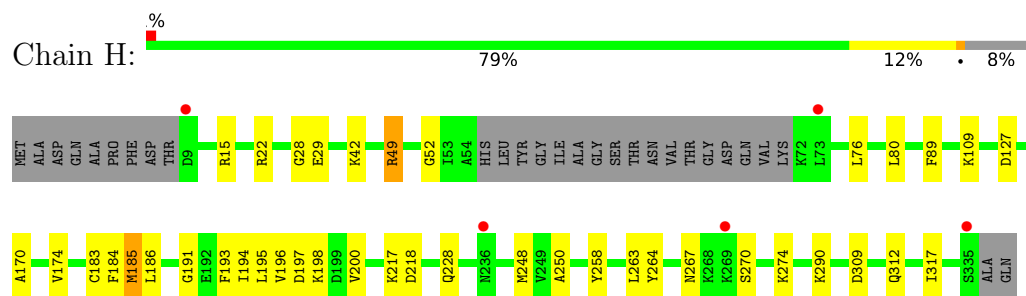
- Molecule 1: Fructose-1,6-bisphosphatase 1



- 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	66.44Å 294.19Å 83.57Å 90.00° 97.56° 90.00°	Depositor
Resolution (Å)	29.50 – 2.80 29.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.50-2.80) 99.9 (29.50-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.80Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.193 , 0.261 0.193 , 0.261	Depositor DCC
R_{free} test set	3891 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtrriage
Anisotropy	0.586	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19352	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: 947

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	0.40	0/2442	0.62	0/3296
1	B	0.41	0/2426	0.63	0/3275
1	C	0.47	0/2415	0.67	0/3261
1	D	0.48	0/2426	0.68	0/3275
1	E	0.41	0/2442	0.61	0/3296
1	F	0.42	0/2426	0.63	0/3275
1	G	0.49	0/2426	0.67	0/3275
1	H	0.46	0/2415	0.66	0/3261
All	All	0.44	0/19418	0.65	0/26214

There are no bond length outliers.

There are no bond angle outliers.

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	2395	0	2447	32	0
1	B	2380	0	2429	30	0
1	C	2374	0	2420	30	0
1	D	2380	0	2429	28	0
1	E	2396	0	2451	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2379	0	2425	30	0
1	G	2379	0	2425	43	0
1	H	2374	0	2420	38	0
2	A	27	0	0	1	0
2	B	27	0	0	3	0
2	C	27	0	0	2	0
2	D	27	0	0	4	0
2	E	27	0	0	3	0
2	F	27	0	0	2	0
2	G	27	0	0	1	0
2	H	27	0	0	1	0
3	A	13	0	0	0	0
3	B	6	0	0	0	0
3	C	10	0	0	0	0
3	D	11	0	0	0	0
3	E	8	0	0	0	0
3	F	3	0	0	0	0
3	G	10	0	0	1	0
3	H	18	0	0	1	0
All	All	19352	0	19446	235	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 (235) 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:49:ARG:NH2	1:E:168:GLY:O	2.10	0.84
1:H:195:LEU:HD21	1:H:198:LYS:HG3	1.61	0.81
1:B:49:ARG:NH2	1:B:168:GLY:O	2.14	0.80
1:F:49:ARG:NH2	1:F:168:GLY:O	2.15	0.80
1:A:274:LYS:O	1:A:313:ARG:NH1	2.19	0.76
1:A:213:GLU:OE1	1:A:231:LYS:NZ	2.17	0.74
1:A:29:GLU:HG3	1:C:22:ARG:HH12	1.54	0.73
1:A:245:VAL:HG22	1:B:245:VAL:HG22	1.71	0.73
1:E:245:VAL:HG22	1:F:245:VAL:HG22	1.69	0.73
1:A:49:ARG:NH2	1:A:168:GLY:O	2.21	0.72
1:C:79:ASP:O	1:C:83:ASN:ND2	2.24	0.70
