



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:40 PM UTC

PDB ID : 7YHJ / pdb_00007yhj
Title : Effector binding domain of LysR-Type transcription factor LrhA from E. coli
Authors : Xie, C.; Jiang, X.
Deposited on : 2022-07-13
Resolution : 3.24 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

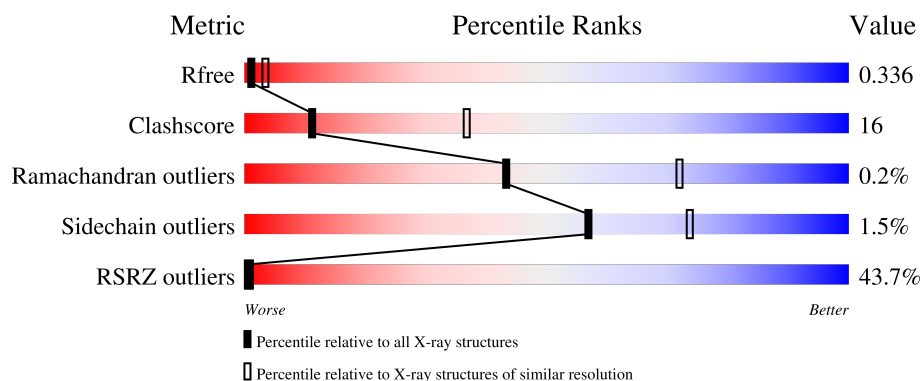
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	319	
1	B	319	
1	C	319	
1	D	319	
1	E	319	

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Mol	Chain	Length	Quality of chain
1	F	319	
1	G	319	
1	H	319	

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	PEG	G	401	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11848 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 Probable HTH-type transcriptional regulator LrhA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1478	946	245	278	9			
1	B	191	Total	C	N	O	S	0	0	0
			1464	935	241	279	9			
1	C	190	Total	C	N	O	S	0	0	0
			1472	946	243	274	9			
1	D	190	Total	C	N	O	S	0	0	0
			1467	939	243	276	9			
1	E	193	Total	C	N	O	S	0	0	0
			1490	951	248	282	9			
1	F	192	Total	C	N	O	S	0	0	0
			1479	947	246	277	9			
1	G	191	Total	C	N	O	S	0	0	0
			1472	943	242	278	9			
1	H	193	Total	C	N	O	S	0	0	0
			1487	950	248	280	9			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P36771
A	-5	HIS	-	expression tag	UNP P36771
A	-4	HIS	-	expression tag	UNP P36771
A	-3	HIS	-	expression tag	UNP P36771
A	-2	HIS	-	expression tag	UNP P36771
A	-1	HIS	-	expression tag	UNP P36771
A	0	HIS	-	expression tag	UNP P36771
B	-6	MET	-	initiating methionine	UNP P36771
B	-5	HIS	-	expression tag	UNP P36771
B	-4	HIS	-	expression tag	UNP P36771
B	-3	HIS	-	expression tag	UNP P36771
B	-2	HIS	-	expression tag	UNP P36771
B	-1	HIS	-	expression tag	UNP P36771

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP P36771
C	-6	MET	-	initiating methionine	UNP P36771
C	-5	HIS	-	expression tag	UNP P36771
C	-4	HIS	-	expression tag	UNP P36771
C	-3	HIS	-	expression tag	UNP P36771
C	-2	HIS	-	expression tag	UNP P36771
C	-1	HIS	-	expression tag	UNP P36771
C	0	HIS	-	expression tag	UNP P36771
D	-6	MET	-	initiating methionine	UNP P36771
D	-5	HIS	-	expression tag	UNP P36771
D	-4	HIS	-	expression tag	UNP P36771
D	-3	HIS	-	expression tag	UNP P36771
D	-2	HIS	-	expression tag	UNP P36771
D	-1	HIS	-	expression tag	UNP P36771
D	0	HIS	-	expression tag	UNP P36771
E	-6	MET	-	initiating methionine	UNP P36771
E	-5	HIS	-	expression tag	UNP P36771
E	-4	HIS	-	expression tag	UNP P36771
E	-3	HIS	-	expression tag	UNP P36771
E	-2	HIS	-	expression tag	UNP P36771
E	-1	HIS	-	expression tag	UNP P36771
E	0	HIS	-	expression tag	UNP P36771
F	-6	MET	-	initiating methionine	UNP P36771
F	-5	HIS	-	expression tag	UNP P36771
F	-4	HIS	-	expression tag	UNP P36771
F	-3	HIS	-	expression tag	UNP P36771
F	-2	HIS	-	expression tag	UNP P36771
F	-1	HIS	-	expression tag	UNP P36771
F	0	HIS	-	expression tag	UNP P36771
G	-6	MET	-	initiating methionine	UNP P36771
G	-5	HIS	-	expression tag	UNP P36771
G	-4	HIS	-	expression tag	UNP P36771
G	-3	HIS	-	expression tag	UNP P36771
G	-2	HIS	-	expression tag	UNP P36771
G	-1	HIS	-	expression tag	UNP P36771
G	0	HIS	-	expression tag	UNP P36771
H	-6	MET	-	initiating methionine	UNP P36771
H	-5	HIS	-	expression tag	UNP P36771
H	-4	HIS	-	expression tag	UNP P36771
H	-3	HIS	-	expression tag	UNP P36771
H	-2	HIS	-	expression tag	UNP P36771
H	-1	HIS	-	expression tag	UNP P36771

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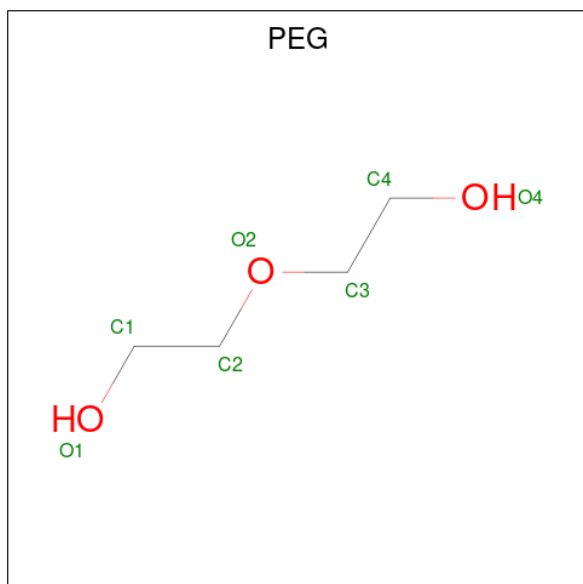
Chain	Residue	Modelled	Actual	Comment	Reference
H	0	HIS	-	expression tag	UNP P36771

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			7	4	3		

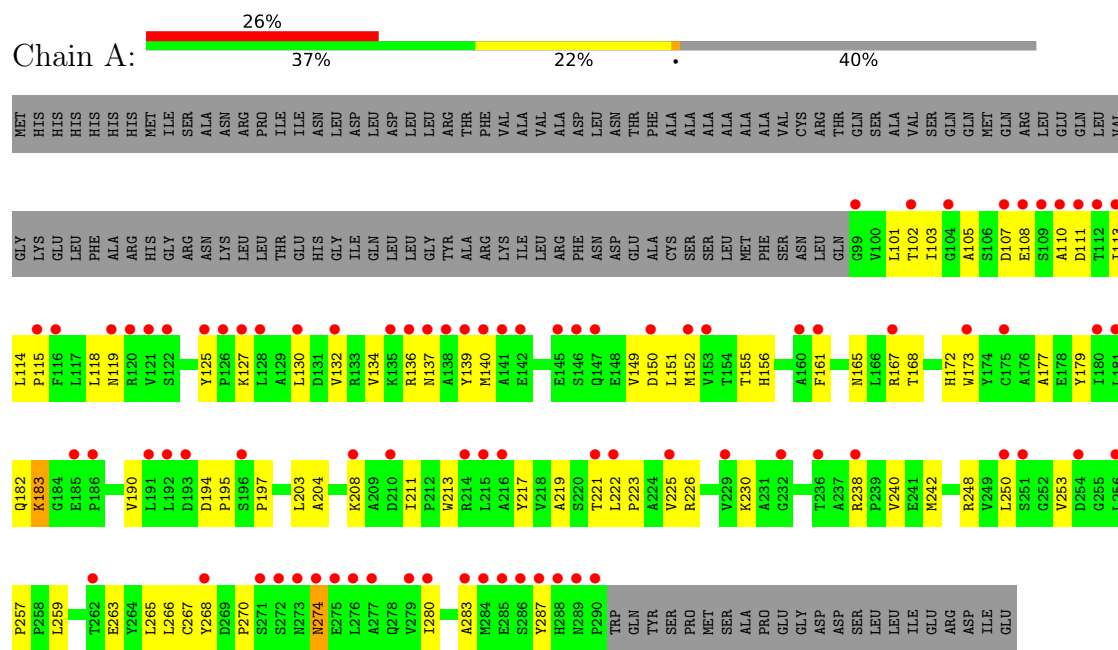
- Molecule 4 is water.

