



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2016 – 05:17 PM EDT

PDB ID : 5A5H  
Title : The crystal structure of the GST-like domains complex of EPRS  
C92SC105SC123S mutant-AIMP2  
Authors : Cho, H.Y.; Kang, B.S.  
Deposited on : 2015-06-18  
Resolution : 2.32 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20027790

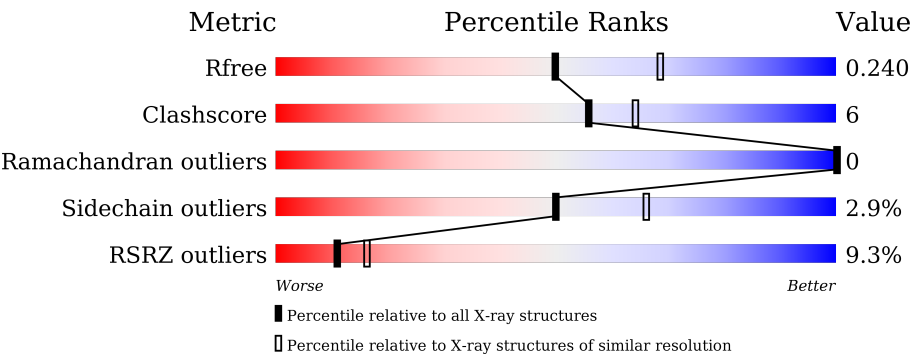
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 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))
$R_{free}$	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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  $\geq 3$ , 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	175	<div><div>2%</div><div>88%</div><div>7%</div><div>.</div><div>.</div></div>
1	C	175	<div><div>2%</div><div>89%</div><div>7%</div><div>.</div></div>
1	E	175	<div><div>4%</div><div>91%</div><div>5%</div><div>.</div></div>
1	G	175	<div><div>7%</div><div>86%</div><div>10%</div><div>.</div></div>
2	B	240	<div><div>10%</div><div>74%</div><div>11%</div><div>.</div><div>13%</div></div>
2	D	240	<div><div>12%</div><div>80%</div><div>9%</div><div>11%</div></div>

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

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11755 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 LIG-ASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	Se	0	0	0
			1293	820	218	254	1			
1	C	168	Total	C	N	O	Se	0	0	0
			1303	827	219	256	1			
1	E	168	Total	C	N	O	Se	0	0	0
			1302	827	219	255	1			
1	G	169	Total	C	N	O	Se	0	0	0
			1308	829	220	258	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	SER	CYS	ENGINEERED MUTATION	UNP P07814
A	105	SER	CYS	ENGINEERED MUTATION	UNP P07814
A	123	SER	CYS	ENGINEERED MUTATION	UNP P07814
C	92	SER	CYS	ENGINEERED MUTATION	UNP P07814
C	105	SER	CYS	ENGINEERED MUTATION	UNP P07814
C	123	SER	CYS	ENGINEERED MUTATION	UNP P07814
E	92	SER	CYS	ENGINEERED MUTATION	UNP P07814
E	105	SER	CYS	ENGINEERED MUTATION	UNP P07814
E	123	SER	CYS	ENGINEERED MUTATION	UNP P07814
G	92	SER	CYS	ENGINEERED MUTATION	UNP P07814
G	105	SER	CYS	ENGINEERED MUTATION	UNP P07814
G	123	SER	CYS	ENGINEERED MUTATION	UNP P07814

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1597	1026	276	286	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	213	Total	C	N	O	S	0	0	0
			1607	1030	279	290	8			
2	F	195	Total	C	N	O	S	0	0	0
			1492	958	260	266	8			
2	H	189	Total	C	N	O	S	0	0	0
			1444	929	247	259	9			