1:H:184:PHE:HB3	1:H:193:PHE:HB3	1.73	0.70
1:C:251:ASP:OD1	1:C:254:ARG:NH2	2.22	0.69
1:D:270:SER:OG	1:D:274:LYS:HE2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:MET:HE3	1:D:15:ARG:HH22	1.61	0.66
1:E:107:PRO:HA	1:E:110:ARG:HB2	1.80	0.64
1:E:29:GLU:HG3	1:G:22:ARG:HH12	1.65	0.62
1:E:133:GLY:HA3	1:E:249:VAL:HG21	1.81	0.61
1:A:131:SER:HB3	1:A:166:LEU:HD11	1.81	0.61
1:G:267:ASN:ND2	3:G:501:HOH:O	2.25	0.61
1:C:49:ARG:NH2	1:C:168:GLY:O	2.34	0.60
1:D:28:GLY:HA2	2:D:401:947:C5	2.32	0.60
1:E:29:GLU:OE1	1:E:112:LYS:HG2	2.01	0.60
1:B:138:ILE:HD12	1:B:161:ALA:HB3	1.83	0.59
1:F:28:GLY:HA2	2:F:401:947:O17	2.02	0.59
1:G:184:PHE:HB3	1:G:193:PHE:HB3	1.84	0.59
1:C:28:GLY:HA2	2:C:401:947:C5	2.32	0.59
1:B:140[B]:ARG:NH1	1:B:141:LYS:O	2.36	0.59
1:E:125:ASN:O	1:E:130:VAL:HG12	2.03	0.58
1:H:89:PHE:HD2	1:H:109:LYS:HA	1.69	0.58
1:F:28:GLY:HA2	2:F:401:947:C5	2.34	0.57
1:C:89:PHE:CD1	1:C:109:LYS:HA	2.39	0.57
1:B:133:GLY:HA3	1:B:249:VAL:HG21	1.87	0.57
1:E:89:PHE:HE1	1:E:109:LYS:HG2	1.69	0.57
1:G:275:LEU:HD12	1:G:316:VAL:HG11	1.87	0.57
1:E:191:GLY:HA3	1:G:191:GLY:HA3	1.88	0.56
1:G:28:GLY:HA2	2:G:401:947:C5	2.35	0.56
1:A:29:GLU:HG3	1:C:22:ARG:NH1	2.19	0.55
1:B:28:GLY:HA2	2:B:401:947:C5	2.35	0.55
1:C:22:ARG:O	1:C:25:ARG:HD3	2.06	0.55
1:G:212:ASN:HB2	1:G:244:TYR:CE2	2.41	0.55
1:D:274:LYS:O	1:D:313:ARG:NH1	2.40	0.55
1:H:267:ASN:OD1	1:H:270:SER:N	2.24	0.55
1:A:133:GLY:HA3	1:A:249:VAL:HG21	1.87	0.55
1:A:129:LEU:HD12	1:B:166:LEU:HD23	1.88	0.54
1:G:218:ASP:HB3	1:G:268:LYS:H	1.72	0.54
1:D:131:SER:HB3	1:D:166:LEU:HD11	1.89	0.54
1:A:22:ARG:NE	1:C:27:THR:O	2.40	0.54
1:B:166:LEU:HD13	1:B:249:VAL:HG12	1.90	0.54
1:G:49:ARG:NH2	1:G:168:GLY:O	2.41	0.53
1:F:29:GLU:OE2	1:F:112:LYS:HG2	2.09	0.53
1:H:28:GLY:HA2	2:H:401:947:C5	2.39	0.53
1:B:72:LYS:HE3	1:B:73:LEU:N	2.23	0.53
1:H:309:ASP:HB3	1:H:312:GLN:HB3	1.90	0.52
1:A:265:PRO:HB3	1:A:317:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HG3	1:B:73:LEU:H	1.73	0.52
1:F:72:LYS:HG3	1:F:73:LEU:H	1.74	0.52
1:E:217:LYS:HA	1:F:232:PHE:CE2	2.45	0.52
1:C:164:TYR:OH	1:C:253:HIS:ND1	2.29	0.52
1:G:277:LEU:HA	1:G:281:CYS:HB2	1.90	0.52
1:A:184:PHE:HB3	1:A:193:PHE:HB3	1.91	0.51
1:C:116:CYS:SG	1:C:278:LEU:HD12	2.51	0.51