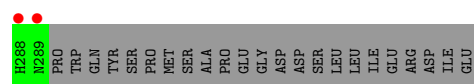
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	4	Total	O	0	0
			4	4		
4	D	3	Total	O	0	0
			3	3		
4	E	1	Total	O	0	0
			1	1		
4	F	6	Total	O	0	0
			6	6		
4	G	4	Total	O	0	0
			4	4		
4	H	3	Total	O	0	0
			3	3		

3 Residue-property plots

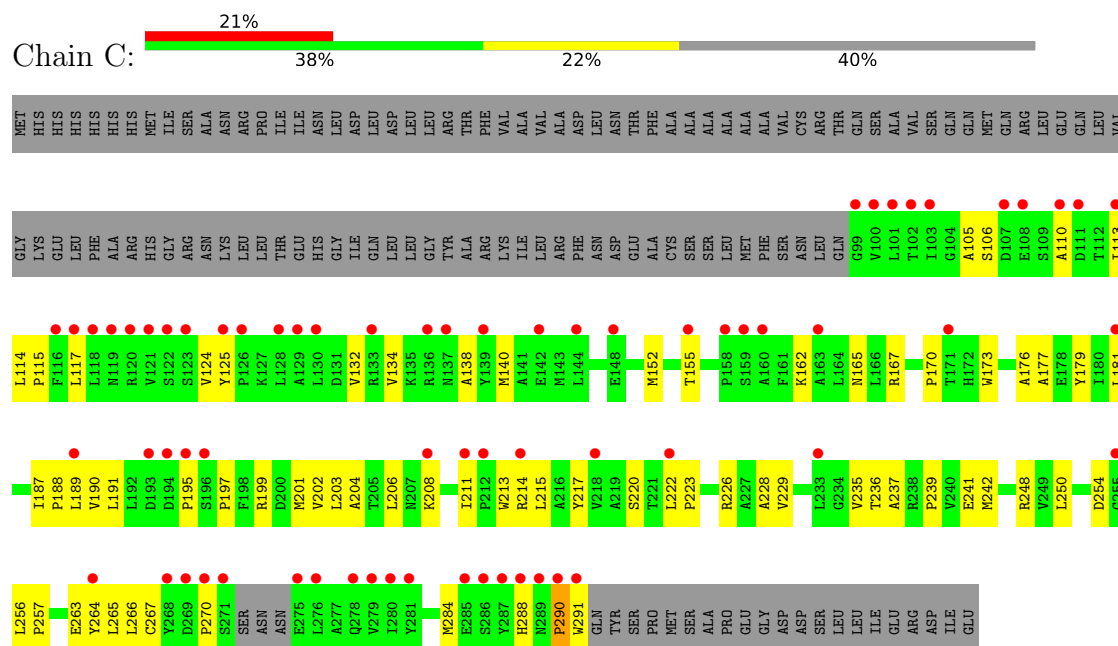
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Probable HTH-type transcriptional regulator LrhA

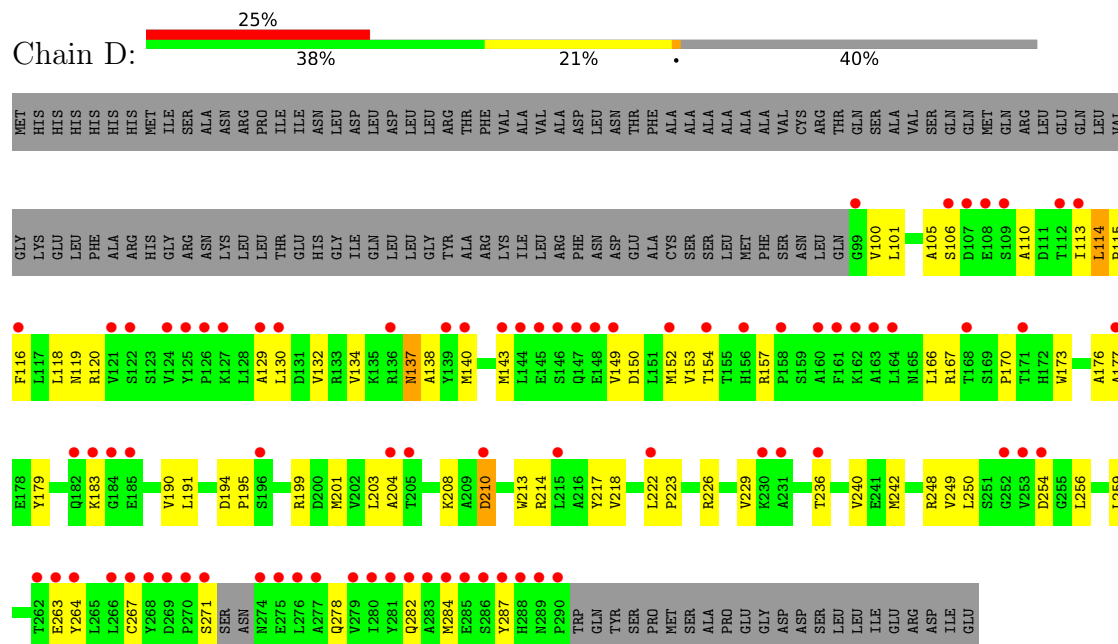




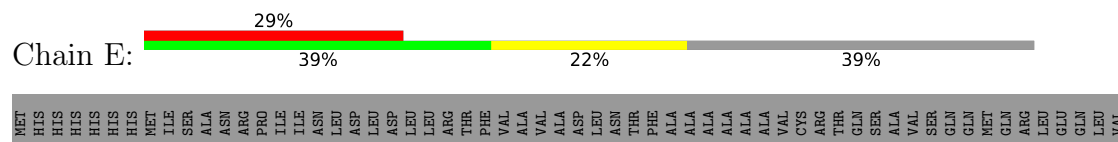
- Molecule 1: Probable HTH-type transcriptional regulator LrhA

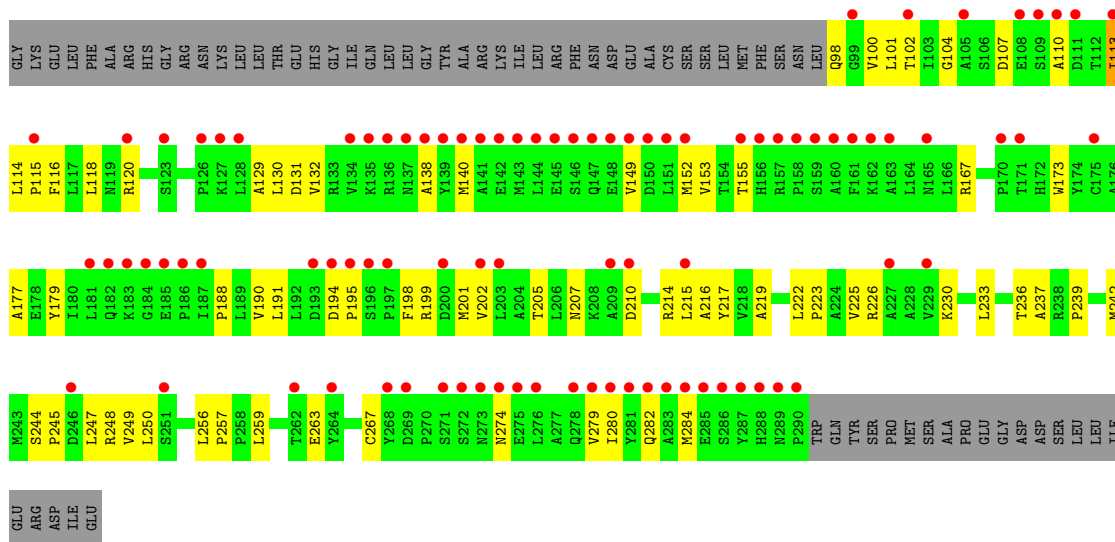


- Molecule 1: Probable HTH-type transcriptional regulator LrhA

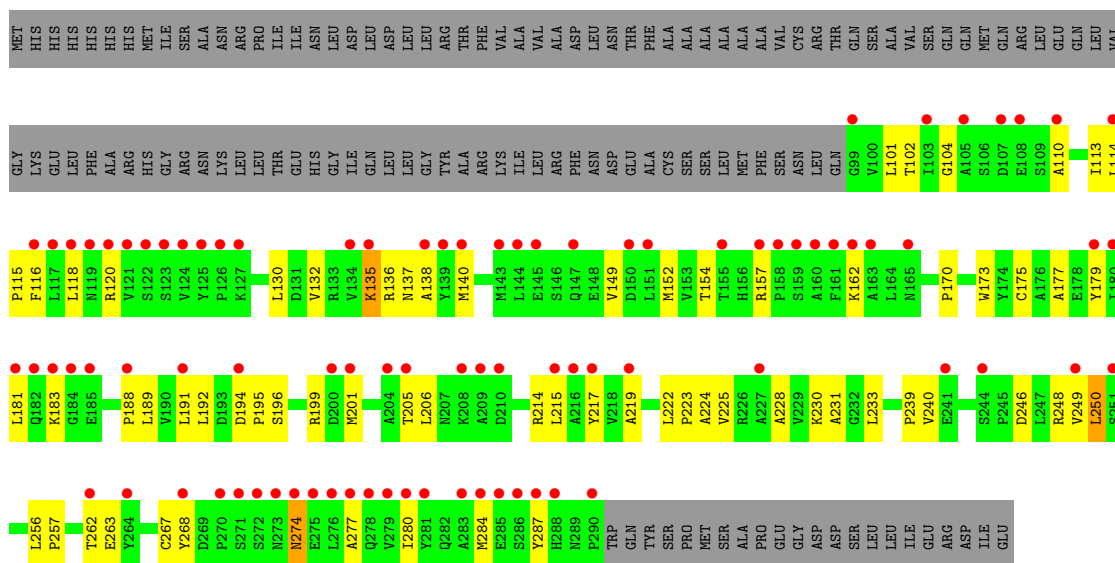


- Molecule 1: Probable HTH-type transcriptional regulator LrhA

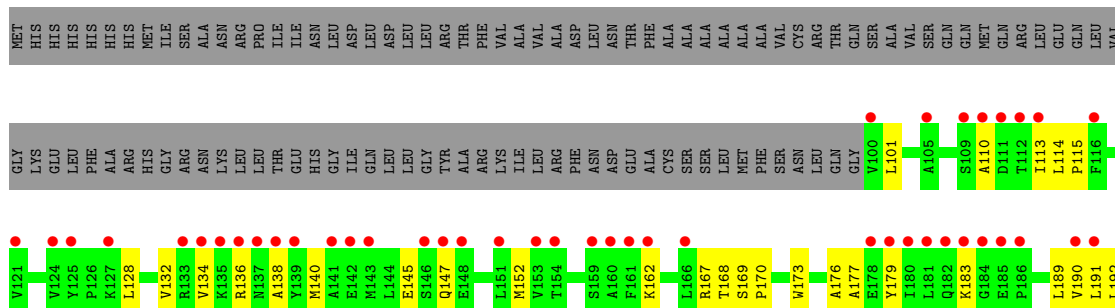
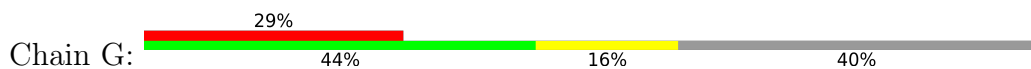


