Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 11:12 PM JST

PDB ID	:	7YHJ
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)

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

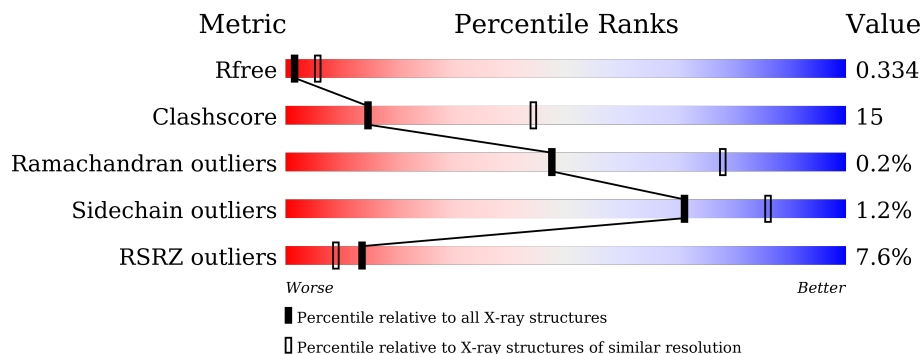|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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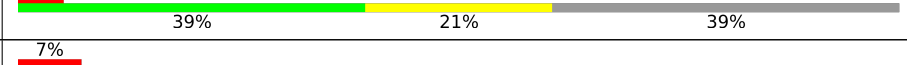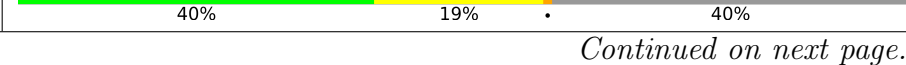*X-RAY DIFFRACTION*

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.
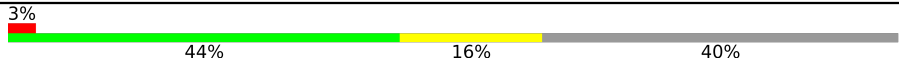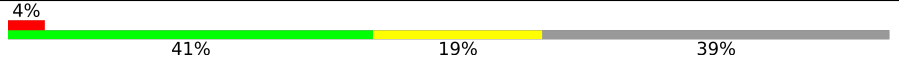
Metric	Percentile Ranks	Value
Rfree		0.334
Clashscore		15
Ramachandran outliers		0.2%
Sidechain outliers		1.2%
RSRZ outliers		7.6%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (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 <=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	3% / 38% / 22% / 40%
1	B	319	4% / 45% / 15% / 40%
1	C	319	5% / 39% / 21% / 40%
1	D	319	5% / 39% / 19% / • / 40%
1	E	319	5% / 39% / 21% / 39%
1	F	319	7% / 40% / 19% / • / 40%

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
1	G	319	3% 44% 16% 40%
1	H	319	4% 41% 19% 39%

