Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 01:31 am GMT

PDB ID	:	5A34
Title	:	The crystal structure of the GST-like domains complex of EPRS-AIMP2
Authors	:	Cho, H.Y.; Kang, B.S.
Deposited on	:	2015-05-27
Resolution	:	2.60 Å(reported)

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

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

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

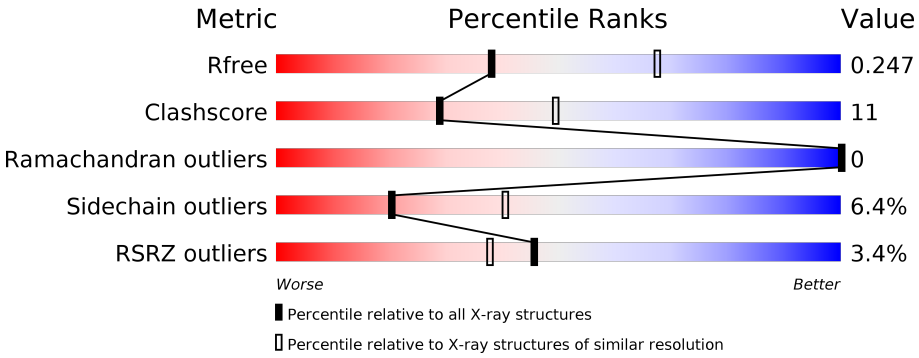
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	175	77% 17%
1	C	175	% 80% 15%
1	E	175	78% 15% 5%
1	G	175	5% 77% 19%
2	B	240	3% 67% 16% 15%
2	D	240	5% 59% 21% 18%

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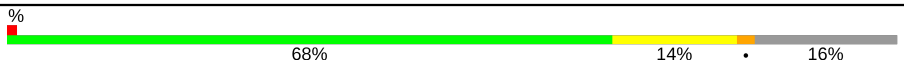
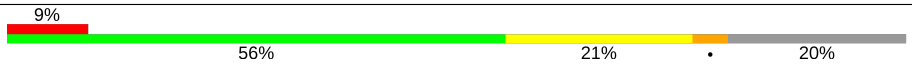
Mol	Chain	Length	Quality of chain
2	F	240	
2	H	240	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	1321	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11266 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 BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1286	816	217	249	4			
1	C	170	Total	C	N	O	S	0	0	0
			1311	832	221	254	4			
1	E	167	Total	C	N	O	S	0	0	0
			1299	826	220	249	4			
1	G	168	Total	C	N	O	S	0	0	0
			1281	815	216	246	4			

- Molecule 2 is a protein called AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONAL PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	2	0
			1556	1001	265	282	8			
2	D	196	Total	C	N	O	S	0	1	0
			1483	957	256	261	9			
2	F	201	Total	C	N	O	S	0	0	0
			1535	990	264	273	8			
2	H	193	Total	C	N	O	S	0	0	0
			1436	924	247	257	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	89	MET	-	EXPRESSION TAG	UNP Q13155
B	321	LEU	-	EXPRESSION TAG	UNP Q13155
B	322	GLU	-	EXPRESSION TAG	UNP Q13155
B	323	HIS	-	EXPRESSION TAG	UNP Q13155
B	324	HIS	-	EXPRESSION TAG	UNP Q13155
B	325	HIS	-	EXPRESSION TAG	UNP Q13155
B	326	HIS	-	EXPRESSION TAG	UNP Q13155

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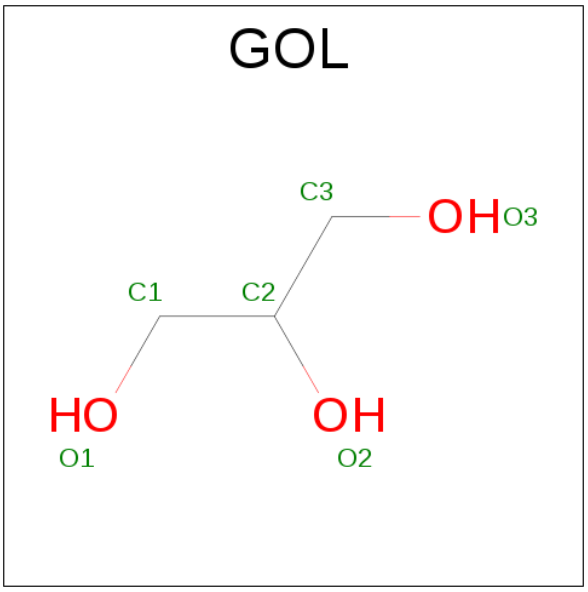
Chain	Residue	Modelled	Actual	Comment	Reference
B	327	HIS	-	EXPRESSION TAG	UNP Q13155
B	328	HIS	-	EXPRESSION TAG	UNP Q13155
D	89	MET	-	EXPRESSION TAG	UNP Q13155
D	321	LEU	-	EXPRESSION TAG	UNP Q13155
D	322	GLU	-	EXPRESSION TAG	UNP Q13155
D	323	HIS	-	EXPRESSION TAG	UNP Q13155
D	324	HIS	-	EXPRESSION TAG	UNP Q13155
D	325	HIS	-	EXPRESSION TAG	UNP Q13155
D	326	HIS	-	EXPRESSION TAG	UNP Q13155
D	327	HIS	-	EXPRESSION TAG	UNP Q13155
D	328	HIS	-	EXPRESSION TAG	UNP Q13155
F	89	MET	-	EXPRESSION TAG	UNP Q13155
F	321	LEU	-	EXPRESSION TAG	UNP Q13155
F	322	GLU	-	EXPRESSION TAG	UNP Q13155
F	323	HIS	-	EXPRESSION TAG	UNP Q13155
F	324	HIS	-	EXPRESSION TAG	UNP Q13155
F	325	HIS	-	EXPRESSION TAG	UNP Q13155
F	326	HIS	-	EXPRESSION TAG	UNP Q13155
F	327	HIS	-	EXPRESSION TAG	UNP Q13155
F	328	HIS	-	EXPRESSION TAG	UNP Q13155
H	89	MET	-	EXPRESSION TAG	UNP Q13155
H	321	LEU	-	EXPRESSION TAG	UNP Q13155
H	322	GLU	-	EXPRESSION TAG	UNP Q13155
H	323	HIS	-	EXPRESSION TAG	UNP Q13155
H	324	HIS	-	EXPRESSION TAG	UNP Q13155
H	325	HIS	-	EXPRESSION TAG	UNP Q13155
H	326	HIS	-	EXPRESSION TAG	UNP Q13155
H	327	HIS	-	EXPRESSION TAG	UNP Q13155
H	328	HIS	-	EXPRESSION TAG	UNP Q13155