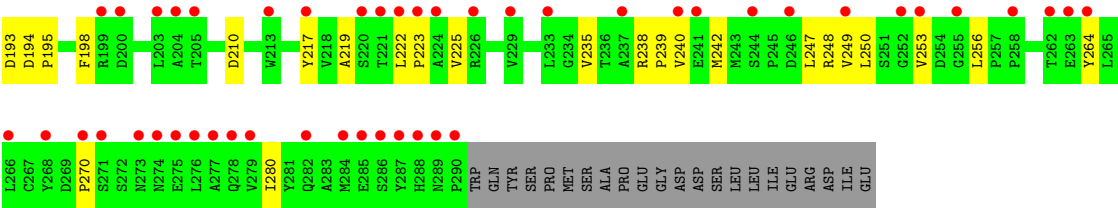


- Molecule 1: Probable HTH-type transcriptional regulator LrhA

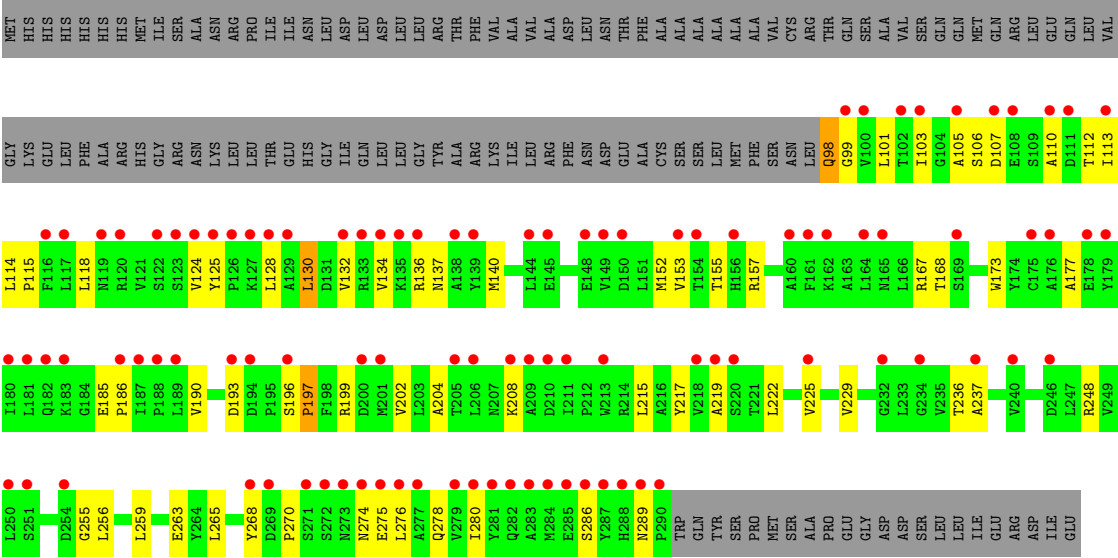


- Molecule 1: Probable HTH-type transcriptional regulator LrhA





● Molecule 1: Probable HTH-type transcriptional regulator LrhA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.68Å 169.31Å 190.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 3.24 48.71 – 3.24	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.71-3.24) 97.9 (48.71-3.24)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.321 , 0.338 0.319 , 0.336	Depositor DCC
R_{free} test set	2153 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	11848	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 46.42 % 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 1.1474e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, PEG

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	0.88	0/1513	1.13	0/2071
1	B	0.87	0/1498	1.13	0/2053
1	C	0.87	0/1507	1.11	0/2061
1	D	0.87	0/1501	1.10	0/2054
1	E	0.87	0/1525	1.10	0/2088
1	F	0.86	0/1514	1.12	0/2072
1	G	0.83	0/1507	1.09	0/2064
1	H	0.88	0/1522	1.12	1/2084 (0.0%)
All	All	0.87	0/12087	1.11	1/16547 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	197	PRO	N-CA-CB	-5.30	97.69	103.25

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	1478	0	1486	58	0
1	B	1464	0	1456	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1472	0	1478	52	0
1	D	1467	0	1473	56	0
1	E	1490	0	1493	68	0
1	F	1479	0	1490	57	0
1	G	1472	0	1478	45	0
1	H	1487	0	1491	45	0
2	D	5	0	0	0	0
2	G	5	0	0	0	0
3	G	7	0	10	0	0
4	A	1	0	0	0	0
4	B	4	0	0	0	0
4	D	3	0	0	0	0
4	E	1	0	0	0	0
4	F	6	0	0	1	0
4	G	4	0	0	0	0
4	H	3	0	0	1	0
All	All	11848	0	11855	387	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 16.