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

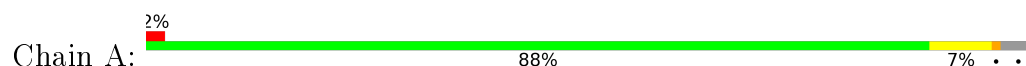
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total 54	O 54	0	0
3	B	42	Total 42	O 42	0	0
3	C	100	Total 100	O 100	0	0
3	D	44	Total 44	O 44	0	0
3	E	72	Total 72	O 72	0	0
3	F	66	Total 66	O 66	0	0
3	G	26	Total 26	O 26	0	0
3	H	5	Total 5	O 5	0	0

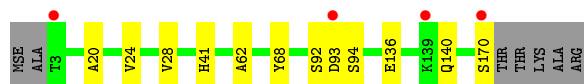
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

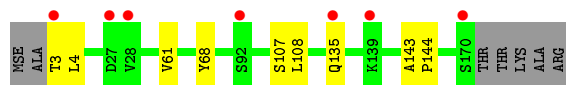
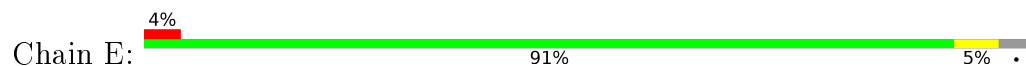
- Molecule 1: BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE



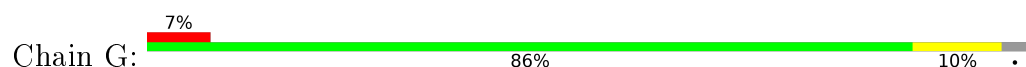
- Molecule 1: BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE



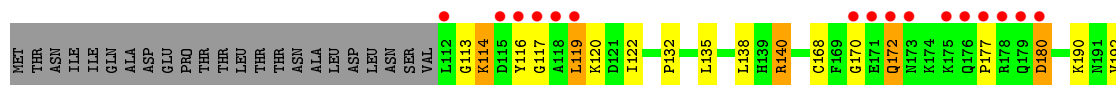
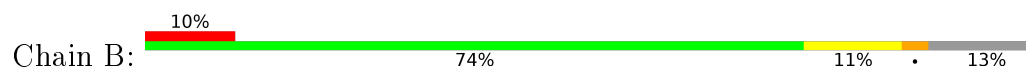
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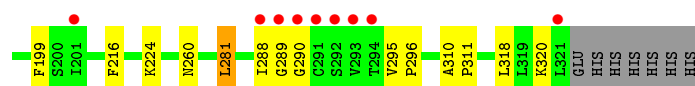


- Molecule 1: BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE

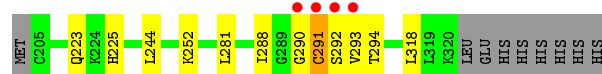
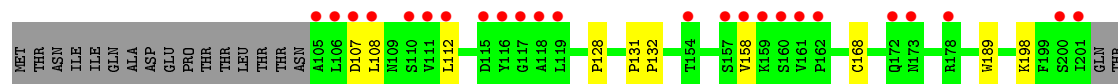
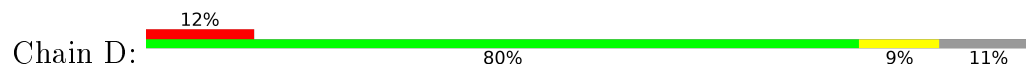


- Molecule 2: AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONAL PROTEIN 2

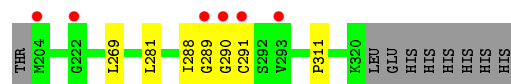
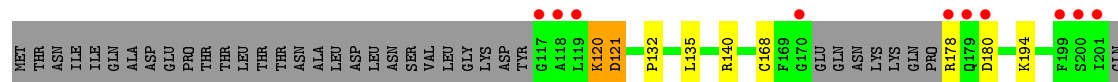
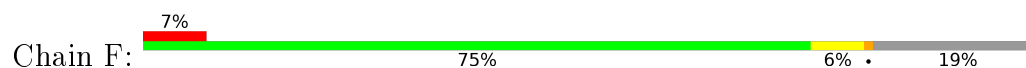