2 Entry composition (i)

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 (three-letter code: SO4) (formula: O_4S).
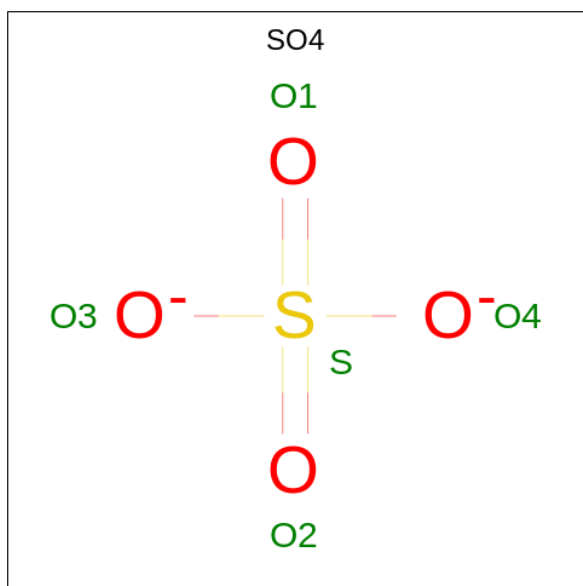
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total 5	O 4	S 1	0	0
2	G	1	Total 5	O 4	S 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
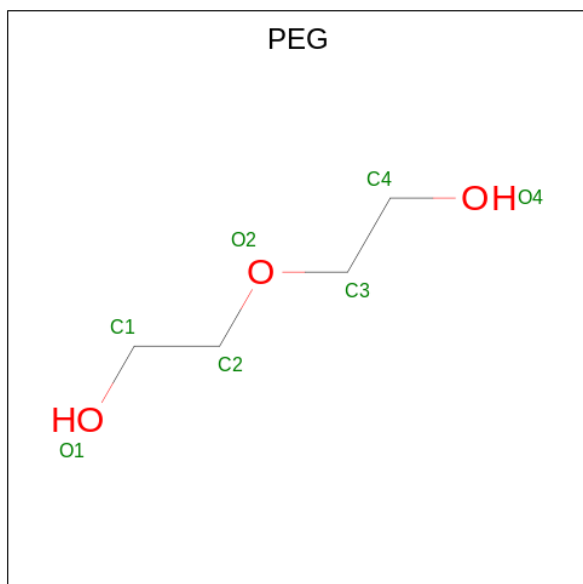
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total 7	C 4	O 3	0	0

- Molecule 4 is water.

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

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

Chain A:

• Molecule 1: Probable HTH-type transcriptional regulator LrhA

Chain B:

• Molecule 1: Probable HTH-type transcriptional regulator LrhA

Chain C:

• Molecule 1: Probable HTH-type transcriptional regulator LrhA

Chain D:

• Molecule 1: Probable HTH-type transcriptional regulator LrhA

Chain E:

A219 L222 P223 A224 V225 R226 K230 L233 T236 A237 R238 P239 M242 M243 S244 P245 D246 L247 R248 V249 L250 L256 P257 P258 L259 E263 N273 N274 Q278 V279 I280 Y281 Q282 E285 S286 Y287 H288 N289 P290 TRP TYR SER MET SER ALA PRO GLU GLY
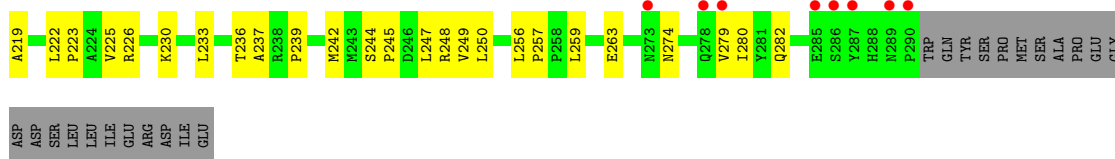
ASP ASP SER LEU LEU ILE GLU ARG ASP ILE GLU

• Molecule 1: Probable HTH-type transcriptional regulator LrhA

Chain F:

MET HIS HIS HIS HIS HIS MET ILE SER ALA ASN ARG PRO ILE ILE ASN LEU ASP LEU ASP LEU LEU ARG PHE VAL ALA VAL ALA ASP LEU ASN THR PHE ALA ALA ALA ALA VAL CYS ARG THR GLN SER ALA VAL SER GLN GLN MET GLN ARG LEU GLU GLN LEU VAL

GLY LYS GLU LEU PHE ALA ARG HIS GLY ARG ASN LYS LEU LEU THR GLU HIS GLY ILE GLN LEU LEU GLY TYR ALA ARG LYS ILE LEU LEU ARG PHE ASN ASP GLU ALA CYS SER SER LEU MET PHE SER ASN LEU GLN G99 V100 L101 T102 A110 I113 L114 P115 L118 N119 R120 V121

S122 L130 D131 V132 K135 R136 N137 A138 Y139 M140 M143 L144 E145 S146 Q147 E148 V149 M152 V153 T154 R157 P158 K162 P170 W173 Y174 C175 A176 A177 E178 Y179 I180 L181 Q182 K183 P188 L189 V190 L191 L192 D193 D194 P195 S196 R199 D200 M201 T205 L206