All (387) 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:H:276:LEU:HD12	4:H:401:HOH:O	1.74	0.87
1:A:132:VAL:HG12	1:E:217:TYR:OH	1.75	0.87
1:A:118:LEU:HD21	1:E:233:LEU:HD11	1.55	0.86
1:F:239:PRO:HG3	1:F:262:THR:HG21	1.55	0.86
1:D:113:ILE:HD13	1:D:264:TYR:HB3	1.57	0.85
1:A:226:ARG:HG3	1:A:242:MET:HE3	1.60	0.83
1:B:113:ILE:HD11	1:B:166:LEU:HB3	1.60	0.82
1:A:253:VAL:HG21	1:G:168:THR:HG21	1.62	0.81
1:F:217:TYR:HE1	1:F:219:ALA:HB2	1.46	0.80
1:A:134:VAL:HG21	1:E:223:PRO:HG2	1.63	0.80
1:H:98:GLN:HE21	1:H:98:GLN:N	1.80	0.79
1:E:113:ILE:HD11	1:E:153:VAL:HG11	1.62	0.79
1:B:226:ARG:HG3	1:B:242:MET:HE3	1.66	0.77
1:D:110:ALA:O	1:D:114:LEU:HB2	1.85	0.76
1:A:107:ASP:HB2	1:A:222:LEU:HD12	1.66	0.76
1:B:253:VAL:HG21	1:H:168:THR:HG21	1.68	0.76
1:B:113:ILE:HD11	1:B:166:LEU:CB	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:LYS:HA	4:F:401:HOH:O	1.87	0.74
1:B:196:SER:HB3	1:B:199:ARG:HB3	1.69	0.73
1:C:110:ALA:O	1:C:114:LEU:HB3	1.90	0.72
1:E:101:LEU:HD22	1:E:280:ILE:HD13	1.70	0.72
1:A:217:TYR:OH	1:E:132:VAL:HG12	1.90	0.71
1:B:110:ALA:O	1:B:114:LEU:HB3	1.90	0.71
1:D:183:LYS:NZ	1:D:254:ASP:O	2.23	0.71
1:E:100:VAL:HG22	1:E:129:ALA:HB3	1.72	0.71
1:F:114:LEU:HD21	1:F:132:VAL:HG11	1.72	0.71
1:E:116:PHE:HB3	1:E:120:ARG:HH12	1.55	0.70
1:A:110:ALA:O	1:A:114:LEU:HB3	1.90	0.70
1:D:167:ARG:HD2	1:F:248:ARG:HG3	1.73	0.70
1:H:190:VAL:HG13	1:H:217:TYR:HD2	1.55	0.70
1:E:120:ARG:HD2	1:E:284:MET:HE1	1.74	0.69
1:A:118:LEU:HD21	1:E:233:LEU:CD1	2.23	0.68
1:C:176:ALA:HB3	1:C:179:TYR:HB2	1.74	0.67
1:F:102:THR:HG22	1:F:149:VAL:HG12	1.77	0.67
1:E:110:ALA:O	1:E:114:LEU:HB3	1.93	0.67
1:G:217:TYR:CE2	1:G:219:ALA:HB2	2.29	0.67
1:G:242:MET:HE2	1:G:247:LEU:HD11	1.76	0.67
1:H:98:GLN:N	1:H:98:GLN:NE2	2.43	0.67
1:F:110:ALA:O	1:F:114:LEU:HB3	1.94	0.67
1:A:190:VAL:HG12	1:A:225:VAL:HG13	1.77	0.67
1:A:221:THR:HG22	1:A:223:PRO:HD2	1.76	0.66
1:E:194:ASP:OD2	1:E:199:ARG:NH1	2.28	0.66
1:B:190:VAL:HG12	1:B:225:VAL:HG13	1.77	0.66
1:F:250:LEU:HB3	1:F:256:LEU:HD12	1.76	0.66
1:H:110:ALA:HA	1:H:114:LEU:HD13	1.77	0.66
1:B:273:ASN:HD21	1:G:210:ASP:HB2	1.60	0.65
1:A:102:THR:HG22	1:A:149:VAL:HG12	1.77	0.65
1:E:190:VAL:HG22	1:E:217:TYR:HB3	1.78	0.65
1:H:110:ALA:O	1:H:114:LEU:HB2	1.97	0.65
1:A:168:THR:HG21	1:G:253:VAL:HG21	1.78	0.65
1:C:226:ARG:HG3	1:C:242:MET:HE3	1.77	0.65
1:D:210:ASP:HB3	1:E:215:LEU:HD11	1.78	0.64
1:E:177:ALA:HA	1:E:248:ARG:HB2	1.80	0.63
1:H:204:ALA:HB1	1:H:208:LYS:HE2	1.79	0.63
1:A:108:GLU:OE1	1:A:238:ARG:NH1	2.32	0.63
1:D:249:VAL:HG11	1:F:170:PRO:HD2	1.80	0.63
1:H:112:THR:HG22	1:H:113:ILE:HG23	1.80	0.63
1:F:222:LEU:HA	1:F:225:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:ALA:O	1:G:114:LEU:HB3	1.99	0.61
1:D:140:MET:HB3	1:D:152:MET:SD	2.41	0.61
1:B:140:MET:HB3	1:B:152:MET:SD	2.41	0.61
1:E:217:TYR:CE2	1:E:219:ALA:HB2	2.35	0.61
1:G:189:LEU:HD13	1:G:191:LEU:HD11	1.82	0.61
1:C:165:ASN:HA	1:C:265:LEU:HD23	1.83	0.61
1:A:240:VAL:HG11	1:G:249:VAL:HG21	1.82	0.60
1:C:124:VAL:HG13	1:C:125:TYR:CD2	2.36	0.60
1:A:140:MET:HB3	1:A:152:MET:SD	2.41	0.60
1:C:162:LYS:HD3	1:C:270:PRO:HG3	1.82	0.60
1:H:217:TYR:CE2	1:H:219:ALA:HB2	2.35	0.60
1:D:137:ASN:ND2	1:D:154:THR:OG1	2.34	0.60
1:H:140:MET:HB3	1:H:152:MET:SD	2.41	0.60
1:E:102:THR:HG22	1:E:149:VAL:HG12	1.82	0.60
1:F:120:ARG:NH2	1:F:287:TYR:HB3	2.16	0.60
1:E:279:VAL:O	1:E:282:GLN:HG2	2.00	0.60
1:B:107:ASP:HB3	1:B:222:LEU:HD12	1.84	0.59
1:B:151:LEU:HD13	1:B:266:LEU:HD11	1.83	0.59
1:F:205:THR:HG22	1:F:257:PRO:HG2	1.84	0.59
1:A:114:LEU:HD21	1:A:132:VAL:HG21	1.84	0.59
1:A:125:TYR:C	1:A:127:LYS:H	2.09	0.59
1:B:118:LEU:HD11	1:B:132:VAL:HG21	1.84	0.59
1:D:100:VAL:HG22	1:D:129:ALA:HB3	1.85	0.59
1:A:151:LEU:HD13	1:A:266:LEU:HD11	1.83	0.59
1:A:248:ARG:HG3	1:G:167:ARG:HD2	1.85	0.59
1:D:278:GLN:NE2	1:D:282:GLN:OE1	2.34	0.59
1:F:118:LEU:HD22	1:F:130:LEU:HD13	1.85	0.59
1:F:120:ARG:CZ	1:F:287:TYR:HB3	2.32	0.58
1:H:286:SER:HA	1:H:289:ASN:O	2.03	0.58
1:E:140:MET:HB3	1:E:152:MET:SD	2.44	0.58
1:E:173:TRP:HB2	1:E:250:LEU:HB2	1.84	0.58
1:B:273:ASN:ND2	1:G:210:ASP:HB2	2.19	0.58
1:E:188:PRO:HB2	1:E:216:ALA:HB2	1.85	0.58
1:G:169:SER:HB3	1:G:240:VAL:HG12	1.84	0.58
1:D:249:VAL:CG1	1:F:170:PRO:HD2	2.34	0.58
1:A:136:ARG:HD3	1:A:195:PRO:O	2.03	0.58
1:C:191:LEU:HD12	1:C:215:LEU:HD22	1.86	0.58
1:C:152:MET:HE2	1:C:267:CYS:HB2	1.85	0.58
1:C:177:ALA:HA	1:C:248:ARG:HB2	1.86	0.57
1:H:173:TRP:CG	1:H:256:LEU:HD13	2.40	0.57
1:C:140:MET:HB3	1:C:152:MET:SD	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:SER:HB3	1:H:199:ARG:HB3	1.87	0.57
1:H:190:VAL:HG13	1:H:217:TYR:CD2	2.38	0.57
1:C:248:ARG:HG3	1:E:167:ARG:HD2	1.86	0.57
1:B:161:PHE:HB3	1:B:268:TYR:O	2.04	0.57
1:D:203:LEU:HD22	1:D:213:TRP:CE2	2.41	0.56
1:E:250:LEU:HB3	1:E:256:LEU:HD12	1.86	0.56
1:F:217:TYR:CE1	1:F:219:ALA:HB2	2.36	0.56
1:C:114:LEU:N	1:C:115:PRO:HD2	2.20	0.56
1:D:140:MET:CE	1:D:152:MET:HG3	2.36	0.56
1:C:138:ALA:CB	1:C:195:PRO:HG2	2.36	0.56
1:H:113:ILE:HD11	1:H:153:VAL:CG1	2.35	0.56
1:B:276:LEU:O	1:B:280:ILE:HD12	2.06	0.56
1:A:177:ALA:HA	1:A:248:ARG:HB2	1.87	0.55
1:C:181:LEU:HD22	1:C:250:LEU:HD13	1.87	0.55
1:E:102:THR:HB	1:E:149:VAL:HA	1.88	0.55
1:D:140:MET:HE2	1:D:152:MET:HG3	1.88	0.55
1:D:173:TRP:CG	1:D:256:LEU:HD23	2.41	0.55
1:E:114:LEU:HD21	1:E:132:VAL:HG21	1.88	0.55
1:B:143:MET:HE2	1:B:149:VAL:CG1	2.37	0.55
1:B:100:VAL:HA	1:B:129:ALA:HB3	1.89	0.55
1:D:170:PRO:HD2	1:F:249:VAL:HG11	1.88	0.55
1:D:177:ALA:HA	1:D:248:ARG:HB2	1.86	0.55
1:H:177:ALA:HA	1:H:248:ARG:HB2	1.89	0.55
1:E:190:VAL:HG12	1:E:225:VAL:HG13	1.89	0.55
1:F:137:ASN:ND2	1:F:154:THR:OG1	2.32	0.55
1:G:217:TYR:HE2	1:G:219:ALA:HB2	1.71	0.55
1:H:190:VAL:HG12	1:H:225:VAL:HG13	1.88	0.55
1:A:211:ILE:CD1	1:A:257:PRO:HD3	2.38	0.54
1:E:205:THR:HG22	1:E:257:PRO:HG2	1.89	0.54
1:C:223:PRO:HG2	1:G:134:VAL:HG21	1.89	0.54
1:H:107:ASP:HB3	1:H:222:LEU:HD12	1.89	0.54
1:C:155:THR:HA	1:C:263:GLU:O	2.07	0.54
1:C:188:PRO:HB3	1:C:214:ARG:HE	1.72	0.54
1:G:136:ARG:NH1	1:G:193:ASP:OD1	2.32	0.54
1:B:273:ASN:OD1	1:G:210:ASP:HB2	2.07	0.54
1:D:248:ARG:HH21	1:D:250:LEU:HD21	1.73	0.54
1:F:152:MET:HE2	1:F:267:CYS:HB2	1.88	0.53
1:G:140:MET:HB3	1:G:152:MET:SD	2.48	0.53
1:F:222:LEU:N	1:F:223:PRO:HD2	2.24	0.53
1:C:204:ALA:O	1:C:208:LYS:HG2	2.08	0.53
1:E:152:MET:HE2	1:E:267:CYS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ARG:HD2	1:E:248:ARG:HG3	1.90	0.53
1:C:173:TRP:HB2	1:C:250:LEU:O	2.09	0.53
1:C:229:VAL:HG21	1:C:236:THR:CG2	2.39	0.53
1:D:173:TRP:CD2	1:D:256:LEU:HD23	2.44	0.53
1:B:114:LEU:N	1:B:115:PRO:HD2	2.23	0.52
1:D:152:MET:HE2	1:D:267:CYS:HB2	1.91	0.52
1:B:176:ALA:HB3	1:B:179:TYR:HB2	1.91	0.52
1:G:176:ALA:HB3	1:G:179:TYR:HB2	1.91	0.52
1:B:113:ILE:HD11	1:B:166:LEU:HB2	1.90	0.52
1:A:136:ARG:HB3	1:A:139:TYR:HD2	1.74	0.52
1:D:229:VAL:HG21	1:D:236:THR:CG2	2.39	0.52
1:F:114:LEU:N	1:F:115:PRO:HD2	2.25	0.52
1:F:140:MET:CE	1:F:152:MET:HG3	2.40	0.52
1:F:173:TRP:HB2	1:F:250:LEU:O	2.09	0.52
1:A:132:VAL:CG1	1:E:217:TYR:OH	2.55	0.52
1:E:190:VAL:HG13	1:E:217:TYR:HD2	1.75	0.51
1:B:219:ALA:HB3	1:B:225:VAL:HG23	1.90	0.51
1:C:206:LEU:HD13	1:C:213:TRP:HB3	1.93	0.51
1:A:161:PHE:HB3	1:A:268:TYR:O	2.09	0.51
1:D:113:ILE:HD12	1:D:166:LEU:HD12	1.92	0.51
1:F:101:LEU:HD22	1:F:280:ILE:HD13	1.93	0.51
1:A:114:LEU:N	1:A:115:PRO:HD2	2.26	0.51
1:C:179:TYR:O	1:C:248:ARG:NH1	2.42	0.51
1:C:190:VAL:HG11	1:C:228:ALA:HB3	1.93	0.51
1:G:190:VAL:HG12	1:G:225:VAL:HG13	1.93	0.51
1:C:188:PRO:HB3	1:C:214:ARG:NE	2.26	0.50
1:E:179:TYR:O	1:E:248:ARG:NH1	2.43	0.50
1:E:191:LEU:HD13	1:E:199:ARG:HG3	1.91	0.50
1:G:138:ALA:CB	1:G:195:PRO:HG2	2.41	0.50
1:D:118:LEU:HD22	1:D:130:LEU:HD13	1.93	0.50
1:E:188:PRO:CB	1:E:216:ALA:HB2	2.41	0.50
1:G:177:ALA:HA	1:G:248:ARG:HB2	1.93	0.50
1:H:173:TRP:CD2	1:H:256:LEU:HD13	2.45	0.50
1:G:136:ARG:HH22	1:G:192:LEU:HB3	1.76	0.50
1:H:136:ARG:NH2	1:H:193:ASP:O	2.44	0.50
1:G:222:LEU:N	1:G:223:PRO:HD2	2.26	0.50
1:G:136:ARG:NH2	1:G:192:LEU:HB3	2.26	0.50
1:A:203:LEU:HG	1:A:213:TRP:CZ2	2.46	0.50
1:D:152:MET:HE2	1:D:267:CYS:CB	2.42	0.50
1:D:143:MET:HE2	1:D:149:VAL:HG11	1.93	0.49
1:E:138:ALA:CB	1:E:195:PRO:HG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:ILE:O	1:H:132:VAL:HA	2.12	0.49
1:C:190:VAL:HG13	1:C:217:TYR:HD2	1.76	0.49
1:D:113:ILE:HD11	1:D:153:VAL:CG1	2.42	0.49
1:D:213:TRP:CE3	1:E:207:ASN:HB3	2.47	0.49
1:F:219:ALA:HB1	1:F:224:ALA:HB3	1.93	0.49
1:H:137:ASN:ND2	1:H:155:THR:H	2.10	0.49
1:D:226:ARG:HG2	1:D:242:MET:HE3	1.94	0.49
1:A:156:HIS:HB2	1:A:197:PRO:HG2	1.95	0.49
1:C:199:ARG:O	1:C:203:LEU:HG	2.12	0.49
1:D:204:ALA:O	1:D:208:LYS:HD3	2.13	0.49
1:F:136:ARG:HH21	1:F:192:LEU:HD13	1.78	0.49
1:D:176:ALA:HB3	1:D:179:TYR:HB2	1.93	0.48
1:F:162:LYS:HD2	1:F:268:TYR:CE2	2.49	0.48
1:G:113:ILE:HG13	1:G:264:TYR:CG	2.49	0.48
1:F:177:ALA:HA	1:F:248:ARG:HB2	1.95	0.48
1:A:101:LEU:HD21	1:A:103:ILE:HD11	1.96	0.48
1:D:118:LEU:HD11	1:D:132:VAL:HG21	1.95	0.48