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

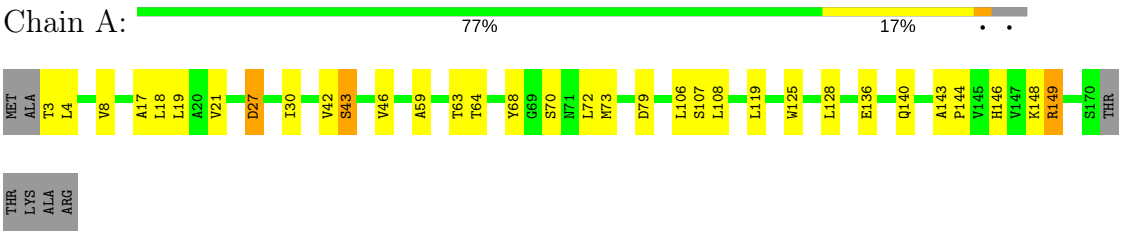
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total O 11 11	0	0
4	B	6	Total O 6 6	0	0
4	C	14	Total O 14 14	0	0
4	D	10	Total O 10 10	0	0
4	E	11	Total O 11 11	0	0
4	F	9	Total O 9 9	0	0
4	G	3	Total O 3 3	0	0
4	H	3	Total O 3 3	0	0

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.

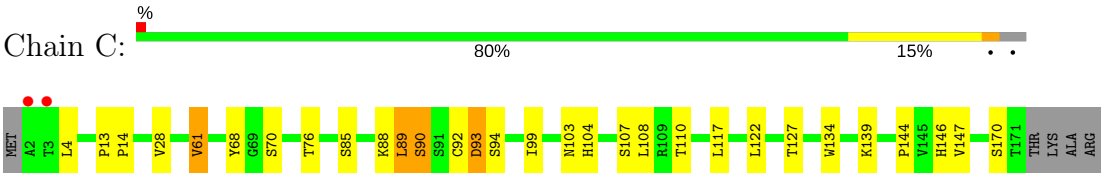
• Molecule 1: BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE

Chain A:



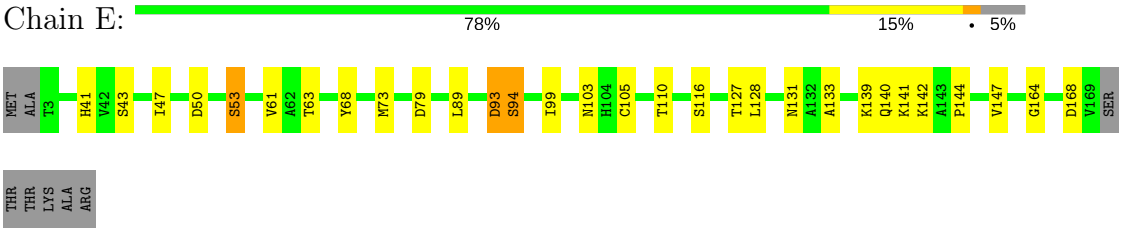
• Molecule 1: BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE

Chain C:



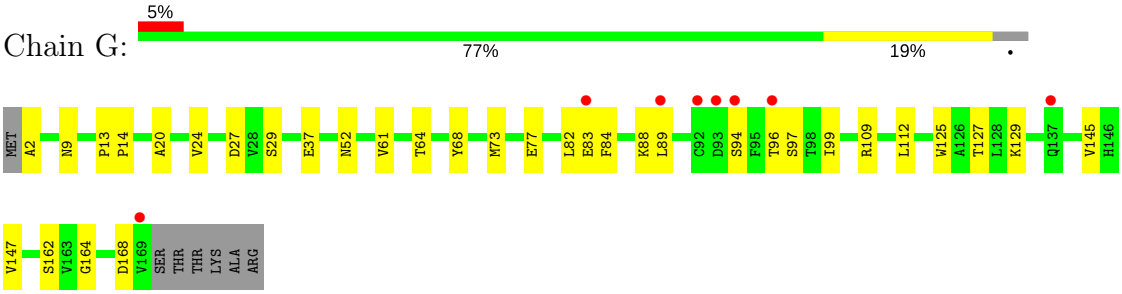
• Molecule 1: BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE

Chain E:



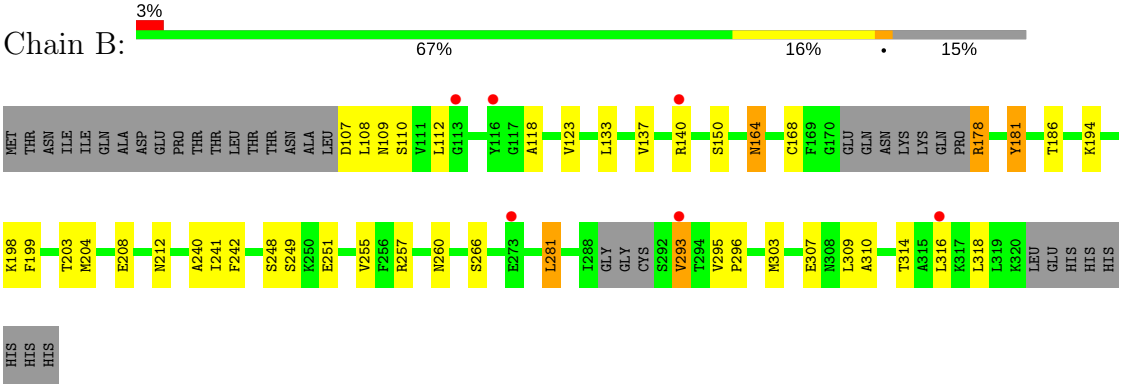
• Molecule 1: BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE

Chain G:



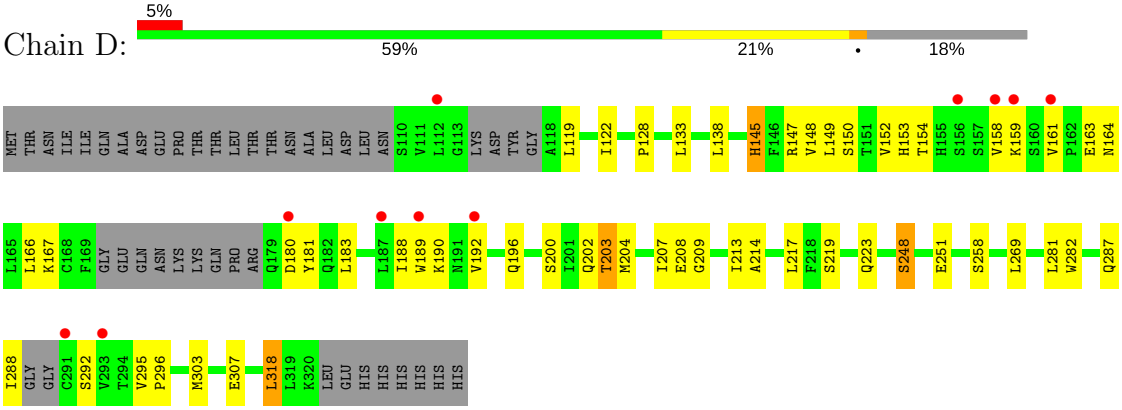
• Molecule 2: AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONAL PROTEIN 2

Chain B:



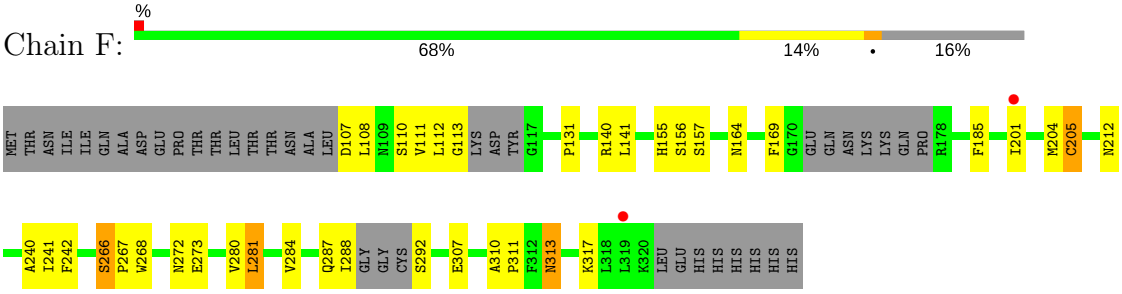
• Molecule 2: AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONAL PROTEIN 2

Chain D:



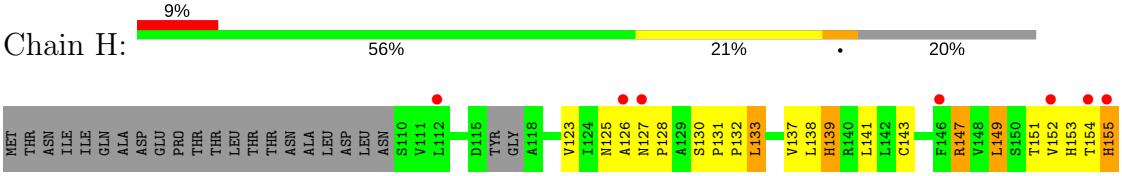
• Molecule 2: AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONAL PROTEIN 2

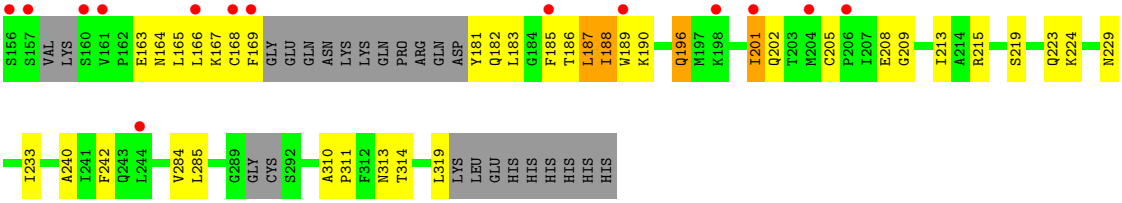
Chain F:



• Molecule 2: AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONAL PROTEIN 2

Chain H:




S156 S157 VAL LYS S160 V161 P162 E163 N164 L165 L166 K167 C168 F169 GLY GLU GLN ASN LYS LYS GLN PRO ARG GLN ASP Y181 Q182 L183 G184 F185 T186 L187 I188 W189 K190 Q196 M197 K198 I201 Q202 T203 M204 C205 P206 I207 E208 G209 I213 A214 R215 S219 Q223 K224 N229
I233 A240 I241 F242 Q243 L244 V284 L285 G289 GLY CYS S292 A310 P311 F312 N313 T314 L319 LYS LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.67Å 111.77Å 181.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.50 – 2.60 46.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.50-2.60) 97.7 (46.34-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.189 , 0.247 0.202 , 0.247	Depositor DCC
R_{free} test set	1997 reflections (3.35%)	DCC
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11266	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.75 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.1252e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.70	0/1313	0.62	0/1793
1	C	0.70	0/1338	0.64	0/1823
1	E	0.85	0/1326	0.65	0/1805
1	G	0.55	0/1308	0.58	0/1786
2	B	0.65	0/1595	1.04	10/2174 (0.5%)
2	D	0.60	0/1516	0.72	0/2065
2	F	0.70	0/1566	0.71	0/2128
2	H	0.58	0/1463	0.75	0/1994
All	All	0.67	0/11425	0.74	10/15568 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	181[A]	TYR	CA-C-O	-15.80	86.91	120.10
2	B	181[B]	TYR	CA-C-O	-15.80	86.91	120.10
2	B	181[A]	TYR	CA-C-N	14.51	149.13	117.20
2	B	181[B]	TYR	CA-C-N	14.51	149.13	117.20
2	B	257[A]	ARG	CA-C-O	7.95	136.80	120.10
2	B	257[B]	ARG	CA-C-O	7.95	136.80	120.10
2	B	181[A]	TYR	N-CA-C	7.23	130.53	111.00
2	B	181[B]	TYR	N-CA-C	7.23	130.53	111.00
2	B	257[A]	ARG	CA-C-N	-6.59	102.71	117.20
2	B	257[B]	ARG	CA-C-N	-6.59	102.71	117.20

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	1286	0	1240	24	0
1	C	1311	0	1280	18	0
1	E	1299	0	1281	22	0
1	G	1281	0	1239	21	0
2	B	1556	0	1528	37	0
2	D	1483	0	1482	44	0
2	F	1535	0	1546	29	0
2	H	1436	0	1412	66	0
3	B	6	0	8	0	0
3	D	6	0	8	0	0
4	A	11	0	0	0	0
4	B	6	0	0	0	0
4	C	14	0	0	0	0
4	D	10	0	0	0	0
4	E	11	0	0	0	0
4	F	9	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
All	All	11266	0	11024	243	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 11.