A209 D210 R214 L215 A216 Y217 V218 A219 L222 P223 A224 V225 A228 V229 K230 A231 G232 L233 P239 V240 D246 L247 R248 V249 L250 L256 P257 T262 E263 Y268 D269 P270 N273 N274 A277 Q278 V279 I280 E285 S286 Y287 P290 TRP GLN TYR SER PRO
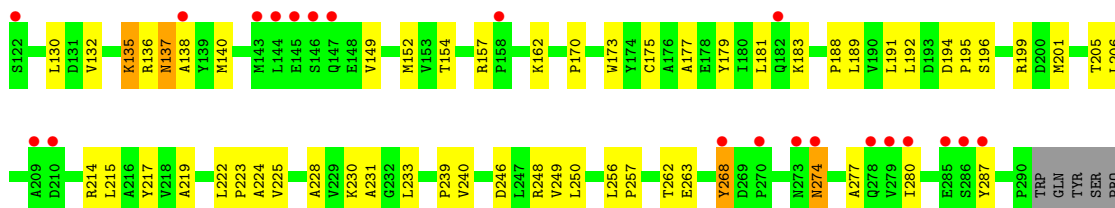
MET SER ALA PRO GLU GLY ASP ASP SER LEU LEU ILE GLU ARG ASP ILE GLU

• Molecule 1: Probable HTH-type transcriptional regulator LrhA

Chain G:

MET HIS HIS HIS HIS HIS MET ILE SER ALA ASN ARG PRO ILE ILE ASN LEU ASP LEU ASP LEU LEU ARG THR PHE VAL ALA VAL ALA ASP LEU ASN THR PHE ALA ALA ALA ALA VAL CYS ARG THR GLN SER ALA VAL SER GLN GLN MET GLN ARG LEU GLU GLU GLN LEU VAL

GLY LYS GLU LEU PHE ALA ARG HIS GLY ARG ASN LYS LEU LEU THR GLU HIS GLY ILE GLN LEU LEU GLY TYR ALA ARG LYS ILE LEU LEU ARG ASN ASP ALA CYS SER SER LEU MET PHE SER ASN LEU GLN GLY V100 L101 A110 I113 L114 P115 V124 L128 V132

R133 V134 K135 R136 N137 A138 Y139 M140 M152 K162 R167 T168 S169 P170 W173 A176 A177 E178 Y179 K183 G184 L189 V190 L191 L192 D193 D194 P195 F198 R199 D200 D210 Y217 V218 A219 S220 T221 L222 P223 A224 V225 R226 V235 R238 P239 V240 E241 M242