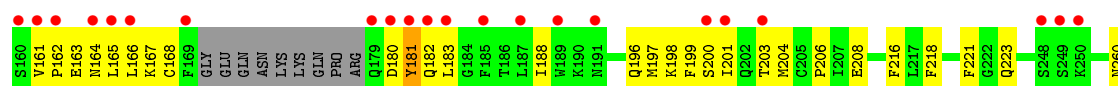
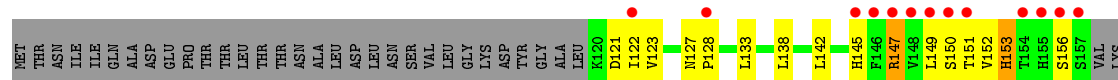
• Molecule 2: AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONAL PROTEIN 2



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.69Å 112.79Å 181.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.80 – 2.32 36.81 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.80-2.32) 95.0 (36.81-2.32)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.67 (at 2.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.172 , 0.227 0.189 , 0.240	Depositor DCC
$R_{free}$ test set	1959 reflections (2.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0/1319	0.51	0/1798
1	C	0.49	0/1329	0.56	0/1809
1	E	0.44	0/1328	0.52	0/1807
1	G	0.33	0/1334	0.47	0/1817
2	B	0.53	0/1633	0.73	5/2221 (0.2%)
2	D	0.50	0/1641	0.57	0/2235
2	F	0.54	0/1524	0.61	2/2070 (0.1%)
2	H	0.54	0/1476	0.68	1/2011 (0.0%)
All	All	0.48	0/11584	0.59	8/15768 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	117	GLY	N-CA-C	-11.12	85.31	113.10
2	F	290	GLY	N-CA-C	-10.31	87.33	113.10
2	B	290	GLY	N-CA-C	6.85	130.23	113.10
2	B	281	LEU	CA-CB-CG	-5.72	102.15	115.30
2	B	180	ASP	N-CA-C	5.56	126.00	111.00
2	B	289	GLY	N-CA-C	5.47	126.78	113.10
2	F	291	CYS	CA-CB-SG	-5.17	104.69	114.00
2	H	147	ARG	N-CA-C	-5.12	97.17	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1293	0	1253	9	0
1	C	1303	0	1272	6	0
1	E	1302	0	1275	3	0
1	G	1308	0	1275	11	0
2	B	1597	0	1587	26	0
2	D	1607	0	1586	12	0
2	F	1492	0	1492	9	0
2	H	1444	0	1430	66	0
3	A	54	0	0	2	0
3	B	42	0	0	0	0
3	C	100	0	0	1	0
3	D	44	0	0	0	0
3	E	72	0	0	1	0
3	F	66	0	0	0	0
3	G	26	0	0	0	0
3	H	5	0	0	0	0
All	All	11755	0	11170	140	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 (140) 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)
2:D:291:CYS:SG	2:D:292:SER:N	2.19	1.12
2:H:149:LEU:HD22	2:H:181:TYR:CE2	1.85	1.11
2:H:201:ILE:HG13	2:H:203:THR:HG22	1.41	1.03
2:H:149:LEU:HD22	2:H:181:TYR:HE2	1.16	0.96
2:H:151:THR:CG2	2:H:153:HIS:HE1	1.79	0.96
2:B:177:PRO:CB	2:B:180:ASP:HB2	2.00	0.92
2:H:151:THR:HG22	2:H:153:HIS:CE1	2.09	0.88
2:H:201:ILE:CG1	2:H:203:THR:HG22	2.05	0.86
2:B:177:PRO:HB2	2:B:180:ASP:HB2	1.59	0.83