1:B:218:ASP:O	1:B:267:ASN:HB2	2.11	0.51
1:D:133:GLY:HA3	1:D:249:VAL:HG21	1.91	0.51
1:E:20:GLU:HB3	2:E:401:947:C23	2.39	0.51
1:G:110:ARG:HD3	1:G:147:PRO:HG3	1.93	0.51
1:G:258:TYR:OH	1:H:127:ASP:HB2	2.11	0.51
1:D:297:THR:HB	1:D:315:PRO:HG2	1.92	0.51
1:F:263:LEU:HD23	1:F:317:ILE:HG12	1.92	0.51
1:E:129:LEU:HD12	1:F:166:LEU:HD23	1.92	0.50
1:C:276:ARG:HG3	1:C:279:TYR:CE1	2.46	0.50
1:A:171:THR:HB	1:A:186:LEU:HB3	1.92	0.50
1:H:89:PHE:CD2	1:H:109:LYS:HA	2.46	0.50
1:G:72:LYS:HG3	1:G:73:LEU:H	1.77	0.50
1:B:72:LYS:HE3	1:B:73:LEU:H	1.76	0.50
1:F:116:CYS:SG	1:F:278:LEU:HD12	2.51	0.50
1:D:218:ASP:O	1:D:267:ASN:HB2	2.11	0.50
1:G:131:SER:CB	1:G:250:ALA:HB2	2.41	0.49
1:G:251:ASP:OD1	1:G:254:ARG:NH2	2.46	0.49
1:C:245:VAL:HG22	1:D:245:VAL:HG22	1.95	0.49
1:A:297:THR:HB	1:A:315:PRO:HG2	1.92	0.49
1:C:253:HIS:O	1:C:257:VAL:HG23	2.13	0.49
1:E:252:VAL:HG11	1:E:284:MET:SD	2.53	0.49
1:F:29:GLU:HG3	1:H:22:ARG:HH12	1.77	0.49
1:G:133:GLY:HA3	1:G:249:VAL:HG21	1.93	0.49
1:G:52:GLY:HA3	1:H:185:MET:HE1	1.95	0.49
1:F:184:PHE:HB3	1:F:193:PHE:HB3	1.93	0.49
1:A:195:LEU:HD21	1:A:198:LYS:HG3	1.95	0.48
1:H:49:ARG:NH2	1:H:168:GLY:O	2.46	0.48
1:A:188:PRO:HD2	1:B:50:LYS:HG2	1.95	0.48
1:E:28:GLY:HA2	2:E:401:947:C5	2.44	0.48
1:F:277:LEU:HD23	1:F:307:PRO:HB3	1.95	0.48
1:C:89:PHE:HD1	1:C:109:LYS:HA	1.79	0.47
1:F:183:CYS:HB2	1:F:197:ASP:HB2	1.96	0.47
1:G:297:THR:HB	1:G:315:PRO:HG2	1.94	0.47
1:C:40:ALA:HB2	1:C:84:MET:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:ASP:HB2	1:H:258:TYR:OH	2.14	0.47
1:A:130:VAL:HG21	1:A:245:VAL:HG13	1.95	0.47
1:F:37:LEU:HD13	1:F:85:LEU:HD21	1.96	0.47
1:G:129:LEU:HD22	1:H:170:ALA:HB3	1.97	0.47
1:F:22:ARG:HH12	1:H:29:GLU:HG3	1.79	0.47
1:B:130:VAL:HG21	1:B:245:VAL:HG13	1.96	0.47
1:E:28:GLY:HA2	2:E:401:947:O17	2.14	0.47
1:F:12:THR:HG21	1:F:192:GLU:HG2	1.97	0.46
1:H:42:LYS:NZ	1:H:191:GLY:O	2.45	0.46
1:H:195:LEU:HD21	1:H:198:LYS:HE2	1.97	0.46
1:B:191:GLY:HA3	1:D:191:GLY:HA3	1.98	0.46
1:F:93:VAL:HB	1:F:114:VAL:HG22	1.96	0.46
1:A:84:MET:HA	1:A:84:MET:CE	2.46	0.46
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.82	0.46
1:B:162:ALA:HB3	1:B:286:TYR:HD1	1.80	0.46
1:D:20:GLU:HB2	2:D:401:947:C24	2.46	0.46