All (243) 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:105:CYS:HB2	2:F:205:CYS:SG	1.88	1.14
2:H:163:GLU:HA	2:H:166:LEU:HD12	1.35	1.03
2:F:112:LEU:HD12	2:F:113:GLY:N	1.78	0.99
2:H:152:VAL:HG13	2:H:187:LEU:HD23	1.58	0.86
2:D:149:LEU:CD1	2:D:181:TYR:CB	2.55	0.84
2:D:149:LEU:HD11	2:D:181:TYR:CB	2.08	0.84
1:E:105:CYS:HB2	2:F:205:CYS:HG	1.43	0.81
1:E:105:CYS:CB	2:F:205:CYS:SG	2.68	0.81
2:B:248:SER:OG	2:B:251:GLU:HG3	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:201:ILE:O	2:H:201:ILE:HD12	1.84	0.78
2:H:165:LEU:O	2:H:168:CYS:HB3	1.84	0.78
2:B:110:SER:HB3	2:B:118:ALA:HB1	1.66	0.77
1:G:20:ALA:O	1:G:24:VAL:HG22	1.85	0.76
2:H:147:ARG:HG3	2:H:182:GLN:HG3	1.69	0.75
1:E:105:CYS:CB	2:F:205:CYS:HG	2.01	0.73
2:D:318:LEU:N	2:D:318:LEU:HD23	2.04	0.73
2:B:112:LEU:HD23	2:B:112:LEU:N	2.05	0.72
1:E:93:ASP:N	1:E:93:ASP:OD1	2.22	0.72
2:B:178:ARG:HB3	2:B:178:ARG:CZ	2.19	0.72
2:H:188:ILE:HD11	2:H:190:LYS:CB	2.19	0.72
2:B:178:ARG:HB3	2:B:178:ARG:NH1	2.05	0.71
2:H:126:ALA:O	2:H:189:TRP:CE3	2.43	0.71
2:H:127:ASN:HA	2:H:189:TRP:HE3	1.54	0.71
2:D:161:VAL:HG23	2:D:166:LEU:HG	1.73	0.71
2:H:163:GLU:CA	2:H:166:LEU:HD12	2.17	0.71
2:H:319:LEU:N	2:H:319:LEU:HD12	2.05	0.71
2:F:131:PRO:O	2:F:287:GLN:NE2	2.23	0.71
2:H:163:GLU:O	2:H:167:LYS:N	2.23	0.71
1:G:27:ASP:OD2	1:G:64:THR:HB	1.90	0.70
1:E:103:ASN:OD1	1:E:144:PRO:HB2	1.91	0.70
1:A:27:ASP:N	1:A:27:ASP:OD1	2.21	0.69
1:G:9:ASN:HB2	1:G:37:GLU:HA	1.74	0.69
1:A:21:VAL:HG13	1:A:30:ILE:HD13	1.76	0.68
2:H:313:ASN:OD1	2:H:314:THR:N	2.27	0.67
1:A:106:LEU:O	1:A:149:ARG:NH2	2.28	0.66
1:C:89:LEU:HB3	1:C:127:THR:HG21	1.78	0.66
2:B:178:ARG:HG3	2:B:178:ARG:HH11	1.61	0.66
2:D:288:ILE:C	2:D:288:ILE:HD12	2.16	0.66
2:H:188:ILE:HD12	2:H:188:ILE:C	2.15	0.66
2:H:163:GLU:O	2:H:166:LEU:N	2.29	0.65
2:F:112:LEU:HD12	2:F:112:LEU:C	2.15	0.65
2:D:202:GLN:O	2:D:203:THR:HB	1.96	0.64
1:E:103:ASN:OD1	1:E:144:PRO:CB	2.45	0.64
2:B:178:ARG:CG	2:B:178:ARG:HH11	2.11	0.64
2:H:127:ASN:HA	2:H:189:TRP:CE3	2.33	0.64
2:H:188:ILE:HD12	2:H:189:TRP:N	2.14	0.63
2:F:107:ASP:OD1	2:F:108:LEU:N	2.25	0.63
1:A:42:VAL:HB	1:A:46:VAL:HG22	1.81	0.63
1:G:94:SER:HB2	1:G:97:SER:HB3	1.80	0.62
1:C:28:VAL:HG21	1:C:61:VAL:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:GLY:O	1:G:168:ASP:HB2	1.99	0.61
2:H:168:CYS:SG	2:H:169:PHE:CD2	2.94	0.61
2:H:139:HIS:CE1	2:H:143:CYS:SG	2.94	0.61
2:B:109:ASN:OD1	2:B:110:SER:N	2.33	0.61
2:B:310:ALA:O	2:B:314:THR:HG23	2.00	0.61
2:H:168:CYS:SG	2:H:169:PHE:CE2	2.94	0.61
2:H:168:CYS:SG	2:H:169:PHE:CZ	2.94	0.61
2:H:168:CYS:SG	2:H:169:PHE:CG	2.94	0.61
1:E:50:ASP:CG	1:E:53:SER:HB2	2.21	0.61
2:F:111:VAL:HG12	2:F:111:VAL:O	2.00	0.61
2:D:152:VAL:O	2:D:153:HIS:HD2	1.85	0.60
2:D:133:LEU:HB3	2:D:287:GLN:OE1	2.01	0.60
2:H:164:ASN:OD1	2:H:165:LEU:N	2.32	0.60
2:H:319:LEU:H	2:H:319:LEU:HD12	1.67	0.60
1:E:41:HIS:HA	1:E:47:ILE:HG22	1.84	0.60
2:H:168:CYS:SG	2:H:169:PHE:CE1	2.94	0.60
2:H:127:ASN:C	2:H:189:TRP:CZ3	2.75	0.59
2:H:188:ILE:HD12	2:H:189:TRP:C	2.23	0.58
1:C:88:LYS:NZ	2:D:208:GLU:OE1	2.36	0.58
1:G:88:LYS:NZ	2:H:208:GLU:OE1	2.36	0.58
1:G:52:ASN:OD1	1:G:82:LEU:HB3	2.04	0.58
2:D:153:HIS:HB2	2:D:188:ILE:HG13	1.86	0.57
1:E:105:CYS:SG	2:F:205:CYS:SG	3.02	0.57
1:G:83:GLU:HG2	2:H:242:PHE:HZ	1.70	0.57
2:D:190:LYS:HD2	2:D:192:VAL:HG13	1.87	0.57
2:F:273:GLU:OE1	2:F:273:GLU:N	2.35	0.57
2:H:153:HIS:O	2:H:188:ILE:HA	2.05	0.57
1:A:72:LEU:HD23	2:B:112:LEU:HD13	1.87	0.56
1:C:103:ASN:OD1	1:C:144:PRO:HB2	2.05	0.56
1:A:136:GLU:O	1:A:140:GLN:HG3	2.05	0.56
2:D:303:MET:O	2:D:307:GLU:HG3	2.06	0.56
2:F:112:LEU:CD1	2:F:113:GLY:N	2.63	0.56
1:C:117:LEU:HD21	1:C:122:LEU:HD21	1.88	0.55
2:F:267:PRO:HG2	2:F:272:ASN:HA	1.87	0.55
2:F:108:LEU:O	2:F:112:LEU:HD23	2.06	0.55
2:F:140:ARG:HB2	2:F:311:PRO:HB3	1.89	0.55
2:D:161:VAL:CG2	2:D:166:LEU:HG	2.37	0.54