2:H:151:THR:CG2	2:H:153:HIS:CE1	2.63	0.81
2:H:152:VAL:O	2:H:153:HIS:ND1	2.15	0.80
2:H:147:ARG:HD2	2:H:180:ASP:O	1.80	0.80
2:B:177:PRO:HB3	2:B:180:ASP:HB2	1.66	0.77
2:B:122:ILE:HG12	2:B:199:PHE:HE1	1.51	0.76
2:B:172:GLN:O	2:B:172:GLN:HG3	1.88	0.73
2:B:140:ARG:NH2	2:B:168:CYS:O	2.22	0.72
2:H:201:ILE:CG2	2:H:203:THR:HG22	2.18	0.72
2:H:166:LEU:HD12	2:H:166:LEU:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:LEU:HD12	2:B:120:LYS:N	2.08	0.68
2:B:119:LEU:HD12	2:B:119:LEU:C	2.14	0.68
1:A:125:TRP:HZ2	1:A:155:GLU:HG3	1.60	0.65
2:B:170:GLY:O	2:B:172:GLN:N	2.28	0.65
2:H:133:LEU:HB2	2:H:287:GLN:OE1	1.97	0.65
2:H:201:ILE:HG13	2:H:203:THR:CG2	2.22	0.65
2:H:201:ILE:HG13	2:H:203:THR:H	1.62	0.64
1:G:3:THR:OG1	1:G:4:LEU:N	2.31	0.64
2:D:291:CYS:HG	2:D:292:SER:H	1.39	0.63
2:H:182:GLN:C	2:H:183:LEU:HG	2.19	0.63
2:H:203:THR:HG23	2:H:204:MET:N	2.14	0.62
2:H:201:ILE:HG23	2:H:203:THR:HG22	1.82	0.61
2:H:223:GLN:OE1	2:H:223:GLN:HA	2.01	0.61
2:B:114:LYS:HG2	2:B:114:LYS:O	2.00	0.60
2:H:152:VAL:C	2:H:153:HIS:ND1	2.53	0.60
2:H:133:LEU:CB	2:H:287:GLN:OE1	2.51	0.59
2:H:181:TYR:H	2:H:181:TYR:HD1	1.45	0.58
2:H:166:LEU:H	2:H:166:LEU:HD12	1.66	0.58
2:H:162:PRO:HD2	2:H:165:LEU:HD12	1.86	0.57
2:H:161:VAL:HG12	2:H:166:LEU:HD11	1.87	0.57
2:D:128:PRO:HG2	2:D:158:VAL:HG11	1.87	0.56
2:H:182:GLN:O	2:H:183:LEU:HG	2.05	0.56
2:D:168:CYS:HB2	2:D:318:LEU:HD13	1.88	0.55
2:F:140:ARG:NH2	2:F:168:CYS:O	2.40	0.55
1:A:20:ALA:O	1:A:24:VAL:HB	2.06	0.55
2:F:180:ASP:OD1	2:F:180:ASP:N	2.36	0.54
2:H:201:ILE:CG2	2:H:203:THR:CG2	2.85	0.54
2:H:138:LEU:HD21	2:H:218:PHE:HD2	1.73	0.54
2:H:181:TYR:CD1	2:H:181:TYR:N	2.73	0.53
2:H:122:ILE:HG23	2:H:197:MET:HE2	1.89	0.53
2:H:166:LEU:N	2:H:166:LEU:CD1	2.73	0.52
2:H:147:ARG:CD	2:H:180:ASP:O	2.52	0.52
2:H:138:LEU:HD21	2:H:218:PHE:CD2	2.45	0.52
2:B:168:CYS:HB2	2:B:318:LEU:HD13	1.92	0.51
2:H:196:GLN:HE21	2:H:206:PRO:HB3	1.76	0.51
2:H:180:ASP:CG	2:H:181:TYR:CD1	2.84	0.51
2:D:107:ASP:OD1	2:D:108:LEU:N	2.43	0.51
2:B:122:ILE:HG12	2:B:199:PHE:CE1	2.40	0.50
2:B:170:GLY:C	2:B:172:GLN:H	2.14	0.50
2:H:201:ILE:CG1	2:H:203:THR:CG2	2.85	0.50
2:B:170:GLY:C	2:B:172:GLN:N	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:166:LEU:H	2:H:166:LEU:CD1	2.24	0.49