1:E:185:MET:HE1	1:F:129:LEU:HD21	1.96	0.46
1:E:29:GLU:HG3	1:G:22:ARG:NH1	2.28	0.46
1:G:49:ARG:HH12	1:G:167:TYR:HB3	1.81	0.46
1:E:163:GLY:HA3	1:E:174:VAL:O	2.15	0.46
1:G:131:SER:HB2	1:G:250:ALA:HB2	1.98	0.45
1:H:174:VAL:HG22	1:H:183:CYS:SG	2.56	0.45
1:A:204:LYS:NZ	1:A:322:ASP:OD1	2.49	0.45
1:B:131:SER:HB2	1:B:250:ALA:HB2	1.98	0.45
1:B:283:PRO:O	1:B:287:VAL:HG23	2.17	0.45
1:H:218:ASP:O	1:H:267:ASN:HB2	2.16	0.45
1:D:85:LEU:HA	1:D:85:LEU:HD23	1.67	0.45
1:F:220:ASP:OD2	1:F:268:LYS:NZ	2.50	0.45
1:H:184:PHE:HA	1:H:194:ILE:O	2.15	0.45
1:A:29:GLU:OE1	1:A:112:LYS:HG2	2.15	0.45
1:C:138:ILE:HD12	1:C:161:ALA:HB3	1.97	0.45
1:G:146:GLU:HG3	1:G:147:PRO:HD2	1.97	0.45
1:C:226:TYR:O	1:C:230:LYS:HG2	2.16	0.45
1:G:195:LEU:HD21	1:G:198:LYS:HG2	1.99	0.45
1:D:17:VAL:HG12	1:D:31:THR:HG23	1.98	0.45
1:A:53:ILE:HG13	1:A:53:ILE:O	2.17	0.45
1:E:162:ALA:HB3	1:E:286:TYR:HD1	1.81	0.45
1:E:72:LYS:HD2	1:E:72:LYS:HA	1.60	0.45
1:H:270:SER:OG	1:H:274:LYS:HE2	2.17	0.45
1:A:85:LEU:HD13	1:A:115:VAL:HG21	1.99	0.44
1:C:218:ASP:HB3	1:C:268:LYS:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASP:N	1:B:133:GLY:O	2.44	0.44
1:B:22:ARG:HG3	2:B:401:947:C12	2.47	0.44
1:B:20:GLU:HB3	2:B:401:947:C23	2.48	0.44
1:G:208:ILE:HA	1:G:241:GLY:O	2.18	0.44
1:G:72:LYS:CG	1:G:73:LEU:H	2.31	0.44
1:D:49:ARG:NH2	1:D:168:GLY:O	2.50	0.44
1:E:217:LYS:HA	1:F:232:PHE:HE2	1.83	0.44
1:H:185:MET:HE3	1:H:196:VAL:HG11	2.00	0.44
1:G:232:PHE:CE2	1:H:217:LYS:HA	2.52	0.44
1:B:96:SER:O	1:B:311:HIS:HE1	2.01	0.43
1:C:184:PHE:CE2	1:C:195:LEU:HD13	2.54	0.43
1:B:278:LEU:HD12	1:B:310:ILE:HA	2.00	0.43
1:E:181:VAL:HG21	1:E:291:ALA:HB2	1.99	0.43
1:H:131:SER:HB2	1:H:250:ALA:HB2	2.00	0.43
1:A:173:LEU:HB3	1:A:184:PHE:HB2	1.99	0.43
1:C:288:MET:HG3	1:C:318:LEU:HD13	2.01	0.43
1:C:37:LEU:HD21	1:C:136:PHE:CG	2.54	0.43
1:D:110:ARG:HD3	1:D:147:PRO:HG3	2.01	0.43
1:F:172:MET:HG3	1:F:173:LEU:N	2.32	0.43
1:G:185:MET:HE1	1:H:52:GLY:H	1.84	0.43
1:A:131:SER:HB2	1:A:250:ALA:HB2	1.99	0.43
1:A:176:ALA:HB2	1:A:181:VAL:HG22	2.00	0.43
1:E:171:THR:HB	1:E:186:LEU:HB3	2.01	0.43
1:F:166:LEU:O	1:F:171:THR:HA	2.19	0.43
1:E:208:ILE:HA	1:E:241:GLY:O	2.18	0.43
1:F:91:THR:HG21	1:F:94:LEU:HD21	2.01	0.43