1:D:249:VAL:HG11	1:F:240:VAL:HG11	1.95	0.48
1:H:99:GLY:C	1:H:128:LEU:HD12	2.38	0.48
1:C:113:ILE:HG21	1:C:264:TYR:HB3	1.95	0.48
1:E:155:THR:HA	1:E:263:GLU:O	2.13	0.48
1:G:114:LEU:N	1:G:115:PRO:HD2	2.28	0.48
1:G:136:ARG:HH21	1:G:192:LEU:HD13	1.79	0.48
1:B:278:GLN:HG2	1:B:282:GLN:OE1	2.14	0.48
1:D:222:LEU:HB3	1:D:223:PRO:HD3	1.94	0.48
1:H:113:ILE:HD11	1:H:153:VAL:HG11	1.95	0.48
1:H:114:LEU:N	1:H:115:PRO:HD2	2.29	0.48
1:A:113:ILE:HD13	1:A:167:ARG:HD3	1.96	0.48
1:C:114:LEU:HD21	1:C:132:VAL:HG11	1.96	0.48
1:A:136:ARG:HG2	1:A:137:ASN:N	2.28	0.47
1:E:230:LYS:HG2	1:E:247:LEU:HD21	1.97	0.47
1:B:177:ALA:HA	1:B:248:ARG:HB2	1.97	0.47
1:E:226:ARG:HG2	1:E:242:MET:SD	2.54	0.47
1:F:228:ALA:O	1:F:233:LEU:HB2	2.15	0.47
1:B:268:TYR:HD1	1:B:277:ALA:HB1	1.79	0.47
1:F:196:SER:HB3	1:F:199:ARG:HB3	1.96	0.47
1:A:194:ASP:HA	1:A:195:PRO:HA	1.67	0.47
1:A:219:ALA:HB3	1:A:225:VAL:CG2	2.45	0.47
1:C:167:ARG:HH11	1:E:248:ARG:HG3	1.79	0.47
1:D:213:TRP:CZ3	1:E:207:ASN:HB3	2.50	0.47
1:E:173:TRP:CG	1:E:256:LEU:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:LYS:HG2	1:G:270:PRO:HG3	1.97	0.47
1:D:201:MET:SD	1:D:259:LEU:HD22	2.54	0.47
1:C:290:PRO:O	1:C:291:TRP:C	2.57	0.47
1:D:114:LEU:N	1:D:115:PRO:HD2	2.29	0.47
1:E:173:TRP:CZ2	1:E:259:LEU:HD21	2.49	0.47
1:E:188:PRO:HB3	1:E:214:ARG:CZ	2.45	0.47
1:F:192:LEU:O	1:F:199:ARG:HD2	2.15	0.47
1:G:189:LEU:HD23	1:G:235:VAL:HG23	1.97	0.47
1:D:208:LYS:HE3	1:E:194:ASP:OD1	2.14	0.46
1:D:240:VAL:HG11	1:F:249:VAL:HG11	1.97	0.46
1:D:214:ARG:HD2	1:E:210:ASP:OD1	2.16	0.46
1:C:248:ARG:HH21	1:C:250:LEU:HD21	1.81	0.46
1:E:226:ARG:HG2	1:E:242:MET:CE	2.46	0.46
1:F:116:PHE:CE2	1:F:284:MET:HE1	2.50	0.46
1:B:152:MET:HE3	1:B:267:CYS:SG	2.56	0.46
1:C:181:LEU:HD11	1:C:187:ILE:HD12	1.96	0.46
1:F:230:LYS:NZ	1:F:246:ASP:HB2	2.30	0.46
1:A:118:LEU:CD2	1:E:233:LEU:HD11	2.35	0.46
1:D:190:VAL:HG13	1:D:217:TYR:CD1	2.51	0.46
1:E:114:LEU:N	1:E:115:PRO:HD2	2.30	0.46
1:F:114:LEU:H	1:F:115:PRO:HD2	1.81	0.46
1:F:191:LEU:HD12	1:F:215:LEU:HD21	1.98	0.46
1:G:101:LEU:HD22	1:G:280:ILE:HD13	1.96	0.46
1:F:231:ALA:HB3	1:F:233:LEU:HD13	1.97	0.46
1:B:109:SER:O	1:B:113:ILE:HG22	2.16	0.46
1:B:273:ASN:CG	1:G:210:ASP:HB2	2.40	0.46
1:H:215:LEU:O	1:H:215:LEU:HD12	2.16	0.46
1:B:143:MET:HE2	1:B:149:VAL:HG13	1.98	0.45
1:D:105:ALA:O	1:D:134:VAL:HA	2.16	0.45
1:D:116:PHE:CE2	1:D:284:MET:HE1	2.51	0.45
1:E:113:ILE:HD11	1:E:153:VAL:CG1	2.40	0.45
1:C:138:ALA:HB2	1:C:195:PRO:HG2	1.97	0.45
1:H:105:ALA:O	1:H:134:VAL:HA	2.17	0.45
1:C:187:ILE:HG13	1:C:256:LEU:HD21	1.98	0.45
1:F:152:MET:HE2	1:F:267:CYS:CB	2.46	0.45
1:A:204:ALA:O	1:A:208:LYS:HG3	2.16	0.45
1:B:152:MET:HE2	1:B:267:CYS:HB2	1.99	0.45
1:F:175:CYS:SG	1:F:250:LEU:HD13	2.56	0.45
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.85	0.45
1:E:107:ASP:HB3	1:E:222:LEU:HD12	1.99	0.45
1:G:250:LEU:HB3	1:G:256:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ALA:O	1:A:134:VAL:HA	2.16	0.45
1:B:122:SER:O	1:B:122:SER:OG	2.26	0.45
1:C:284:MET:O	1:C:288:HIS:HB2	2.16	0.45
1:H:157:ARG:HA	1:H:265:LEU:HD12	1.98	0.45
1:E:118:LEU:HD22	1:E:130:LEU:HD13	1.99	0.45
1:E:244:SER:HB2	1:E:245:PRO:HD2	1.98	0.45
1:H:101:LEU:HD22	1:H:280:ILE:HD13	1.98	0.45
1:F:217:TYR:CD1	1:F:217:TYR:C	2.95	0.45
1:G:238:ARG:HB3	1:G:239:PRO:HD2	1.98	0.45
1:C:190:VAL:HG13	1:C:217:TYR:CD2	2.51	0.45
1:D:120:ARG:HB3	1:D:287:TYR:HE2	1.82	0.44
1:A:111:ASP:OD2	1:E:226:ARG:NH2	2.46	0.44
1:E:217:TYR:HE2	1:E:219:ALA:HB2	1.79	0.44
1:F:138:ALA:CB	1:F:195:PRO:HG2	2.48	0.44
1:G:136:ARG:NH2	1:G:192:LEU:HD13	2.32	0.44
1:E:98:GLN:O	1:E:98:GLN:HG2	2.17	0.44
1:F:152:MET:HE3	1:F:154:THR:HG22	1.99	0.44
1:G:113:ILE:HG13	1:G:264:TYR:CB	2.47	0.44
1:H:275:GLU:HA	1:H:278:GLN:OE1	2.17	0.44
1:A:173:TRP:HB2	1:A:250:LEU:HB2	1.99	0.44
1:C:170:PRO:HG3	1:E:249:VAL:HG11	1.99	0.44
1:D:138:ALA:CB	1:D:195:PRO:HG2	2.48	0.44
1:E:132:VAL:HG13	1:E:132:VAL:O	2.18	0.44
1:F:181:LEU:HD12	1:F:181:LEU:HA	1.85	0.44
1:G:194:ASP:HA	1:G:195:PRO:HA	1.74	0.44
1:F:189:LEU:HD11	1:F:206:LEU:HD12	1.99	0.44
1:G:113:ILE:HG13	1:G:264:TYR:HB3	2.00	0.44
1:H:118:LEU:HD22	1:H:130:LEU:HD13	2.00	0.44
1:E:173:TRP:HA	1:E:236:THR:O	2.17	0.44
1:B:101:LEU:HB2	1:B:128:LEU:HD21	2.00	0.44
1:E:104:GLY:C	1:E:140:MET:HE1	2.43	0.44
1:B:273:ASN:ND2	1:G:210:ASP:O	2.51	0.43
1:D:106:SER:O	1:D:110:ALA:HB2	2.17	0.43
1:H:185:GLU:HB3	1:H:186:PRO:HD2	1.99	0.43
1:D:191:LEU:O	1:D:218:VAL:HA	2.19	0.43
1:D:113:ILE:CD1	1:D:264:TYR:HB3	2.40	0.43
1:F:274:ASN:HB3	1:F:277:ALA:HB3	2.01	0.43
1:A:107:ASP:OD1	1:A:134:VAL:HG23	2.18	0.43
1:E:102:THR:HA	1:E:131:ASP:O	2.17	0.43
1:H:124:VAL:HG12	1:H:125:TYR:CE1	2.53	0.43
1:A:226:ARG:HG2	1:A:230:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:PRO:HB2	1:C:241:GLU:OE1	2.18	0.43
1:A:172:HIS:CE1	1:G:170:PRO:HG3	2.53	0.43
1:A:270:PRO:HB2	1:H:255:GLY:HA2	2.01	0.43
1:F:135:LYS:HD2	1:F:135:LYS:HA	1.68	0.43
1:F:231:ALA:CB	1:F:233:LEU:HD13	2.49	0.43
1:G:134:VAL:HG23	1:G:134:VAL:O	2.19	0.43
1:D:120:ARG:HB3	1:D:287:TYR:CE2	2.53	0.43
1:E:113:ILE:HA	1:E:116:PHE:HD2	1.84	0.43
1:G:198:PHE:CZ	1:G:239:PRO:HD3	2.53	0.43
1:A:136:ARG:HB3	1:A:139:TYR:CD2	2.52	0.43
1:A:173:TRP:CE2	1:A:259:LEU:HD11	2.53	0.43
1:B:118:LEU:HD22	1:B:130:LEU:HD13	2.01	0.43
1:D:101:LEU:HD12	1:D:150:ASP:HB2	2.00	0.43
1:F:188:PRO:HB3	1:F:214:ARG:CZ	2.48	0.43
1:A:152:MET:HE3	1:A:267:CYS:SG	2.59	0.42
1:A:219:ALA:HB3	1:A:225:VAL:HG23	2.01	0.42
1:E:116:PHE:HB3	1:E:120:ARG:NH1	2.29	0.42
1:G:101:LEU:HB2	1:G:128:LEU:HD21	2.01	0.42
1:B:101:LEU:HD13	1:B:280:ILE:HD13	2.01	0.42
1:C:211:ILE:CD1	1:C:257:PRO:HD3	2.49	0.42
1:D:116:PHE:O	1:D:119:ASN:HB3	2.18	0.42
1:D:137:ASN:HD22	1:D:137:ASN:C	2.27	0.42
1:F:104:GLY:C	1:F:140:MET:HE1	2.44	0.42
1:A:115:PRO:O	1:A:119:ASN:HB2	2.19	0.42
1:A:155:THR:HA	1:A:263:GLU:O	2.19	0.42
1:F:194:ASP:HA	1:F:195:PRO:HA	1.75	0.42
1:H:229:VAL:HG21	1:H:236:THR:HG22	2.01	0.42
1:C:181:LEU:HD23	1:C:254:ASP:HB3	2.02	0.42
1:C:197:PRO:O	1:C:201:MET:N	2.48	0.42
1:H:157:ARG:HH21	1:H:263:GLU:CD	2.27	0.42
1:B:263:GLU:HB3	1:B:265:LEU:HD21	2.01	0.42
1:F:140:MET:HE3	1:F:152:MET:HG3	2.01	0.42
1:A:283:ALA:O	1:A:287:TYR:HD2	2.03	0.42
1:C:229:VAL:HG21	1:C:236:THR:HG21	2.01	0.42
1:G:114:LEU:HD21	1:G:132:VAL:HG11	2.01	0.42
1:A:179:TYR:O	1:A:248:ARG:NH2	2.48	0.42
1:E:194:ASP:HA	1:E:195:PRO:HA	1.70	0.42
1:F:113:ILE:HG13	1:F:113:ILE:O	2.20	0.42
1:C:138:ALA:HB1	1:C:195:PRO:HG2	2.02	0.41
1:E:202:VAL:CG1	1:E:237:ALA:HB3	2.50	0.41
1:A:165:ASN:HA	1:A:265:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:CD1	1:C:266:LEU:HD13	2.50	0.41
1:A:150:ASP:CG	1:A:274:ASN:ND2	2.79	0.41
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.90	0.41
1:D:179:TYR:O	1:D:248:ARG:NH1	2.53	0.41
1:G:145:GLU:C	1:G:147:GLN:H	2.28	0.41
1:B:251:SER:OG	1:B:253:VAL:HG23	2.20	0.41
1:C:105:ALA:O	1:C:134:VAL:HA	2.21	0.41
1:H:268:TYR:CE2	1:H:270:PRO:HD3	2.55	0.41
1:B:152:MET:CE	1:B:267:CYS:HB2	2.50	0.41
1:B:211:ILE:CD1	1:B:257:PRO:HD3	2.51	0.41
1:E:101:LEU:HD23	1:E:130:LEU:CD2	2.50	0.41
1:F:157:ARG:NH1	1:F:263:GLU:OE1	2.53	0.41
1:G:242:MET:HE2	1:G:247:LEU:CD1	2.49	0.41
1:B:206:LEU:HD23	1:B:206:LEU:HA	1.91	0.41
1:C:202:VAL:CG1	1:C:237:ALA:HB3	2.51	0.41
1:C:202:VAL:HG11	1:C:237:ALA:HB3	2.01	0.41
1:E:188:PRO:HB2	1:E:216:ALA:CB	2.51	0.41
1:A:125:TYR:C	1:A:127:LYS:N	2.78	0.41
1:F:152:MET:HE3	1:F:154:THR:CG2	2.50	0.41
1:H:274:ASN:O	1:H:278:GLN:OE1	2.39	0.41
1:C:106:SER:HA	1:C:140:MET:HE3	2.03	0.41
1:C:189:LEU:HA	1:C:235:VAL:O	2.20	0.41
1:D:157:ARG:NH1	1:D:263:GLU:OE1	2.53	0.41
1:D:194:ASP:HA	1:D:195:PRO:HA	1.78	0.41
1:E:198:PHE:CZ	1:E:239:PRO:HD3	2.55	0.41
1:H:106:SER:O	1:H:110:ALA:HB2	2.21	0.41
1:A:130:LEU:HD12	1:A:130:LEU:O	2.21	0.41
1:B:143:MET:HE2	1:B:149:VAL:HG11	2.02	0.41
1:D:183:LYS:NZ	1:D:254:ASP:C	2.78	0.41
1:D:191:LEU:HD13	1:D:199:ARG:HG3	2.02	0.41
1:H:155:THR:HA	1:H:263:GLU:O	2.21	0.41
1:H:173:TRP:CE2	1:H:259:LEU:HD11	2.55	0.41
1:H:190:VAL:HA	1:H:217:TYR:O	2.21	0.41
1:A:101:LEU:HD13	1:A:280:ILE:HD12	2.03	0.40
1:B:248:ARG:HG3	1:H:167:ARG:HD2	2.03	0.40
1:G:173:TRP:HB2	1:G:250:LEU:HB2	2.03	0.40
1:F:179:TYR:O	1:F:248:ARG:NH2	2.54	0.40
1:H:202:VAL:HG22	1:H:237:ALA:HB3	2.03	0.40
1:A:238:ARG:HA	1:A:238:ARG:HD3	1.88	0.40
1:F:140:MET:HB3	1:F:152:MET:SD	2.60	0.40
1:C:222:LEU:HA	1:C:222:LEU:HD23	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:MET:HB3	1:A:267:CYS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	190/319 (60%)	181 (95%)	7 (4%)	2 (1%)	11	40
1	B	189/319 (59%)	186 (98%)	3 (2%)	0	100	100
1	C	186/319 (58%)	180 (97%)	5 (3%)	1 (0%)	24	56
1	D	186/319 (58%)	179 (96%)	7 (4%)	0	100	100
1	E	191/319 (60%)	184 (96%)	7 (4%)	0	100	100
1	F	190/319 (60%)	184 (97%)	6 (3%)	0	100	100
1	G	189/319 (59%)	183 (97%)	6 (3%)	0	100	100
1	H	191/319 (60%)	183 (96%)	8 (4%)	0	100	100
All	All	1512/2552 (59%)	1460 (97%)	49 (3%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	290	PRO
1	A	183	LYS
1	A	274	ASN