2:H:180:ASP:CG	2:H:181:TYR:HD1	2.15	0.49
2:H:180:ASP:OD2	2:H:181:TYR:HD1	1.96	0.49
1:A:24:VAL:HG22	1:A:62:ALA:CB	2.43	0.48
1:G:80:HIS:CE1	2:H:208:GLU:HG2	2.48	0.48
2:D:128:PRO:HG3	2:D:189:TRP:HB3	1.94	0.48
2:F:140:ARG:HB2	2:F:311:PRO:HB3	1.94	0.48
1:A:36:LYS:O	1:A:36:LYS:HG2	2.14	0.47
1:C:20:ALA:O	1:C:24:VAL:HB	2.15	0.47
2:F:269:LEU:HD11	2:F:281:LEU:HD23	1.97	0.47
1:G:21:VAL:O	1:G:25:LYS:HB3	2.15	0.47
2:H:199:PHE:HD2	2:H:204:MET:HE2	1.79	0.47
2:H:161:VAL:CG1	2:H:166:LEU:HD11	2.45	0.47
2:H:182:GLN:O	2:H:183:LEU:HD23	2.15	0.47
1:C:93:ASP:OD1	1:C:94:SER:N	2.48	0.47
2:H:149:LEU:HD22	2:H:181:TYR:CD2	2.43	0.47
2:F:288:ILE:HG13	2:F:289:GLY:N	2.30	0.46
2:H:151:THR:HG21	2:H:153:HIS:HE1	1.73	0.46
1:C:136:GLU:OE2	1:C:140:GLN:NE2	2.49	0.46
2:B:190:LYS:HG2	2:B:192:VAL:HG13	1.97	0.46
1:C:24:VAL:HG13	1:C:28:VAL:HG22	1.98	0.46
1:G:109:ARG:NH2	2:H:203:THR:O	2.49	0.46
2:D:112:LEU:HD23	2:D:112:LEU:HA	1.68	0.45
1:A:91:SER:HB3	1:A:93:ASP:HB3	1.99	0.45
2:H:300:GLN:O	2:H:304:ARG:HG3	2.16	0.45
1:E:107:SER:HB3	1:E:108:LEU:HD12	1.97	0.45
2:B:132:PRO:HB2	2:B:135:LEU:HG	1.99	0.45
2:H:180:ASP:OD1	2:H:181:TYR:CE1	2.70	0.45
2:H:153:HIS:HB2	2:H:188:ILE:HG13	1.97	0.45
2:B:168:CYS:HA	2:B:318:LEU:HD22	1.98	0.44
2:H:182:GLN:O	2:H:183:LEU:CG	2.66	0.44
2:H:180:ASP:OD2	2:H:181:TYR:CD1	2.70	0.44
2:H:203:THR:HG23	2:H:204:MET:H	1.83	0.44
2:B:177:PRO:CB	2:B:180:ASP:CB	2.85	0.44
2:H:196:GLN:NE2	2:H:198:LYS:HE2	2.32	0.44
2:F:120:LYS:HA	2:F:120:LYS:HD2	1.77	0.44
2:B:177:PRO:HB3	2:B:180:ASP:CB	2.44	0.44
2:H:142:LEU:HD23	2:H:221:PHE:CZ	2.53	0.44
2:D:223:GLN:HG3	2:D:225:HIS:CE1	2.53	0.44
2:H:122:ILE:HG22	2:H:123:VAL:N	2.33	0.44
1:A:75:HIS:HE1	3:A:2022:HOH:O	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:TRP:CH2	1:G:129:LYS:HD2	2.53	0.43
2:H:164:ASN:O	2:H:167:LYS:CB	2.67	0.43
1:G:128:LEU:HA	1:G:128:LEU:HD12	1.81	0.43
2:D:293:VAL:HG12	2:D:294:THR:N	2.34	0.43
2:H:127:ASN:OD1	2:H:128:PRO:HD2	2.19	0.43
2:D:244:LEU:HD12	2:D:252:LYS:HG2	2.01	0.43
2:H:163:GLU:HA	2:H:166:LEU:HD13	1.99	0.43
1:G:143:ALA:HA	1:G:144:PRO:HD3	1.93	0.43
2:B:113:GLY:O	2:B:114:LYS:HB3	2.19	0.42
1:G:137:GLN:NE2	1:G:144:PRO:HD3	2.34	0.42