2:H:127:ASN:CA	2:H:189:TRP:CE3	2.90	0.54
1:E:50:ASP:OD1	1:E:53:SER:HB2	2.08	0.54
2:H:310:ALA:HB3	2:H:311:PRO:HD3	1.90	0.54
1:A:73:MET:SD	2:B:199:PHE:CE2	3.01	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:VAL:HG13	2:B:295:VAL:HG23	1.89	0.54
2:F:240:ALA:HB2	2:F:281:LEU:HG	1.88	0.54
2:H:149:LEU:HD22	2:H:181:TYR:CB	2.38	0.54
1:A:21:VAL:HG13	1:A:30:ILE:HG21	1.90	0.54
2:B:251:GLU:O	2:B:255:VAL:HG23	2.08	0.54
2:H:133:LEU:HD22	2:H:137:VAL:HG23	1.90	0.54
1:E:164:GLY:O	1:E:168:ASP:HB2	2.08	0.53
2:H:151:THR:HG22	2:H:152:VAL:N	2.23	0.53
2:H:126:ALA:O	2:H:189:TRP:HE3	1.90	0.53
1:C:104:HIS:NE2	2:D:204:MET:HE2	2.23	0.53
2:D:223:GLN:OE1	2:D:223:GLN:N	2.41	0.53
2:F:112:LEU:HD12	2:F:113:GLY:CA	2.38	0.53
2:D:292:SER:OG	2:D:292:SER:O	2.26	0.53
1:A:59:ALA:HB2	1:A:119:LEU:HD21	1.91	0.52
1:C:85:SER:O	1:C:90:SER:OG	2.28	0.52
2:D:196:GLN:HG2	2:D:208:GLU:HG2	1.92	0.52
2:H:215:ARG:O	2:H:219:SER:OG	2.25	0.52
2:B:133:LEU:O	2:B:137:VAL:HG23	2.09	0.52
2:H:123:VAL:HG12	2:H:186:THR:HB	1.91	0.52
2:H:152:VAL:CG1	2:H:187:LEU:HD23	2.35	0.52
1:E:79:ASP:HB3	2:F:212:ASN:OD1	2.10	0.52
2:B:178:ARG:NH1	2:B:178:ARG:CB	2.73	0.52
2:F:141:LEU:HD23	2:F:311:PRO:HG2	1.92	0.52
2:H:209:GLY:O	2:H:213:ILE:HG13	2.10	0.51
2:D:164:ASN:ND2	2:D:318:LEU:O	2.44	0.51
1:C:107:SER:CB	1:C:146:HIS:CE1	2.94	0.51
1:E:140:GLN:O	1:E:140:GLN:HG3	2.10	0.50
2:F:108:LEU:HG	2:F:110:SER:H	1.77	0.50
2:D:128:PRO:HD3	2:D:189:TRP:HE3	1.75	0.50
1:G:2:ALA:HB2	1:G:29:SER:OG	2.12	0.50
2:H:223:GLN:O	2:H:224:LYS:HD3	2.12	0.50
2:D:148:VAL:HG22	2:D:183:LEU:HB3	1.93	0.50
2:H:154:THR:HG22	2:H:155:HIS:N	2.27	0.49
1:G:89:LEU:HB3	1:G:127:THR:HG21	1.95	0.49
1:C:104:HIS:NE2	2:D:204:MET:CE	2.76	0.49
1:C:107:SER:HA	1:C:146:HIS:ND1	2.28	0.48
2:B:194:LYS:HD2	2:B:208:GLU:HB3	1.93	0.48
2:B:260:ASN:CG	2:B:296:PRO:HB3	2.34	0.48
2:B:240:ALA:HB2	2:B:281:LEU:HG	1.95	0.48
2:B:123:VAL:HG22	2:B:186:THR:HB	1.95	0.48
2:F:266:SER:HB2	2:F:268:TRP:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:ARG:CD	2:D:180:ASP:O	2.61	0.48
1:C:93:ASP:OD1	1:C:93:ASP:N	2.46	0.48
2:D:158:VAL:CG1	2:D:159:LYS:N	2.77	0.48
2:H:127:ASN:O	2:H:131:PRO:HA	2.12	0.48
2:D:158:VAL:HG12	2:D:159:LYS:N	2.30	0.47
2:F:164:ASN:N	2:F:164:ASN:OD1	2.47	0.47
1:G:96:THR:HA	1:G:99:ILE:HG22	1.97	0.47
1:C:76:THR:HG22	2:D:207:ILE:HG12	1.98	0.46
2:B:260:ASN:OD1	2:B:296:PRO:CB	2.63	0.46
2:H:152:VAL:HG22	2:H:169:PHE:CE2	2.49	0.46
1:E:93:ASP:O	1:E:94:SER:HB2	2.14	0.46
1:G:2:ALA:CB	1:G:29:SER:OG	2.62	0.46
2:B:178:ARG:CG	2:B:178:ARG:NH1	2.72	0.46
2:H:125:ASN:CB	2:H:196:GLN:HG2	2.46	0.46
2:H:128:PRO:HA	2:H:131:PRO:HG3	1.98	0.45
2:H:285:LEU:HA	2:H:285:LEU:HD23	1.75	0.45
1:A:8:VAL:HG11	1:A:18:LEU:HD21	1.97	0.45
2:B:178:ARG:CB	2:B:178:ARG:CZ	2.91	0.45
2:D:200:SER:HB2	2:D:202:GLN:HB3	1.96	0.45
1:G:99:ILE:HD11	1:G:147:VAL:HG11	1.97	0.45
2:H:126:ALA:O	2:H:189:TRP:HA	2.17	0.45
2:D:209:GLY:O	2:D:213:ILE:HG13	2.17	0.45
2:H:147:ARG:NH1	2:H:182:GLN:HG2	2.31	0.45
2:D:161:VAL:HG23	2:D:166:LEU:CG	2.45	0.45
2:H:319:LEU:N	2:H:319:LEU:CD1	2.77	0.45
1:A:30:ILE:HG23	1:A:30:ILE:O	2.16	0.45
2:B:241:ILE:HG22	2:B:242:PHE:CD1	2.52	0.45
1:C:110:THR:HG23	1:E:110:THR:HG23	1.98	0.45
2:B:164:ASN:OD1	2:B:164:ASN:N	2.39	0.45
2:D:288:ILE:CD1	2:D:288:ILE:C	2.85	0.45
1:A:107:SER:OG	1:A:108:LEU:HG	2.16	0.45
1:A:73:MET:SD	2:B:199:PHE:HE2	2.40	0.44
1:A:108:LEU:HD23	1:G:145:VAL:HG13	1.98	0.44
1:A:17:ALA:O	1:A:21:VAL:HG23	2.17	0.44
2:D:282:TRP:CZ2	2:D:307:GLU:HG2	2.52	0.44
1:E:99:ILE:HD11	1:E:147:VAL:HG11	1.99	0.44
2:B:178:ARG:N	2:B:181[B]:TYR:HH	2.15	0.44
1:C:4:LEU:HD12	1:C:4:LEU:HA	1.82	0.44
2:H:147:ARG:HG3	2:H:182:GLN:CG	2.45	0.44
2:B:303:MET:O	2:B:307:GLU:HG3	2.18	0.44
2:D:122:ILE:HD12	2:D:183:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:VAL:CG2	2:D:166:LEU:CG	2.95	0.44