1:G:297:THR:HG22	1:G:315:PRO:O	2.18	0.43
1:D:28:GLY:HA2	2:D:401:947:O17	2.18	0.43
1:H:195:LEU:CD2	1:H:198:LYS:HE2	2.49	0.43
1:A:221:PRO:HB2	1:A:334:HIS:ND1	2.34	0.42
1:B:37:LEU:HD12	1:B:37:LEU:HA	1.79	0.42
1:D:223:VAL:O	1:D:227:ILE:HG12	2.19	0.42
1:G:181:VAL:O	1:G:200:VAL:HG23	2.19	0.42
1:H:89:PHE:HA	1:H:109:LYS:O	2.19	0.42
1:D:263:LEU:HD23	1:D:317:ILE:HG12	2.00	0.42
1:H:274:LYS:HD3	1:H:274:LYS:HA	1.74	0.42
1:D:184:PHE:HA	1:D:194:ILE:O	2.19	0.42
1:B:218:ASP:OD2	1:B:269:LYS:HD3	2.19	0.42
1:D:184:PHE:HB3	1:D:193:PHE:HB3	2.01	0.42
1:D:89:PHE:HE1	1:D:109:LYS:HG2	1.84	0.42
1:H:185:MET:HB2	1:H:185:MET:HE2	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LYS:HB2	1:B:329:LYS:HE3	1.68	0.42
1:C:223:VAL:O	1:C:227:ILE:HG12	2.19	0.42
1:D:20:GLU:HB3	2:D:401:947:C23	2.49	0.42
1:G:225:GLU:O	1:G:229:ARG:HG3	2.20	0.42
1:A:176:ALA:CB	1:A:181:VAL:HG22	2.50	0.42
1:C:264:TYR:OH	1:C:274:LYS:HD2	2.19	0.42
1:G:37:LEU:HD21	1:G:136:PHE:CG	2.55	0.42
1:D:265:PRO:HB3	1:D:317:ILE:HD11	2.02	0.42
1:E:184:PHE:HB3	1:E:193:PHE:HB3	2.01	0.42
1:A:264:TYR:CE1	1:A:274:LYS:HB2	2.55	0.42
1:B:278:LEU:HA	1:B:278:LEU:HD23	1.81	0.42
1:E:172:MET:HB2	1:E:172:MET:HE3	1.86	0.42
1:E:136:PHE:O	1:E:283:PRO:HB3	2.20	0.42
1:F:29:GLU:HG3	1:H:22:ARG:NH1	2.33	0.42
1:G:50:LYS:HB2	1:G:50:LYS:HE3	1.77	0.42
1:C:212:ASN:HB2	1:C:244:TYR:CE2	2.55	0.41
1:D:120:LEU:HD12	1:D:120:LEU:HA	1.88	0.41
1:F:270:SER:OG	1:F:274:LYS:HE2	2.20	0.41
1:H:184:PHE:CB	1:H:193:PHE:HB3	2.46	0.41
1:A:20:GLU:HB3	2:A:401:947:C23	2.50	0.41
1:D:275:LEU:HD12	1:D:316:VAL:HG11	2.02	0.41
1:E:297:THR:HB	1:E:315:PRO:HG2	2.02	0.41
1:E:309:ASP:HB3	1:E:312:GLN:HB3	2.02	0.41
1:E:326:GLU:O	1:E:330:VAL:HG23	2.20	0.41
1:F:99:ASP:O	1:F:311:HIS:NE2	2.51	0.41
1:G:85:LEU:HA	1:G:85:LEU:HD23	1.77	0.41
1:F:22:ARG:NH1	1:H:29:GLU:HG3	2.36	0.41
1:H:89:PHE:HE2	1:H:109:LYS:HG2	1.84	0.41
1:B:178:ASP:HA	1:B:290:LYS:NZ	2.35	0.41
1:G:107:PRO:HG3	1:G:110:ARG:NH2	2.35	0.41
1:E:181:VAL:HB	1:E:200:VAL:HG22	2.02	0.41
1:B:11:ASN:OD1	1:B:15:ARG:HG2	2.21	0.41
1:C:37:LEU:HD21	1:C:136:PHE:CD1	2.55	0.41
1:H:15:ARG:NE	3:H:503:HOH:O	2.54	0.41
1:A:72:LYS:HD2	1:A:72:LYS:HA	1.70	0.41
1:G:278:LEU:HA	1:G:278:LEU:HD23	1.61	0.41
1:D:213:GLU:OE1	1:D:231:LYS:NZ	2.32	0.41