2:H:267:PRO:O	2:H:301:ARG:NH2	2.52	0.42
2:F:132:PRO:HB2	2:F:135:LEU:HG	2.02	0.42
2:H:152:VAL:HG12	2:H:153:HIS:N	2.33	0.42
1:A:125:TRP:CH2	1:A:129:LYS:HD2	2.54	0.42
2:H:197:MET:HE1	2:H:216:PHE:CE2	2.55	0.42
1:A:75:HIS:HD2	3:A:2025:HOH:O	2.02	0.42
2:D:288:ILE:HG13	2:D:290:GLY:H	1.84	0.42
2:F:120:LYS:HG3	2:F:121:ASP:OD1	2.19	0.42
2:B:224:LYS:HB2	2:B:224:LYS:HE3	1.72	0.42
2:B:310:ALA:HB3	2:B:311:PRO:HD3	2.02	0.42
2:H:199:PHE:CD2	2:H:204:MET:CE	3.03	0.42
1:G:41:HIS:HA	1:G:47:ILE:HD13	2.01	0.41
2:H:145:HIS:ND1	2:H:145:HIS:O	2.52	0.41
1:E:3:THR:OG1	1:E:4:LEU:N	2.51	0.41
2:B:119:LEU:CD1	2:B:119:LEU:C	2.85	0.41
3:E:2039:HOH:O	2:F:194:LYS:HE3	2.20	0.41
2:B:295:VAL:HA	2:B:296:PRO:HD3	1.78	0.41
1:E:143:ALA:HA	1:E:144:PRO:HD3	1.95	0.41
1:G:77:GLU:O	1:G:80:HIS:HB3	2.20	0.41
2:H:260:ASN:OD1	2:H:298:ASN:HB2	2.20	0.41
1:G:155:GLU:O	1:G:161:GLN:NE2	2.54	0.41
1:C:41:HIS:HB3	3:C:2031:HOH:O	2.20	0.41
1:C:24:VAL:HG22	1:C:62:ALA:CB	2.51	0.41
2:B:260:ASN:OD1	2:B:296:PRO:HB2	2.21	0.41
2:H:182:GLN:O	2:H:183:LEU:CD2	2.69	0.41
2:B:199:PHE:HZ	2:B:216:PHE:CE2	2.39	0.41
2:H:201:ILE:HG21	2:H:203:THR:CG2	2.52	0.40
1:A:128:LEU:HD12	1:A:128:LEU:HA	1.96	0.40
2:D:131:PRO:HA	2:D:132:PRO:HD3	1.97	0.40
2:H:266:SER:HB2	2:H:267:PRO:HD2	2.02	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	166/175 (95%)	160 (96%)	6 (4%)	0	100	100
1	C	166/175 (95%)	163 (98%)	3 (2%)	0	100	100
1	E	166/175 (95%)	163 (98%)	3 (2%)	0	100	100
1	G	167/175 (95%)	163 (98%)	4 (2%)	0	100	100
2	B	208/240 (87%)	198 (95%)	10 (5%)	0	100	100
2	D	209/240 (87%)	205 (98%)	4 (2%)	0	100	100
2	F	189/240 (79%)	183 (97%)	6 (3%)	0	100	100
2	H	183/240 (76%)	174 (95%)	9 (5%)	0	100	100
All	All	1454/1660 (88%)	1409 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	142/149 (95%)	138 (97%)	4 (3%)	51	67
1	C	144/149 (97%)	141 (98%)	3 (2%)	61	78
1	E	144/149 (97%)	141 (98%)	3 (2%)	61	78
1	G	145/149 (97%)	144 (99%)	1 (1%)	88	95
2	B	171/211 (81%)	162 (95%)	9 (5%)	28	37
2	D	171/211 (81%)	168 (98%)	3 (2%)	66	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	162/211 (77%)	159 (98%)	3 (2%)	65	80
2	H	158/211 (75%)	148 (94%)	10 (6%)	22	29
All	All	1237/1440 (86%)	1201 (97%)	36 (3%)	50	66