2:D:147:ARG:HD3	2:D:180:ASP:O	2.18	0.44
2:H:164:ASN:N	2:H:164:ASN:OD1	2.50	0.44
1:A:143:ALA:HA	1:A:144:PRO:HD3	1.87	0.44
1:A:43:SER:OG	1:A:46:VAL:HG13	2.17	0.44
2:H:163:GLU:HA	2:H:166:LEU:CD1	2.26	0.43
1:A:79:ASP:HB3	2:B:212:ASN:OD1	2.17	0.43
1:E:89:LEU:HB3	1:E:127:THR:HG21	1.99	0.43
2:F:310:ALA:HA	2:F:313:ASN:ND2	2.33	0.43
2:H:168:CYS:SG	2:H:169:PHE:CD1	2.94	0.43
2:D:163:GLU:O	2:D:167:LYS:N	2.51	0.43
2:F:307:GLU:O	2:F:313:ASN:OD1	2.37	0.43
2:H:168:CYS:SG	2:H:169:PHE:N	2.92	0.43
2:B:168:CYS:HB2	2:B:318:LEU:HD23	2.00	0.43
2:D:147:ARG:HD2	2:D:180:ASP:O	2.18	0.43
1:C:99:ILE:HA	1:C:99:ILE:HD12	1.89	0.43
1:G:84:PHE:HE1	1:G:89:LEU:HD22	1.84	0.43
2:H:224:LYS:HD3	2:H:224:LYS:HA	1.71	0.43
2:D:152:VAL:C	2:D:153:HIS:HD2	2.23	0.42
1:G:125:TRP:CH2	1:G:129:LYS:HD2	2.54	0.42
2:B:260:ASN:OD1	2:B:296:PRO:HB3	2.19	0.42
2:D:138:LEU:HD13	2:D:217:LEU:HB2	2.01	0.42
2:F:169:PHE:HZ	2:F:185:PHE:HE1	1.67	0.42
2:F:280:VAL:O	2:F:284:VAL:HG23	2.19	0.42
2:H:201:ILE:HD12	2:H:201:ILE:C	2.40	0.42
2:H:310:ALA:O	2:H:313:ASN:OD1	2.37	0.42
2:F:241:ILE:HG22	2:F:242:PHE:CD1	2.54	0.42
2:B:260:ASN:OD1	2:B:296:PRO:HB2	2.19	0.42
1:E:89:LEU:HD21	1:E:128:LEU:HD13	2.02	0.42
2:B:110:SER:HB3	2:B:118:ALA:CB	2.44	0.42
2:B:107:ASP:O	2:B:108:LEU:HB3	2.20	0.42
2:F:169:PHE:HZ	2:F:185:PHE:CE1	2.37	0.42
1:C:134:TRP:CH2	1:C:147:VAL:HG12	2.55	0.42
2:H:127:ASN:C	2:H:189:TRP:HZ3	2.23	0.42
2:H:127:ASN:CA	2:H:189:TRP:CZ3	3.03	0.42
1:A:128:LEU:HD12	1:A:128:LEU:HA	1.85	0.41
1:C:13:PRO:HA	1:C:14:PRO:HD2	1.91	0.41
1:A:107:SER:HA	1:A:146:HIS:CE1	2.55	0.41
2:D:295:VAL:HA	2:D:296:PRO:HD3	1.76	0.41
2:H:164:ASN:CG	2:H:165:LEU:N	2.73	0.41
1:A:107:SER:HA	1:A:146:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:HB	1:A:4:LEU:H	1.52	0.41
1:E:103:ASN:OD1	1:E:144:PRO:HB3	2.17	0.41
1:G:109:ARG:NH1	1:G:112:LEU:O	2.54	0.41
2:H:139:HIS:C	2:H:139:HIS:ND1	2.73	0.41
2:H:152:VAL:HG13	2:H:187:LEU:CD2	2.41	0.41
2:H:163:GLU:O	2:H:164:ASN:C	2.58	0.41
1:A:19:LEU:HD11	1:A:125:TRP:CZ3	2.56	0.41
2:D:318:LEU:HD23	2:D:318:LEU:H	1.83	0.41
1:G:13:PRO:HA	1:G:14:PRO:HD3	1.98	0.41
2:H:229:ASN:O	2:H:233:ILE:HG13	2.21	0.41
2:D:138:LEU:CD1	2:D:214:ALA:HA	2.50	0.41
1:C:108:LEU:HA	1:C:108:LEU:HD23	1.89	0.41
1:G:89:LEU:HD12	1:G:89:LEU:HA	1.91	0.41
2:D:269:LEU:HD11	2:D:281:LEU:HD23	2.02	0.41
2:B:316:LEU:HA	2:B:316:LEU:HD12	1.90	0.41
1:G:84:PHE:CE1	1:G:89:LEU:HD22	2.56	0.40
2:B:309:LEU:HD23	2:B:309:LEU:HA	1.91	0.40
2:B:203:THR:OG1	2:B:204:MET:N	2.55	0.40
1:E:131:ASN:OD1	1:E:133:ALA:HB3	2.21	0.40
1:G:73:MET:O	1:G:77:GLU:HG3	2.22	0.40
2:H:240:ALA:O	2:H:284:VAL:HG21	2.21	0.40
2:D:152:VAL:O	2:D:153:HIS:CD2	2.70	0.40
2:D:248:SER:HB2	2:D:251:GLU:H	1.87	0.40
2:F:155:HIS:CE1	2:F:157:SER:HG	2.33	0.40
2:H:215:ARG:HH11	2:H:215:ARG:HD2	1.72	0.40
1:A:149:ARG:HG2	1:A:149:ARG:NH1	2.37	0.40
1:E:142:LYS:CG	1:E:142:LYS:O	2.70	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	166/175 (95%)	162 (98%)	4 (2%)	0	100	100
1	C	168/175 (96%)	161 (96%)	7 (4%)	0	100	100
1	E	165/175 (94%)	162 (98%)	3 (2%)	0	100	100
1	G	166/175 (95%)	158 (95%)	8 (5%)	0	100	100
2	B	200/240 (83%)	194 (97%)	6 (3%)	0	100	100
2	D	189/240 (79%)	182 (96%)	7 (4%)	0	100	100
2	F	193/240 (80%)	189 (98%)	4 (2%)	0	100	100
2	H	183/240 (76%)	174 (95%)	9 (5%)	0	100	100
All	All	1430/1660 (86%)	1382 (97%)	48 (3%)	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	140/151 (93%)	132 (94%)	8 (6%)	24	47
1	C	144/151 (95%)	134 (93%)	10 (7%)	18	36
1	E	144/151 (95%)	133 (92%)	11 (8%)	15	30
1	G	138/151 (91%)	135 (98%)	3 (2%)	57	81
2	B	167/211 (79%)	158 (95%)	9 (5%)	26	49
2	D	161/211 (76%)	151 (94%)	10 (6%)	21	42
2	F	168/211 (80%)	158 (94%)	10 (6%)	22	44
2	H	152/211 (72%)	135 (89%)	17 (11%)	7	12
All	All	1214/1448 (84%)	1136 (94%)	78 (6%)	20	40