1:F:309:ASP:HB3	1:F:312:GLN:HB3	2.03	0.41
1:H:186:LEU:HB2	1:H:193:PHE:CE1	2.56	0.41
1:C:91:THR:HB	1:C:94:LEU:HD21	2.03	0.41
1:D:37:LEU:HD12	1:D:37:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ALA:O	1:G:113:TYR:HB2	2.20	0.41
1:E:328:LEU:HD23	1:E:328:LEU:HA	1.91	0.40
1:C:263:LEU:HD23	1:C:317:ILE:HG12	2.03	0.40
1:F:230:LYS:HD3	1:F:240:TYR:CD2	2.56	0.40
1:G:232:PHE:HE2	1:H:217:LYS:HA	1.86	0.40
1:H:263:LEU:HD23	1:H:317:ILE:HG12	2.02	0.40
1:D:274:LYS:HA	1:D:274:LYS:HD3	1.69	0.40
1:G:120:LEU:HA	1:G:120:LEU:HD12	1.82	0.40
1:G:212:ASN:HB2	1:G:244:TYR:CZ	2.57	0.40
1:G:84:MET:HE2	1:G:84:MET:HA	2.02	0.40
1:H:89:PHE:CE2	1:H:109:LYS:HG2	2.57	0.40
1:H:290:LYS:HD3	1:H:290:LYS:HA	1.96	0.40
1:C:28:GLY:HA2	2:C:401:947:O17	2.21	0.40
1:A:37:LEU:HD21	1:A:136:PHE:CD1	2.56	0.40
1:C:133:GLY:HA3	1:C:249:VAL:HG21	2.03	0.40
1:G:181:VAL:HG21	1:G:291:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	309/338 (91%)	298 (96%)	9 (3%)	2 (1%)	27	60
1	B	307/338 (91%)	297 (97%)	9 (3%)	1 (0%)	43	75
1	C	306/338 (90%)	292 (95%)	12 (4%)	2 (1%)	24	57
1	D	307/338 (91%)	298 (97%)	9 (3%)	0	100	100
1	E	309/338 (91%)	301 (97%)	8 (3%)	0	100	100
1	F	307/338 (91%)	297 (97%)	10 (3%)	0	100	100
1	G	307/338 (91%)	297 (97%)	9 (3%)	1 (0%)	43	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	306/338 (90%)	294 (96%)	12 (4%)	0	100	100
All	All	2458/2704 (91%)	2374 (97%)	78 (3%)	6 (0%)	49	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	ALA
1	A	52	GLY
1	A	51	ALA
1	C	53	ILE
1	B	145	ASP
1	G	53	ILE

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	263/281 (94%)	250 (95%)	13 (5%)	27	60
1	B	261/281 (93%)	250 (96%)	11 (4%)	32	66
1	C	260/281 (92%)	246 (95%)	14 (5%)	24	56
1	D	261/281 (93%)	253 (97%)	8 (3%)	43	77
1	E	263/281 (94%)	254 (97%)	9 (3%)	40	74
1	F	261/281 (93%)	253 (97%)	8 (3%)	43	77
1	G	261/281 (93%)	254 (97%)	7 (3%)	48	81
1	H	260/281 (92%)	250 (96%)	10 (4%)	36	70
All	All	2090/2248 (93%)	2010 (96%)	80 (4%)	36	70

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

Mol	Chain	Res	Type
1	A	38	CYS
1	A	49	ARG

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Mol	Chain	Res	Type
1	A	53	ILE
1	A	73	LEU
1	A	76	LEU