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	68	TYR
1	A	91	SER
1	A	97	SER
2	B	114	LYS
2	B	116	TYR
2	B	119	LEU
2	B	138	LEU
2	B	140	ARG
2	B	172	GLN
2	B	281	LEU
2	B	288	ILE
2	B	320	LYS
1	C	68	TYR
1	C	92	SER
1	C	170	SER
2	D	198	LYS
2	D	281	LEU
2	D	291	CYS
1	E	61	VAL
1	E	68	TYR
1	E	135	GLN
2	F	120	LYS
2	F	121	ASP
2	F	178	ARG
1	G	68	TYR
2	H	121	ASP
2	H	150	SER
2	H	153	HIS
2	H	156	SER
2	H	168	CYS
2	H	181	TYR
2	H	200	SER
2	H	281	LEU

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Mol	Chain	Res	Type
2	H	292	SER
2	H	294	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	223	GLN
2	D	225	HIS
2	H	196	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](#)

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	167/175 (95%)	-0.00	4 (2%) 62 71	32, 53, 101, 129	0
1	C	167/175 (95%)	-0.08	4 (2%) 62 71	28, 42, 79, 129	0
1	E	167/175 (95%)	-0.03	7 (4%) 40 48	27, 46, 93, 121	0
1	G	168/175 (96%)	0.20	12 (7%) 19 26	43, 61, 106, 135	0
2	B	210/240 (87%)	0.55	25 (11%) 6 9	25, 52, 119, 158	0
2	D	213/240 (88%)	0.57	28 (13%) 5 7	32, 56, 130, 164	0
2	F	195/240 (81%)	0.36	16 (8%) 14 20	24, 45, 98, 134	0
2	H	189/240 (78%)	0.90	42 (22%) 1 2	30, 81, 138, 160	0
All	All	1476/1660 (88%)	0.33	138 (9%) 11 16	24, 54, 116, 164	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	291	CYS	9.7
2	B	290	GLY	8.5
2	D	118	ALA	8.3
2	F	290	GLY	8.3
2	H	181	TYR	6.7
2	B	178	ARG	6.6
2	B	289	GLY	6.2
2	F	200	SER	6.2
1	G	170	SER	6.0
2	D	117	GLY	6.0
2	H	290	GLY	5.9
2	B	179	GLN	5.7
2	D	292	SER	5.6
2	F	178	ARG	5.4
2	H	289	GLY	5.3
2	H	200	SER	5.3

