



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:37 AM UTC

PDB ID : 8EQW / pdb_00008eqw
Title : Crystal structure of Fub7
Authors : Hai, Y.
Deposited on : 2022-10-10
Resolution : 1.76 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

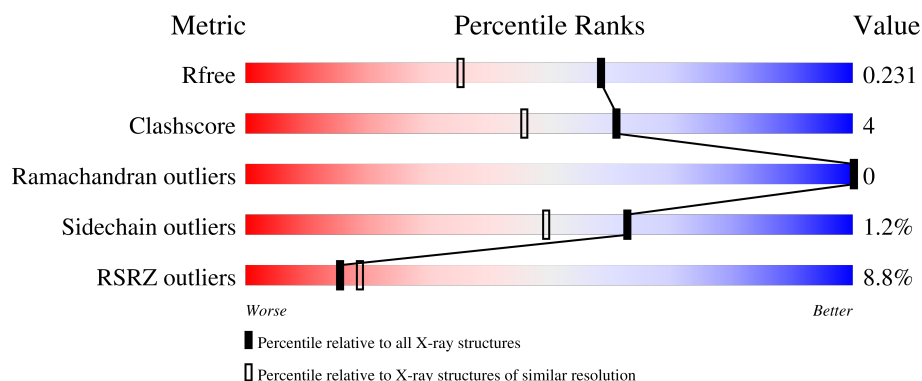
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	450	9% 83%10%6%
1	B	450	9% 80%9%10%
1	C	450	8% 83%10%7%
1	D	450	8% 83%9%8%
1	E	450	8% 84%9%6%