1	A	130	VAL
1	A	197	ASP
1	A	200	VAL
1	A	230	LYS
1	A	236	ASN
1	A	264	TYR
1	A	268	LYS
1	A	329	LYS
1	B	33	LEU
1	B	38	CYS
1	B	49	ARG
1	B	72	LYS
1	B	76	LEU
1	B	144	THR
1	B	145	ASP
1	B	197	ASP
1	B	248	MET
1	B	264	TYR
1	B	299	LYS
1	C	25	ARG
1	C	32	GLN
1	C	38	CYS
1	C	49	ARG
1	C	76	LEU
1	C	130	VAL
1	C	140	ARG
1	C	142	LYS
1	C	144	THR
1	C	185	MET
1	C	197	ASP
1	C	248	MET
1	C	264	TYR
1	C	332	GLU
1	D	38	CYS
1	D	49	ARG
1	D	72	LYS
1	D	130	VAL
1	D	185	MET
1	D	197	ASP

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Mol	Chain	Res	Type
1	D	248	MET
1	D	264	TYR
1	E	38	CYS
1	E	49	ARG
1	E	53	ILE
1	E	76	LEU
1	E	130	VAL
1	E	172	MET
1	E	197	ASP
1	E	248	MET
1	E	264	TYR
1	F	38	CYS
1	F	49	ARG
1	F	76	LEU
1	F	146	GLU
1	F	185	MET
1	F	197	ASP
1	F	264	TYR
1	F	268	LYS
1	G	38	CYS
1	G	49	ARG
1	G	106	GLU
1	G	197	ASP
1	G	236	ASN
1	G	248	MET
1	G	264	TYR
1	H	49	ARG
1	H	76	LEU
1	H	80	LEU
1	H	130	VAL
1	H	185	MET
1	H	197	ASP
1	H	200	VAL
1	H	228	GLN
1	H	248	MET
1	H	264	TYR

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	947	A	401	-	26,29,29	1.07	1 (3%)	32,41,41	0.58	0
2	947	B	401	-	26,29,29	0.71	0	32,41,41	0.63	1 (3%)
2	947	C	401	-	26,29,29	0.62	0	32,41,41	0.61	1 (3%)
2	947	D	401	-	26,29,29	0.77	1 (3%)	32,41,41	0.69	1 (3%)
2	947	E	401	-	26,29,29	0.61	0	32,41,41	0.73	1 (3%)
2	947	F	401	-	26,29,29	0.61	0	32,41,41	0.63	1 (3%)
2	947	G	401	-	26,29,29	0.77	1 (3%)	32,41,41	0.60	1 (3%)
2	947	H	401	-	26,29,29	0.83	1 (3%)	32,41,41	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	947	A	401	-	-	0/19/21/21	0/3/3/3
2	947	B	401	-	-	0/19/21/21	0/3/3/3
2	947	C	401	-	-	0/19/21/21	0/3/3/3
2	947	D	401	-	-	0/19/21/21	0/3/3/3
2	947	E	401	-	-	0/19/21/21	0/3/3/3
2	947	F	401	-	-	0/19/21/21	0/3/3/3
2	947	G	401	-	-	0/19/21/21	0/3/3/3
2	947	H	401	-	-	0/19/21/21	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	947	C10-C11	2.15	1.43	1.40
2	H	401	947	C2-N6	2.82	1.41	1.36
2	G	401	947	C2-N6	2.98	1.41	1.36
2	A	401	947	C21-C11	4.62	1.64	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	947	BR2-C8-C12	2.09	127.58	124.38
2	B	401	947	BR2-C8-C12	2.13	127.64	124.38
2	C	401	947	BR2-C8-C12	2.23	127.80	124.38
2	H	401	947	BR2-C8-C12	2.38	128.02	124.38