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	43	SER

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Mol	Chain	Res	Type
1	A	63	THR
1	A	64	THR
1	A	68	TYR
1	A	70	SER
1	A	148	LYS
1	A	149	ARG
2	B	140	ARG
2	B	150	SER
2	B	164	ASN
2	B	178	ARG
2	B	198	LYS
2	B	249	SER
2	B	266	SER
2	B	281	LEU
2	B	293	VAL
1	C	61	VAL
1	C	68	TYR
1	C	70	SER
1	C	89	LEU
1	C	90	SER
1	C	92	CYS
1	C	93	ASP
1	C	94	SER
1	C	139	LYS
1	C	170	SER
2	D	119	LEU
2	D	145[A]	HIS
2	D	145[B]	HIS
2	D	150	SER
2	D	154	THR
2	D	203	THR
2	D	219	SER
2	D	248	SER
2	D	258	SER
2	D	318	LEU
1	E	43	SER
1	E	53	SER
1	E	61	VAL
1	E	63	THR
1	E	68	TYR
1	E	73	MET
1	E	93	ASP

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Mol	Chain	Res	Type
1	E	94	SER
1	E	116	SER
1	E	139	LYS
1	E	141	LYS
2	F	156	SER
2	F	201	ILE
2	F	204	MET
2	F	205	CYS
2	F	266	SER
2	F	281	LEU
2	F	288	ILE
2	F	292	SER
2	F	313	ASN
2	F	317	LYS
1	G	61	VAL
1	G	68	TYR
1	G	162	SER
2	H	130	SER
2	H	132	PRO
2	H	133	LEU
2	H	138	LEU
2	H	139	HIS
2	H	141	LEU
2	H	147	ARG
2	H	149	LEU
2	H	155	HIS
2	H	183	LEU
2	H	185	PHE
2	H	187	LEU
2	H	188	ILE
2	H	196	GLN
2	H	201	ILE
2	H	202	GLN
2	H	205	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	139	HIS
2	D	153	HIS
1	E	146	HIS
2	F	286	GLN

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Mol	Chain	Res	Type
2	H	153	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	$\#\|Z\| > 2$
3	GOL	B	1321	-	5,5,5	0.30	0	5,5,5	0.39	0
3	GOL	D	1321	-	5,5,5	0.29	0	5,5,5	0.73	0

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
3	GOL	B	1321	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1321	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	168/175 (96%)	-0.31	0 100 100	42, 69, 118, 145	0
1	C	170/175 (97%)	-0.16	2 (1%) 79 75	30, 58, 101, 143	0
1	E	167/175 (95%)	-0.35	0 100 100	25, 55, 101, 120	0
1	G	168/175 (96%)	-0.00	8 (4%) 31 24	48, 71, 106, 152	0
2	B	204/240 (85%)	-0.07	6 (2%) 52 45	38, 72, 127, 153	0
2	D	196/240 (81%)	0.20	11 (5%) 25 19	44, 75, 130, 166	0
2	F	201/240 (83%)	-0.10	2 (0%) 82 79	38, 57, 111, 144	0
2	H	193/240 (80%)	0.47	21 (10%) 6 4	49, 91, 138, 157	0
All	All	1467/1660 (88%)	-0.03	50 (3%) 46 38	25, 68, 125, 166	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	291	CYS	6.4
1	C	2	ALA	5.1
2	H	160	SER	5.0
2	H	189	TRP	4.8
2	H	169	PHE	4.8
2	H	204	MET	4.5
1	G	137	GLN	4.0
2	H	168	CYS	3.8
1	G	169	VAL	3.7
2	D	161	VAL	3.5
2	H	157	SER	3.5
2	H	201	ILE	3.5
2	H	126	ALA	3.4
2	H	156	SER	3.4
2	B	316	LEU	3.2
2	H	161	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	94	SER	3.1
2	D	293	VAL	3.1
2	F	319	LEU	2.9
2	H	154	THR	2.9
2	H	127	ASN	2.9
2	D	159	LYS	2.8
1	G	92	CYS	2.7
2	H	146	PHE	2.7
2	H	206	PRO	2.7
1	G	89	LEU	2.6
2	B	293	VAL	2.6
1	G	93	ASP	2.6
2	D	180	ASP	2.5
2	H	112	LEU	2.5
2	F	201	ILE	2.5
2	D	189	TRP	2.5
2	D	112	LEU	2.5
1	G	83	GLU	2.5
2	D	158	VAL	2.4
1	C	3	THR	2.4
2	H	155	HIS	2.3
2	B	140	ARG	2.3
2	D	187	LEU	2.3
1	G	96	THR	2.2
2	B	113	GLY	2.2
2	D	156	SER	2.2
2	D	192	VAL	2.2
2	B	116	TYR	2.1
2	H	166	LEU	2.1
2	H	185	PHE	2.1
2	B	273	GLU	2.1
2	H	152	VAL	2.1
2	H	244	LEU	2.1
2	H	198	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	B	1321	6/6	0.85	0.27	6.15	102,109,110,112	0
3	GOL	D	1321	6/6	0.83	0.38	-	97,106,110,112	0

6.5 Other polymers (i)

There are no such residues in this entry.