R248 V249 L250 V253 L256 Y264 P270 E275 L276 A277 Q278 V279 I280 Y281 Q282 Y287 P290 TRP GLN TYR SER PRO MET SER ALA PRO GLU GLY ASP ASP SER LEU LEU ILE GLU ARG ASP ILE GLU
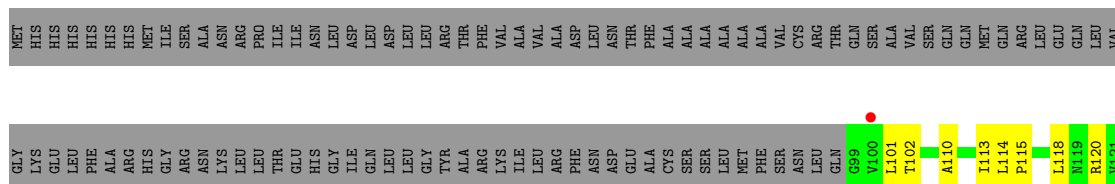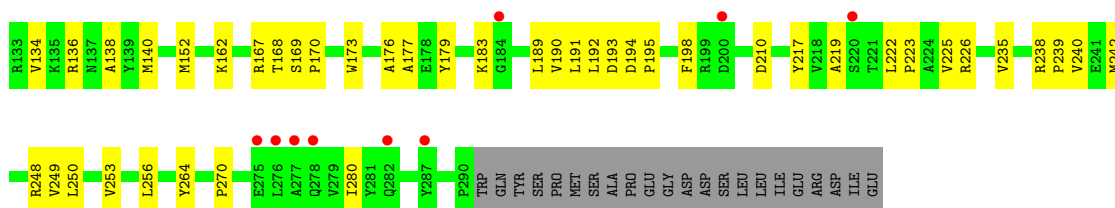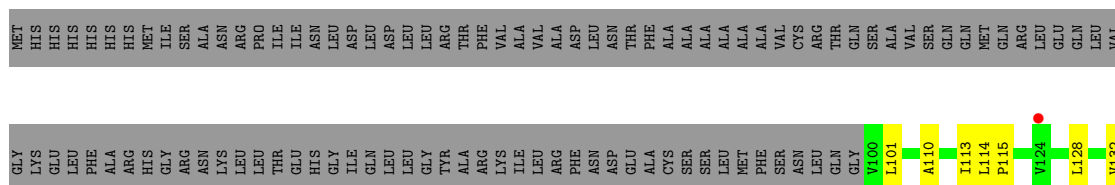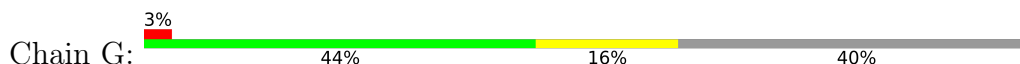
• Molecule 1: Probable HTH-type transcriptional regulator LrhA

Chain H:

MET HIS HIS HIS HIS HIS MET ILE SER ALA ASN ARG PRO ILE ILE ASN LEU ASP LEU ASP LEU LEU ARG THR PHE VAL ALA VAL ALA ASP LEU ASN THR PHE ALA ALA ALA ALA VAL CYS ARG THR GLN SER ALA VAL SER GLN GLN MET GLN ARG LEU GLU GLN LEU VAL

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
$< I/\sigma(I) >$ [1]	1.55 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.321 , 0.338 0.319 , 0.334	Depositor DCC
R_{free} test set	2153 reflections (4.94%)	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)	0.33 , 29.0	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.26$	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.*

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[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: 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	0.60	0/1513	0.78	0/2071
1	B	0.60	0/1498	0.75	0/2053
1	C	0.59	0/1507	0.79	0/2061
1	D	0.60	0/1501	0.76	0/2054
1	E	0.60	0/1525	0.75	0/2088
1	F	0.60	0/1514	0.77	0/2072
1	G	0.57	0/1507	0.73	0/2064
1	H	0.60	0/1522	0.79	0/2084
All	All	0.59	0/12087	0.76	0/16547

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	38	0
1	C	1472	0	1478	50	0
1	D	1467	0	1473	50	0
1	E	1490	0	1493	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1479	0	1490	50	0
1	G	1472	0	1478	43	0
1	H	1487	0	1491	44	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	362	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 15.