2	F	401	947	BR2-C8-C12	2.41	128.08	124.38
2	D	401	947	BR2-C8-C12	2.43	128.10	124.38
2	E	401	947	BR2-C8-C12	2.53	128.25	124.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	947	1	0
2	B	401	947	3	0
2	C	401	947	2	0
2	D	401	947	4	0
2	E	401	947	3	0
2	F	401	947	2	0
2	G	401	947	1	0
2	H	401	947	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	312/338 (92%)	-0.19	7 (2%) 62 52	36, 66, 102, 132	0
1	B	310/338 (91%)	-0.04	6 (1%) 66 59	33, 65, 115, 146	0
1	C	310/338 (91%)	-0.24	6 (1%) 66 59	29, 53, 100, 138	0
1	D	310/338 (91%)	-0.41	2 (0%) 89 86	28, 48, 87, 133	0
1	E	312/338 (92%)	0.02	14 (4%) 33 23	40, 74, 122, 149	0
1	F	310/338 (91%)	-0.10	5 (1%) 72 65	40, 68, 106, 135	0
1	G	310/338 (91%)	-0.29	5 (1%) 72 65	31, 52, 97, 136	0
1	H	310/338 (91%)	-0.35	5 (1%) 72 65	32, 53, 91, 134	0
All	All	2484/2704 (91%)	-0.20	50 (2%) 65 56	28, 59, 105, 149	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	ASP	4.7
1	E	70	VAL	4.7
1	E	71	LYS	4.6
1	C	9	ASP	4.5
1	E	238	ALA	4.3
1	A	70	VAL	3.8
1	C	237	SER	3.6
1	C	54	ALA	3.3
1	C	25	ARG	3.2
1	B	234	PRO	3.2
1	F	72	LYS	3.1
1	E	10	VAL	3.1
1	E	269	LYS	3.1
1	F	335	SER	3.0
1	F	9	ASP	3.0
1	F	271	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	9	ASP	2.8
1	A	146	GLU	2.8
1	B	10	VAL	2.7
1	H	236	ASN	2.6
1	F	10	VAL	2.6
1	H	9	ASP	2.6
1	G	52	GLY	2.5
1	A	71	LYS	2.5
1	G	126	ILE	2.4
1	H	335	SER	2.4
1	D	25	ARG	2.4
1	B	333	LYS	2.4
1	H	269	LYS	2.4
1	E	239	PRO	2.4
1	E	234	PRO	2.4
1	G	238	ALA	2.4
1	E	127	ASP	2.3
1	G	128	CYS	2.3
1	B	271	PRO	2.3
1	A	142	LYS	2.3
1	G	127	ASP	2.2
1	A	140[A]	ARG	2.2
1	C	236	ASN	2.1
1	E	235	ASP	2.1
1	E	232	PHE	2.1
1	B	335	SER	2.1
1	A	38	CYS	2.1
1	C	235	ASP	2.1
1	D	122	GLY	2.0
1	E	163	GLY	2.0
1	A	144	THR	2.0
1	E	107	PRO	2.0
1	E	233	PRO	2.0
1	H	73	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	947	H	401	27/27	0.96	0.18	49,65,82,83	1
2	947	A	401	27/27	0.96	0.15	46,63,85,92	1
2	947	B	401	27/27	0.97	0.15	50,67,83,106	1
2	947	G	401	27/27	0.97	0.14	49,63,70,79	1
2	947	F	401	27/27	0.97	0.16	46,67,87,93	1
2	947	E	401	27/27	0.97	0.16	47,63,70,81	1
2	947	C	401	27/27	0.97	0.16	52,61,71,76	1
2	947	D	401	27/27	0.97	0.16	45,54,69,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.