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	163/273 (60%)	161 (99%)	2 (1%)	63	76
1	B	161/273 (59%)	160 (99%)	1 (1%)	78	83
1	C	161/273 (59%)	160 (99%)	1 (1%)	78	83
1	D	162/273 (59%)	158 (98%)	4 (2%)	42	66
1	E	165/273 (60%)	162 (98%)	3 (2%)	51	71
1	F	163/273 (60%)	159 (98%)	4 (2%)	42	66
1	G	163/273 (60%)	162 (99%)	1 (1%)	78	83
1	H	164/273 (60%)	161 (98%)	3 (2%)	51	71
All	All	1302/2184 (60%)	1283 (98%)	19 (2%)	57	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	183	LYS
1	B	280	ILE
1	C	220	SER
1	D	114	LEU
1	D	137	ASN
1	D	210	ASP
1	D	271	SER
1	E	113	ILE
1	E	201	MET
1	E	274	ASN
1	F	135	LYS
1	F	201	MET
1	F	250	LEU
1	F	274	ASN
1	G	183	LYS
1	H	98	GLN
1	H	130	LEU
1	H	197	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	C	119	ASN
1	C	165	ASN
1	E	165	ASN
1	F	147	GLN
1	F	165	ASN
1	G	165	ASN
1	G	172	HIS
1	H	165	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	SO4	D	401	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	G	402	-	4,4,4	0.27	0	6,6,6	0.11	0
3	PEG	G	401	-	6,6,6	0.11	0	5,5,5	0.08	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	PEG	G	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	401	PEG	O2-C3-C4-O4
3	G	401	PEG	O1-C1-C2-O2