All (362) 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: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: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
1:B:152:MET:HE2	1:B:267:CYS:HB2	1.69	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:125:TYR:C	1:A:127:LYS:H	2.09	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:D:140:MET:HE3	1:D:152:MET:HG3	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:138:ALA:CB	1:E:195:PRO:HG2	2.41	0.49
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: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:B:152:MET:HE2	1:B:267:CYS:CB	2.40	0.49
1:F:140:MET:HE3	1:F:152:MET:HG3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:226:ARG:HG2	1:G:242:MET:HE1	1.94	0.48
1:D:249:VAL:HG11	1:F:240:VAL:HG11	1.95	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:A:132:VAL:HG12	1:E:217:TYR:HH	1.78	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:215:LEU:O	1:H:215:LEU:HD12	2.16	0.46
1:D:105:ALA:O	1:D:134:VAL:HA	2.16	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:A:204:ALA:O	1:A:208:LYS:HG3	2.16	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:99:GLY:C	1:H:128:LEU:HD12	2.38	0.44
1:B:101:LEU:HB2	1:B:128:LEU:HD21	2.00	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
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:226:ARG:HG3	1:A:242:MET:HE3	2.01	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: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:271:SER:HG	1:D:274:ASN:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:226:ARG:HG3	1:A:242:MET:CE	2.49	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:B:263:GLU:HB3	1:B:265:LEU:HD21	2.01	0.42
1:C:290:PRO:O	1:C:291:TRP:C	2.57	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:A:152:MET:HE3	1:A:158:PRO:HG3	2.01	0.41
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
1:C:117:LEU:CD1	1:C:266:LEU:HD13	2.50	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: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:211:ILE:CD1	1:B:257:PRO:HD3	2.51	0.41
1:C:106:SER:HA	1:C:140:MET:HE3	2.03	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: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:B:273:ASN:CG	1:G:210:ASP:HB2	2.40	0.41
1:H:274:ASN:O	1:H:278:GLN:OE1	2.39	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:104:GLY:C	1:E:140:MET:HE1	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD12	1:A:130:LEU:O	2.21	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
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%)	14	48
1	B	189/319 (59%)	186 (98%)	3 (2%)	0	100	100
1	C	186/319 (58%)	180 (97%)	5 (3%)	1 (0%)	29	64
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%)	47	78

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 ⓘ

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%)	162 (99%)	1 (1%)	86	93
1	B	161/273 (59%)	160 (99%)	1 (1%)	86	93
1	C	161/273 (59%)	160 (99%)	1 (1%)	86	93
1	D	162/273 (59%)	158 (98%)	4 (2%)	47	74
1	E	165/273 (60%)	164 (99%)	1 (1%)	86	93
1	F	163/273 (60%)	158 (97%)	5 (3%)	40	70
1	G	163/273 (60%)	162 (99%)	1 (1%)	86	93
1	H	164/273 (60%)	162 (99%)	2 (1%)	71	86
All	All	1302/2184 (60%)	1286 (99%)	16 (1%)	71	86

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LYS
1	B	245	PRO
1	C	137	ASN
1	D	114	LEU
1	D	137	ASN
1	D	210	ASP
1	D	271	SER
1	E	274	ASN
1	F	135	LYS
1	F	137	ASN
1	F	201	MET

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Mol	Chain	Res	Type
1	F	268	TYR
1	F	274	ASN
1	G	183	LYS
1	H	98	GLN
1	H	197	PRO