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Mol	Chain	Res	Type	RSRZ
2	D	291	CYS	5.2
2	B	118	ALA	5.2
2	B	288	ILE	5.2
2	D	106	LEU	5.2
2	D	290	GLY	5.2
2	D	172	GLN	5.1
2	B	321	LEU	5.1
2	B	292	SER	5.1
2	D	119	LEU	5.0
2	H	201	ILE	5.0
2	D	201	ILE	4.9
2	H	160	SER	4.7
1	A	138	LEU	4.5
2	B	170	GLY	4.4
1	E	139	LYS	4.4
2	B	112	LEU	4.4
1	A	3	THR	4.3
2	H	156	SER	4.3
2	B	175	LYS	4.3
2	D	116	TYR	4.1
2	D	173	ASN	4.1
1	E	170	SER	4.1
2	D	158	VAL	4.1
2	H	147	ARG	4.1
2	D	161	VAL	4.0
2	H	128	PRO	4.0
2	H	185	PHE	4.0
1	G	132	ALA	4.0
2	H	148	VAL	4.0
2	H	145	HIS	3.9
2	H	146	PHE	3.9
2	H	169	PHE	3.9
1	A	92	SER	3.9
2	H	155	HIS	3.9
2	B	180	ASP	3.8
2	F	118	ALA	3.7
2	H	187	LEU	3.7
1	C	170	SER	3.6
1	G	140	GLN	3.6
2	H	157	SER	3.6
2	H	191	ASN	3.5
2	B	115	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	169	VAL	3.5
2	F	180	ASP	3.5
2	D	200	SER	3.5
2	F	291	CYS	3.4
2	D	293	VAL	3.3
1	A	170	SER	3.3
2	B	173	ASN	3.3
2	F	170	GLY	3.2
1	G	92	SER	3.2
2	B	293	VAL	3.2
2	H	189	TRP	3.2
2	H	249	SER	3.2
1	G	171	THR	3.2
2	D	105	ALA	3.2
2	F	119	LEU	3.2
2	H	288	ILE	3.1
2	B	172	GLN	3.1
2	F	179	GLN	3.1
2	H	248	SER	3.1
2	F	117	GLY	3.1
2	F	222	GLY	3.1
2	H	180	ASP	3.0
2	B	171	GLU	3.0
2	F	201	ILE	3.0
1	E	92	SER	3.0
1	G	133	ALA	2.9
2	D	159	LYS	2.9
2	F	293	VAL	2.9
2	D	115	ASP	2.9
2	D	160	SER	2.8
1	C	139	LYS	2.8
2	H	318	LEU	2.8
2	D	107	ASP	2.8
2	B	201	ILE	2.8
2	H	179	GLN	2.7
1	G	93	ASP	2.7
2	H	161	VAL	2.7
1	C	93	ASP	2.6
2	H	182	GLN	2.6
2	D	178	ARG	2.6
2	F	204	MET	2.6
2	D	162	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	117	GLY	2.5
2	B	119	LEU	2.5
2	B	294	THR	2.5
2	H	203	THR	2.5
2	B	177	PRO	2.5
2	F	199	PHE	2.4
2	B	116	TYR	2.4
1	G	136	GLU	2.4
2	D	157	SER	2.4
2	B	176	GLN	2.4
2	D	108	LEU	2.4
2	H	122	ILE	2.4
2	F	289	GLY	2.4
2	D	154	THR	2.4
2	H	154	THR	2.4
1	G	90	SER	2.4
1	E	3	THR	2.4
2	H	164	ASN	2.4
1	E	27	ASP	2.3
1	G	3	THR	2.3
2	D	110	SER	2.3
1	E	28	VAL	2.3
2	H	183	LEU	2.3
2	H	151	THR	2.2
1	G	135	GLN	2.2
1	C	3	THR	2.2
2	H	150	SER	2.2
2	H	166	LEU	2.1
1	E	135	GLN	2.1
2	H	165	LEU	2.1
2	H	250	LYS	2.1
2	H	149	LEU	2.1
2	D	111	VAL	2.1
2	H	292	SER	2.1
2	D	112	LEU	2.1
2	H	319	LEU	2.1
2	H	291	CYS	2.0
2	H	162	PRO	2.0

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

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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.