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, 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	192/319 (60%)	2.10	84 (43%) 0 1	15, 33, 58, 74	0
1	B	191/319 (59%)	1.86	70 (36%) 1 1	14, 27, 51, 80	0
1	C	190/319 (59%)	1.95	68 (35%) 1 1	17, 34, 63, 104	0
1	D	190/319 (59%)	2.05	79 (41%) 0 1	14, 32, 72, 94	0
1	E	193/319 (60%)	2.07	91 (47%) 0 1	16, 34, 64, 96	0
1	F	192/319 (60%)	2.13	87 (45%) 0 1	16, 34, 69, 91	0
1	G	191/319 (59%)	2.22	91 (47%) 0 1	17, 36, 60, 85	0
1	H	193/319 (60%)	2.25	100 (51%) 0 1	19, 35, 66, 77	0
All	All	1532/2552 (60%)	2.08	670 (43%) 0 1	14, 33, 64, 104	0

All (670) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	286	SER	8.9
1	B	287	TYR	7.7
1	H	182	GLN	7.5
1	B	182	GLN	7.1
1	D	276	LEU	7.0
1	C	291	TRP	7.0
1	A	137	ASN	6.8
1	C	122	SER	6.7
1	B	289	ASN	6.5
1	A	122	SER	6.4
1	C	100	VAL	6.4
1	C	194	ASP	6.3
1	E	290	PRO	6.3
1	C	289	ASN	6.3
1	G	200	ASP	6.3
1	D	287	TYR	6.2