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

Mol	Chain	Res	Type
1	A	137	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	0.26	0	6,6,6	0.07	0
3	PEG	G	401	-	6,6,6	0.11	0	5,5,5	0.08	0
2	SO4	G	402	-	4,4,4	0.29	0	6,6,6	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	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	192/319 (60%)	0.44	10 (5%)	27	17	15, 33, 58, 74	0
1	B	191/319 (59%)	0.45	13 (6%)	17	12	14, 27, 51, 80	0
1	C	190/319 (59%)	0.54	17 (8%)	9	7	17, 34, 63, 104	0
1	D	190/319 (59%)	0.60	16 (8%)	11	7	14, 32, 72, 94	0
1	E	193/319 (60%)	0.59	17 (8%)	10	7	16, 34, 64, 96	0
1	F	192/319 (60%)	0.67	22 (11%)	4	4	16, 34, 69, 91	0
1	G	191/319 (59%)	0.52	10 (5%)	27	17	17, 36, 60, 85	0
1	H	193/319 (60%)	0.58	12 (6%)	20	13	19, 35, 66, 77	0
All	All	1532/2552 (60%)	0.55	117 (7%)	13	9	14, 33, 64, 104	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	271	SER	5.0
1	H	99	GLY	4.9
1	D	274	ASN	4.9
1	B	289	ASN	4.4
1	E	289	ASN	4.4
1	C	290	PRO	4.4
1	F	278	GLN	4.3
1	D	143	MET	4.2
1	C	289	ASN	4.2
1	D	287	TYR	4.2
1	C	291	TRP	4.0
1	C	275	GLU	4.0
1	E	279	VAL	4.0
1	A	122	SER	4.0
1	E	100	VAL	3.9
1	B	273	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	210	ASP	3.8
1	G	277	ALA	3.7
1	D	276	LEU	3.7
1	E	290	PRO	3.6
1	F	274	ASN	3.5
1	G	276	LEU	3.5
1	D	289	ASN	3.4
1	H	182	GLN	3.4
1	H	102	THR	3.4
1	B	182	GLN	3.4
1	D	275	GLU	3.4
1	E	186	PRO	3.4
1	E	285	GLU	3.4
1	C	288	HIS	3.3
1	H	274	ASN	3.3
1	H	276	LEU	3.3
1	C	122	SER	3.2
1	E	273	ASN	3.2
1	E	99	GLY	3.2
1	D	290	PRO	3.2
1	G	200	ASP	3.1
1	C	269	ASP	3.0
1	B	287	TYR	3.0
1	E	286	SER	3.0
1	H	289	ASN	3.0
1	B	150	ASP	3.0
1	F	285	GLU	2.9
1	F	209	ALA	2.9
1	C	276	LEU	2.9
1	F	286	SER	2.8
1	H	127	LYS	2.8
1	H	128	LEU	2.8
1	E	195	PRO	2.7
1	B	274	ASN	2.7
1	G	275	GLU	2.7
1	H	275	GLU	2.7
1	F	182	GLN	2.7
1	F	138	ALA	2.7
1	G	278	GLN	2.7
1	A	287	TYR	2.7
1	B	282	GLN	2.7
1	G	184	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	269	ASP	2.7
1	A	290	PRO	2.7
1	E	278	GLN	2.7
1	B	127	LYS	2.6
1	C	121	VAL	2.6
1	F	144	LEU	2.6
1	F	279	VAL	2.6
1	F	158	PRO	2.5
1	C	281	TYR	2.5
1	D	136	ARG	2.5
1	F	268	TYR	2.5
1	F	122	SER	2.5
1	C	286	SER	2.4
1	F	145	GLU	2.4
1	D	182	GLN	2.4
1	C	100	VAL	2.4
1	A	289	ASN	2.4
1	F	146	SER	2.4
1	F	100	VAL	2.4
1	E	210	ASP	2.4
1	D	122	SER	2.4
1	B	147	GLN	2.3
1	D	145	GLU	2.3
1	G	220	SER	2.3
1	A	285	GLU	2.3
1	G	282	GLN	2.3
1	F	280	ILE	2.3
1	C	287	TYR	2.3
1	C	194	ASP	2.3
1	E	193	ASP	2.3
1	G	124	VAL	2.3
1	A	146	SER	2.3
1	B	215	LEU	2.2
1	F	273	ASN	2.2
1	F	147	GLN	2.2
1	F	287	TYR	2.2
1	D	139	TYR	2.2
1	B	285	GLU	2.2
1	B	286	SER	2.2
1	B	156	HIS	2.2
1	C	129	ALA	2.2
1	G	287	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	2.2
1	H	186	PRO	2.1
1	H	147	GLN	2.1
1	D	277	ALA	2.1
1	D	288	HIS	2.1
1	A	137	ASN	2.1
1	E	139	TYR	2.1
1	E	287	TYR	2.1
1	F	143	MET	2.1
1	C	268	TYR	2.1
1	H	273	ASN	2.1
1	E	126	PRO	2.0
1	A	214	ARG	2.0
1	E	159	SER	2.0
1	C	195	PRO	2.0
1	F	270	PRO	2.0
1	A	101	LEU	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	G	401	7/7	0.77	0.25	65,65,66,67	0
2	SO4	D	401	5/5	0.81	0.34	43,43,43,44	0
2	SO4	G	402	5/5	0.92	0.35	41,41,41,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.