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Mol	Chain	Res	Type	RSRZ
1	E	289	ASN	6.1
1	H	287	TYR	6.1
1	B	137	ASN	5.8
1	A	287	TYR	5.6
1	G	112	THR	5.6
1	H	99	GLY	5.6
1	C	287	TYR	5.5
1	F	210	ASP	5.5
1	H	279	VAL	5.5
1	C	288	HIS	5.4
1	A	285	GLU	5.4
1	C	275	GLU	5.4
1	G	290	PRO	5.4
1	G	289	ASN	5.3
1	F	158	PRO	5.3
1	G	287	TYR	5.3
1	E	284	MET	5.3
1	D	144	LEU	5.2
1	C	129	ALA	5.2
1	C	125	TYR	5.2
1	F	268	TYR	5.2
1	F	138	ALA	5.2
1	D	139	TYR	5.2
1	E	285	GLU	5.2
1	F	182	GLN	5.2
1	D	279	VAL	5.1
1	A	289	ASN	5.0
1	G	113	ILE	5.0
1	F	278	GLN	5.0
1	D	281	TYR	4.9
1	D	271	SER	4.9
1	F	124	VAL	4.9
1	H	102	THR	4.9
1	G	220	SER	4.9
1	E	287	TYR	4.9
1	A	275	GLU	4.9
1	A	286	SER	4.8
1	F	287	TYR	4.8
1	G	285	GLU	4.8
1	D	268	TYR	4.8
1	B	286	SER	4.8
1	H	128	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	G	127	LYS	4.7
1	H	120	ARG	4.7
1	F	280	ILE	4.7
1	B	111	ASP	4.7
1	G	277	ALA	4.7
1	D	183	LYS	4.6
1	D	122	SER	4.6
1	B	145	GLU	4.6
1	D	288	HIS	4.6
1	A	274	ASN	4.6
1	A	108	GLU	4.6
1	F	273	ASN	4.6
1	H	288	HIS	4.5
1	G	222	LEU	4.5
1	D	162	LYS	4.5
1	C	290	PRO	4.5
1	B	272	SER	4.5
1	F	285	GLU	4.4
1	F	209	ALA	4.4
1	G	278	GLN	4.4
1	A	225	VAL	4.4
1	D	275	GLU	4.4
1	A	109	SER	4.4
1	F	279	VAL	4.4
1	F	161	PHE	4.4
1	E	273	ASN	4.4
1	F	160	ALA	4.3
1	H	274	ASN	4.3
1	H	276	LEU	4.3
1	D	284	MET	4.3
1	G	125	TYR	4.3
1	E	210	ASP	4.2
1	G	273	ASN	4.2
1	D	143	MET	4.2
1	F	127	LYS	4.2
1	E	203	LEU	4.2
1	G	203	LEU	4.2
1	F	108	GLU	4.1
1	C	111	ASP	4.1
1	E	268	TYR	4.1
1	B	278	GLN	4.1
1	C	107	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	139	TYR	4.1
1	A	196	SER	4.1
1	A	180	ILE	4.1
1	D	126	PRO	4.1
1	E	279	VAL	4.1
1	D	182	GLN	4.1
1	E	278	GLN	4.1
1	D	289	ASN	4.0
1	H	272	SER	4.0
1	G	184	GLY	4.0
1	C	286	SER	4.0
1	E	159	SER	4.0
1	G	276	LEU	4.0
1	H	218	VAL	4.0
1	C	121	VAL	4.0
1	D	286	SER	4.0
1	H	183	LYS	4.0
1	B	282	GLN	3.9
1	B	281	TYR	3.9
1	E	193	ASP	3.9
1	A	120	ARG	3.9
1	E	126	PRO	3.9
1	A	273	ASN	3.9
1	F	116	PHE	3.9
1	H	283	ALA	3.9
1	E	272	SER	3.9
1	B	285	GLU	3.9
1	E	99	GLY	3.8
1	B	273	ASN	3.8
1	G	136	ARG	3.8
1	C	148	GLU	3.8
1	C	196	SER	3.8
1	D	109	SER	3.8
1	E	135	LYS	3.8
1	G	179	TYR	3.8
1	G	288	HIS	3.8
1	B	215	LEU	3.8
1	H	111	ASP	3.8
1	G	217	TYR	3.8
1	G	183	LYS	3.7
1	G	282	GLN	3.7
1	A	271	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	120	ARG	3.7
1	G	178	GLU	3.7
1	E	127	LYS	3.7
1	F	122	SER	3.7
1	G	275	GLU	3.7
1	A	146	SER	3.7
1	E	139	TYR	3.7
1	F	139	TYR	3.7
1	A	216	ALA	3.7
1	G	141	ALA	3.7
1	D	282	GLN	3.7
1	D	274	ASN	3.7
1	C	116	PHE	3.7
1	F	290	PRO	3.7
1	H	271	SER	3.7
1	C	285	GLU	3.7
1	H	129	ALA	3.7
1	G	182	GLN	3.7
1	G	213	TRP	3.7
1	E	170	PRO	3.6
1	B	283	ALA	3.6
1	C	268	TYR	3.6
1	G	190	VAL	3.6
1	C	269	ASP	3.6
1	F	107	ASP	3.6
1	A	127	LYS	3.6
1	E	147	GLN	3.6
1	E	195	PRO	3.6
1	F	274	ASN	3.6
1	H	123	SER	3.6
1	H	284	MET	3.6
1	H	154	THR	3.6
1	F	123	SER	3.6
1	F	205	THR	3.6
1	F	120	ARG	3.6
1	A	283	ALA	3.6
1	F	227	ALA	3.6
1	G	274	ASN	3.6
1	H	145	GLU	3.6
1	G	271	SER	3.6
1	G	240	VAL	3.5
1	A	208	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	221	THR	3.5
1	E	184	GLY	3.5
1	A	140	MET	3.5
1	F	155	THR	3.5
1	E	286	SER	3.5
1	A	126	PRO	3.5
1	C	270	PRO	3.5
1	E	186	PRO	3.5
1	G	284	MET	3.5
1	H	280	ILE	3.5
1	F	150	ASP	3.5
1	D	116	PHE	3.4
1	A	132	VAL	3.4
1	H	124	VAL	3.4
1	G	270	PRO	3.4
1	H	144	LEU	3.4
1	B	219	ALA	3.4
1	H	110	ALA	3.4
1	G	180	ILE	3.4
1	G	151	LEU	3.4
1	C	99	GLY	3.4
1	B	138	ALA	3.4
1	C	193	ASP	3.4
1	G	148	GLU	3.4
1	A	222	LEU	3.4
1	E	141	ALA	3.4
1	H	160	ALA	3.4
1	H	201	MET	3.4
1	H	127	LYS	3.4
1	G	146	SER	3.4
1	D	185	GLU	3.4
1	C	120	ARG	3.4
1	H	193	ASP	3.4
1	G	252	GLY	3.4
1	H	289	ASN	3.3
1	E	269	ASP	3.3
1	D	125	TYR	3.3
1	B	158	PRO	3.3
1	G	223	PRO	3.3
1	G	124	VAL	3.3
1	A	268	TYR	3.3
1	D	129	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	215	LEU	3.3
1	H	273	ASN	3.3
1	B	185	GLU	3.3
1	E	108	GLU	3.3
1	D	290	PRO	3.3
1	B	156	HIS	3.3
1	G	137	ASN	3.3
1	E	145	GLU	3.3
1	H	122	SER	3.3
1	D	210	ASP	3.3
1	C	276	LEU	3.3
1	B	108	GLU	3.3
1	A	167	ARG	3.2
1	C	123	SER	3.2
1	H	189	LEU	3.2
1	H	176	ALA	3.2
1	D	121	VAL	3.2
1	F	147	GLN	3.2
1	H	100	VAL	3.2
1	A	113	ILE	3.2
1	H	290	PRO	3.2
1	F	194	ASP	3.2
1	G	111	ASP	3.2
1	A	125	TYR	3.2
1	A	161	PHE	3.2
1	B	116	PHE	3.2
1	D	270	PRO	3.2
1	F	159	SER	3.2
1	D	113	ILE	3.2
1	D	280	ILE	3.2
1	G	262	THR	3.2
1	E	276	LEU	3.2
1	E	288	HIS	3.2
1	H	282	GLN	3.2
1	H	165	ASN	3.1
1	C	264	TYR	3.1
1	E	182	GLN	3.1
1	C	110	ALA	3.1
1	B	214	ARG	3.1
1	D	140	MET	3.1
1	D	204	ALA	3.1
1	A	128	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	205	THR	3.1
1	A	193	ASP	3.1
1	D	253	VAL	3.1
1	A	280	ILE	3.1
1	F	277	ALA	3.1
1	B	275	GLU	3.1
1	C	279	VAL	3.1
1	G	100	VAL	3.1
1	G	186	PRO	3.1
1	H	117	LEU	3.1
1	C	102	THR	3.1
1	H	196	SER	3.1
1	D	161	PHE	3.1
1	F	135	LYS	3.1
1	A	139	TYR	3.1
1	G	166	LEU	3.0
1	F	157	ARG	3.0
1	F	140	MET	3.0
1	E	111	ASP	3.0
1	E	160	ALA	3.0
1	F	144	LEU	3.0
1	G	110	ALA	3.0
1	C	214	ARG	3.0
1	D	145	GLU	3.0
1	D	283	ALA	3.0
1	F	143	MET	3.0
1	A	191	LEU	3.0
1	B	169	SER	3.0
1	E	144	LEU	3.0
1	E	271	SER	3.0
1	H	125	TYR	3.0
1	F	184	GLY	3.0
1	D	124	VAL	3.0
1	D	112	THR	3.0
1	F	201	MET	3.0
1	B	181	LEU	3.0
1	A	147	GLN	3.0
1	C	119	ASN	3.0
1	E	187	ILE	3.0
1	C	117	LEU	2.9
1	F	191	LEU	2.9
1	F	215	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	204	ALA	2.9
1	E	137	ASN	2.9
1	H	186	PRO	2.9
1	G	160	ALA	2.9
1	A	229	VAL	2.9
1	G	153	VAL	2.9
1	A	116	PHE	2.9
1	H	113	ILE	2.9
1	G	133	ARG	2.9
1	D	127	LYS	2.9
1	A	290	PRO	2.9
1	A	276	LEU	2.9
1	C	101	LEU	2.9
1	E	165	ASN	2.9
1	C	136	ARG	2.9
1	E	136	ARG	2.9
1	G	266	LEU	2.9
1	E	138	ALA	2.9
1	G	154	THR	2.9
1	B	213	TRP	2.9
1	E	143	MET	2.9
1	H	187	ILE	2.9
1	A	141	ALA	2.8
1	A	150	ASP	2.8
1	A	254	ASP	2.8
1	D	269	ASP	2.8
1	A	142	GLU	2.8
1	C	142	GLU	2.8
1	H	149	VAL	2.8
1	G	116	PHE	2.8
1	A	272	SER	2.8
1	G	159	SER	2.8
1	C	160	ALA	2.8
1	C	218	VAL	2.8
1	H	178	GLU	2.8
1	H	164	LEU	2.8
1	H	281	TYR	2.8
1	D	147	GLN	2.8
1	F	219	ALA	2.8
1	H	134	VAL	2.8
1	D	215	LEU	2.8
1	B	180	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	152	MET	2.8
1	B	267	CYS	2.8
1	F	283	ALA	2.8
1	G	229	VAL	2.8
1	H	169	SER	2.8
1	C	144	LEU	2.8
1	H	179	TYR	2.8
1	A	214	ARG	2.8
1	G	249	VAL	2.8
1	F	272	SER	2.8
1	G	286	SER	2.8
1	D	107	ASP	2.7
1	B	268	TYR	2.7
1	B	127	LYS	2.7
1	D	149	VAL	2.7
1	H	153	VAL	2.7
1	A	251	SER	2.7
1	B	104	GLY	2.7
1	D	99	GLY	2.7
1	B	274	ASN	2.7
1	F	105	ALA	2.7
1	E	175	CYS	2.7
1	H	188	PRO	2.7
1	H	103	ILE	2.7
1	A	102	THR	2.7
1	C	271	SER	2.7
1	H	162	LYS	2.7
1	A	107	ASP	2.7
1	E	110	ALA	2.7
1	A	192	LEU	2.7
1	D	252	GLY	2.7
1	E	185	GLU	2.7
1	E	155	THR	2.7
1	B	146	SER	2.7
1	E	150	ASP	2.7
1	H	194	ASP	2.7
1	D	222	LEU	2.7
1	H	133	ARG	2.7
1	D	285	GLU	2.7
1	F	183	LYS	2.7
1	H	105	ALA	2.7
1	B	276	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	202	VAL	2.7
1	F	288	HIS	2.7
1	H	210	ASP	2.7
1	D	108	GLU	2.6
1	D	236	THR	2.6
1	B	191	LEU	2.6
1	C	130	LEU	2.6
1	H	209	ALA	2.6
1	B	288	HIS	2.6
1	C	158	PRO	2.6
1	E	274	ASN	2.6
1	F	284	MET	2.6
1	G	142	GLU	2.6
1	B	189	LEU	2.6
1	F	114	LEU	2.6
1	G	181	LEU	2.6
1	G	204	ALA	2.6
1	H	138	ALA	2.6
1	E	281	TYR	2.6
1	H	116	PHE	2.6
1	A	145	GLU	2.6
1	A	236	THR	2.6
1	D	196	SER	2.6
1	F	264	TYR	2.6
1	H	254	ASP	2.6
1	C	128	LEU	2.6
1	A	238	ARG	2.6
1	C	103	ILE	2.6
1	B	159	SER	2.6
1	H	150	ASP	2.6
1	A	250	LEU	2.6
1	C	222	LEU	2.6
1	A	160	ALA	2.6
1	E	227	ALA	2.6
1	E	171	THR	2.6
1	C	281	TYR	2.5
1	H	126	PRO	2.5
1	B	136	ARG	2.5
1	C	137	ASN	2.5
1	F	121	VAL	2.5
1	H	269	ASP	2.5
1	F	216	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	148	GLU	2.5
1	H	219	ALA	2.5
1	E	102	THR	2.5
1	G	221	THR	2.5
1	E	197	PRO	2.5
1	B	251	SER	2.5
1	H	250	LEU	2.5
1	B	253	VAL	2.5
1	D	264	TYR	2.5
1	E	196	SER	2.5
1	G	244	SER	2.5
1	A	185	GLU	2.5
1	C	108	GLU	2.5
1	H	213	TRP	2.5
1	B	126	PRO	2.5
1	D	130	LEU	2.5
1	E	128	LEU	2.5
1	F	249	VAL	2.5
1	A	210	ASP	2.5
1	H	107	ASP	2.5
1	C	155	THR	2.5
1	F	162	LYS	2.5
1	G	147	GLN	2.5
1	A	152	MET	2.4
1	D	263	GLU	2.4
1	E	148	GLU	2.4
1	B	107	ASP	2.4
1	H	200	ASP	2.4
1	F	117	LEU	2.4
1	D	158	PRO	2.4
1	E	115	PRO	2.4
1	F	217	TYR	2.4
1	A	99	GLY	2.4
1	F	134	VAL	2.4
1	G	279	VAL	2.4
1	A	110	ALA	2.4
1	F	180	ILE	2.4
1	B	148	GLU	2.4
1	G	233	LEU	2.4
1	A	112	THR	2.4
1	F	126	PRO	2.4
1	A	232	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	156	HIS	2.4
1	B	160	ALA	2.4
1	H	285	GLU	2.4
1	H	286	SER	2.4
1	E	215	LEU	2.4
1	G	253	VAL	2.4
1	H	268	TYR	2.4
1	D	177	ALA	2.4
1	G	241	GLU	2.4
1	A	288	HIS	2.4
1	B	150	ASP	2.4
1	G	246	ASP	2.4
1	A	277	ALA	2.4
1	H	277	ALA	2.4
1	H	136	ARG	2.4
1	C	189	LEU	2.4
1	C	233	LEU	2.4
1	D	266	LEU	2.4
1	F	181	LEU	2.4
1	H	181	LEU	2.4
1	E	146	SER	2.4
1	C	126	PRO	2.4
1	A	119	ASN	2.3
1	B	135	LYS	2.3
1	B	141	ALA	2.3
1	C	211	ILE	2.3
1	D	160	ALA	2.3
1	E	264	TYR	2.3
1	G	226	ARG	2.3
1	H	139	TYR	2.3
1	H	180	ILE	2.3
1	F	151	LEU	2.3
1	F	241	GLU	2.3
1	A	186	PRO	2.3
1	C	159	SER	2.3
1	D	146	SER	2.3
1	E	262	THR	2.3
1	H	232	GLY	2.3
1	H	237	ALA	2.3
1	E	152	MET	2.3
1	B	210	ASP	2.3
1	E	194	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	108	GLU	2.3
1	C	195	PRO	2.3
1	E	157	ARG	2.3
1	F	270	PRO	2.3
1	C	255	GLY	2.3
1	B	129	ALA	2.3
1	D	171	THR	2.3
1	E	283	ALA	2.3
1	F	179	TYR	2.3
1	E	200	ASP	2.3
1	H	275	GLU	2.3
1	G	255	GLY	2.3
1	B	144	LEU	2.3
1	G	139	TYR	2.3
1	G	268	TYR	2.3
1	H	246	ASP	2.3
1	A	136	ARG	2.3
1	B	149	VAL	2.3
1	D	148	GLU	2.3
1	E	229	VAL	2.3
1	H	225	VAL	2.3
1	E	158	PRO	2.3
1	D	231	ALA	2.3
1	D	205	THR	2.3
1	E	251	SER	2.3
1	F	125	TYR	2.3
1	G	162	LYS	2.3
1	A	279	VAL	2.3
1	E	275	GLU	2.2
1	F	185	GLU	2.2
1	G	263	GLU	2.2
1	E	280	ILE	2.2
1	C	171	THR	2.2
1	D	168	THR	2.2
1	H	161	PHE	2.2
1	C	139	TYR	2.2
1	H	220	SER	2.2
1	H	251	SER	2.2
1	A	175	CYS	2.2
1	E	134	VAL	2.2
1	F	165	ASN	2.2
1	G	121	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	240	VAL	2.2
1	D	254	ASP	2.2
1	F	275	GLU	2.2
1	C	212	PRO	2.2
1	G	138	ALA	2.2
1	F	208	LYS	2.2
1	G	135	LYS	2.2
1	G	199	ARG	2.2
1	B	244	SER	2.2
1	C	278	GLN	2.2
1	A	115	PRO	2.2
1	B	166	LEU	2.2
1	D	163	ALA	2.2
1	E	163	ALA	2.2
1	E	181	LEU	2.2
1	D	230	LYS	2.2
1	A	173	TRP	2.2
1	E	156	HIS	2.2
1	F	262	THR	2.2
1	H	132	VAL	2.2
1	D	106	SER	2.2
1	E	109	SER	2.2
1	G	185	GLU	2.2
1	A	138	ALA	2.2
1	F	110	ALA	2.2
1	F	188	PRO	2.2
1	G	258	PRO	2.2
1	H	234	GLY	2.2
1	D	136	ARG	2.2
1	B	279	VAL	2.2
1	F	244	SER	2.2
1	F	271	SER	2.2
1	E	142	GLU	2.2
1	F	163	ALA	2.2
1	H	208	LYS	2.2
1	H	175	CYS	2.2
1	A	262	THR	2.1
1	F	103	ILE	2.1
1	F	118	LEU	2.1
1	E	183	LYS	2.1
1	C	163	ALA	2.1
1	E	105	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	209	ALA	2.1
1	G	109	SER	2.1
1	F	99	GLY	2.1
1	E	161	PHE	2.1
1	E	246	ASP	2.1
1	B	190	VAL	2.1
1	G	134	VAL	2.1
1	F	281	TYR	2.1
1	A	181	LEU	2.1
1	A	256	LEU	2.1
1	D	164	LEU	2.1
1	E	151	LEU	2.1
1	G	105	ALA	2.1
1	F	119	ASN	2.1
1	D	267	CYS	2.1
1	E	149	VAL	2.1
1	A	135	LYS	2.1
1	C	113	ILE	2.1
1	G	205	THR	2.1
1	H	206	LEU	2.1
1	H	211	ILE	2.1
1	G	264	TYR	2.1
1	G	143	MET	2.1
1	B	147	GLN	2.1
1	G	224	ALA	2.1
1	F	145	GLU	2.1
1	H	119	ASN	2.1
1	B	121	VAL	2.1
1	A	111	ASP	2.1
1	C	208	LYS	2.1
1	B	264	TYR	2.1
1	D	154	THR	2.1
1	D	184	GLY	2.1
1	B	271	SER	2.1
1	A	121	VAL	2.1
1	B	100	VAL	2.1
1	B	162	LYS	2.1
1	H	135	LYS	2.1
1	A	130	LEU	2.1
1	C	118	LEU	2.1
1	D	262	THR	2.1
1	A	153	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	191	LEU	2.0
1	B	284	MET	2.0
1	D	277	ALA	2.0
1	F	200	ASP	2.0
1	A	104	GLY	2.0
1	C	133	ARG	2.0
1	C	181	LEU	2.0
1	B	280	ILE	2.0
1	E	113	ILE	2.0
1	E	123	SER	2.0
1	F	251	SER	2.0
1	A	284	MET	2.0
1	E	140	MET	2.0
1	H	156	HIS	2.0
1	B	110	ALA	2.0
1	G	237	ALA	2.0
1	B	125	TYR	2.0
1	B	217	TYR	2.0
1	B	254	ASP	2.0
1	G	161	PHE	2.0
1	E	162	LYS	2.0
1	E	282	GLN	2.0
1	F	276	LEU	2.0
1	C	280	ILE	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	PEG	G	401	7/7	0.43	0.48	65,65,66,67	0
2	SO4	D	401	5/5	0.57	0.17	43,43,43,44	0
2	SO4	G	402	5/5	0.81	0.15	41,41,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.