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Mol	Chain	Length	Quality of chain
1	F	450	7% 85% 9% 6%
1	G	450	8% 79% 13% 8%
1	H	450	9% 82% 12% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27419 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 Sulphydrylase FUB7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	P	S	0	0	0
			3259	2070	561	620	1	7			
1	B	407	Total	C	N	O	P	S	0	0	0
			3143	2000	538	597	1	7			
1	C	418	Total	C	N	O	P	S	0	0	0
			3220	2046	554	612	1	7			
1	D	414	Total	C	N	O	P	S	0	0	0
			3198	2035	548	607	1	7			
1	E	424	Total	C	N	O	P	S	0	0	0
			3271	2075	563	625	1	7			
1	F	424	Total	C	N	O	P	S	0	0	0
			3272	2074	563	627	1	7			
1	G	415	Total	C	N	O	P	S	0	1	0
			3210	2042	552	608	1	7			
1	H	426	Total	C	N	O	P	S	0	0	0
			3289	2085	566	630	1	7			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP S0DUX5
A	-15	GLY	-	expression tag	UNP S0DUX5
A	-14	SER	-	expression tag	UNP S0DUX5
A	-13	SER	-	expression tag	UNP S0DUX5
A	-12	HIS	-	expression tag	UNP S0DUX5
A	-11	HIS	-	expression tag	UNP S0DUX5
A	-10	HIS	-	expression tag	UNP S0DUX5
A	-9	HIS	-	expression tag	UNP S0DUX5
A	-8	HIS	-	expression tag	UNP S0DUX5
A	-7	HIS	-	expression tag	UNP S0DUX5
A	-6	GLU	-	expression tag	UNP S0DUX5
A	-5	ASN	-	expression tag	UNP S0DUX5
A	-4	LEU	-	expression tag	UNP S0DUX5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP S0DUX5
A	-2	PHE	-	expression tag	UNP S0DUX5
A	-1	GLN	-	expression tag	UNP S0DUX5
A	0	SER	-	expression tag	UNP S0DUX5
A	1	ASN	-	expression tag	UNP S0DUX5
B	-16	MET	-	initiating methionine	UNP S0DUX5
B	-15	GLY	-	expression tag	UNP S0DUX5
B	-14	SER	-	expression tag	UNP S0DUX5
B	-13	SER	-	expression tag	UNP S0DUX5
B	-12	HIS	-	expression tag	UNP S0DUX5
B	-11	HIS	-	expression tag	UNP S0DUX5
B	-10	HIS	-	expression tag	UNP S0DUX5
B	-9	HIS	-	expression tag	UNP S0DUX5
B	-8	HIS	-	expression tag	UNP S0DUX5
B	-7	HIS	-	expression tag	UNP S0DUX5
B	-6	GLU	-	expression tag	UNP S0DUX5
B	-5	ASN	-	expression tag	UNP S0DUX5
B	-4	LEU	-	expression tag	UNP S0DUX5
B	-3	TYR	-	expression tag	UNP S0DUX5
B	-2	PHE	-	expression tag	UNP S0DUX5
B	-1	GLN	-	expression tag	UNP S0DUX5
B	0	SER	-	expression tag	UNP S0DUX5
B	1	ASN	-	expression tag	UNP S0DUX5
C	-16	MET	-	initiating methionine	UNP S0DUX5
C	-15	GLY	-	expression tag	UNP S0DUX5
C	-14	SER	-	expression tag	UNP S0DUX5
C	-13	SER	-	expression tag	UNP S0DUX5
C	-12	HIS	-	expression tag	UNP S0DUX5
C	-11	HIS	-	expression tag	UNP S0DUX5
C	-10	HIS	-	expression tag	UNP S0DUX5
C	-9	HIS	-	expression tag	UNP S0DUX5
C	-8	HIS	-	expression tag	UNP S0DUX5
C	-7	HIS	-	expression tag	UNP S0DUX5
C	-6	GLU	-	expression tag	UNP S0DUX5
C	-5	ASN	-	expression tag	UNP S0DUX5
C	-4	LEU	-	expression tag	UNP S0DUX5
C	-3	TYR	-	expression tag	UNP S0DUX5
C	-2	PHE	-	expression tag	UNP S0DUX5
C	-1	GLN	-	expression tag	UNP S0DUX5
C	0	SER	-	expression tag	UNP S0DUX5
C	1	ASN	-	expression tag	UNP S0DUX5
D	-16	MET	-	initiating methionine	UNP S0DUX5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	GLY	-	expression tag	UNP S0DUX5
D	-14	SER	-	expression tag	UNP S0DUX5
D	-13	SER	-	expression tag	UNP S0DUX5
D	-12	HIS	-	expression tag	UNP S0DUX5
D	-11	HIS	-	expression tag	UNP S0DUX5
D	-10	HIS	-	expression tag	UNP S0DUX5
D	-9	HIS	-	expression tag	UNP S0DUX5
D	-8	HIS	-	expression tag	UNP S0DUX5
D	-7	HIS	-	expression tag	UNP S0DUX5
D	-6	GLU	-	expression tag	UNP S0DUX5
D	-5	ASN	-	expression tag	UNP S0DUX5
D	-4	LEU	-	expression tag	UNP S0DUX5
D	-3	TYR	-	expression tag	UNP S0DUX5
D	-2	PHE	-	expression tag	UNP S0DUX5
D	-1	GLN	-	expression tag	UNP S0DUX5
D	0	SER	-	expression tag	UNP S0DUX5
D	1	ASN	-	expression tag	UNP S0DUX5
E	-16	MET	-	initiating methionine	UNP S0DUX5
E	-15	GLY	-	expression tag	UNP S0DUX5
E	-14	SER	-	expression tag	UNP S0DUX5
E	-13	SER	-	expression tag	UNP S0DUX5
E	-12	HIS	-	expression tag	UNP S0DUX5
E	-11	HIS	-	expression tag	UNP S0DUX5
E	-10	HIS	-	expression tag	UNP S0DUX5
E	-9	HIS	-	expression tag	UNP S0DUX5
E	-8	HIS	-	expression tag	UNP S0DUX5
E	-7	HIS	-	expression tag	UNP S0DUX5
E	-6	GLU	-	expression tag	UNP S0DUX5
E	-5	ASN	-	expression tag	UNP S0DUX5
E	-4	LEU	-	expression tag	UNP S0DUX5
E	-3	TYR	-	expression tag	UNP S0DUX5
E	-2	PHE	-	expression tag	UNP S0DUX5
E	-1	GLN	-	expression tag	UNP S0DUX5
E	0	SER	-	expression tag	UNP S0DUX5
E	1	ASN	-	expression tag	UNP S0DUX5
F	-16	MET	-	initiating methionine	UNP S0DUX5
F	-15	GLY	-	expression tag	UNP S0DUX5
F	-14	SER	-	expression tag	UNP S0DUX5
F	-13	SER	-	expression tag	UNP S0DUX5
F	-12	HIS	-	expression tag	UNP S0DUX5
F	-11	HIS	-	expression tag	UNP S0DUX5
F	-10	HIS	-	expression tag	UNP S0DUX5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	HIS	-	expression tag	UNP S0DUX5
F	-8	HIS	-	expression tag	UNP S0DUX5
F	-7	HIS	-	expression tag	UNP S0DUX5
F	-6	GLU	-	expression tag	UNP S0DUX5
F	-5	ASN	-	expression tag	UNP S0DUX5
F	-4	LEU	-	expression tag	UNP S0DUX5
F	-3	TYR	-	expression tag	UNP S0DUX5
F	-2	PHE	-	expression tag	UNP S0DUX5
F	-1	GLN	-	expression tag	UNP S0DUX5
F	0	SER	-	expression tag	UNP S0DUX5
F	1	ASN	-	expression tag	UNP S0DUX5
G	-16	MET	-	initiating methionine	UNP S0DUX5
G	-15	GLY	-	expression tag	UNP S0DUX5
G	-14	SER	-	expression tag	UNP S0DUX5
G	-13	SER	-	expression tag	UNP S0DUX5
G	-12	HIS	-	expression tag	UNP S0DUX5
G	-11	HIS	-	expression tag	UNP S0DUX5
G	-10	HIS	-	expression tag	UNP S0DUX5
G	-9	HIS	-	expression tag	UNP S0DUX5
G	-8	HIS	-	expression tag	UNP S0DUX5
G	-7	HIS	-	expression tag	UNP S0DUX5
G	-6	GLU	-	expression tag	UNP S0DUX5
G	-5	ASN	-	expression tag	UNP S0DUX5
G	-4	LEU	-	expression tag	UNP S0DUX5
G	-3	TYR	-	expression tag	UNP S0DUX5
G	-2	PHE	-	expression tag	UNP S0DUX5
G	-1	GLN	-	expression tag	UNP S0DUX5
G	0	SER	-	expression tag	UNP S0DUX5
G	1	ASN	-	expression tag	UNP S0DUX5
H	-16	MET	-	initiating methionine	UNP S0DUX5
H	-15	GLY	-	expression tag	UNP S0DUX5
H	-14	SER	-	expression tag	UNP S0DUX5
H	-13	SER	-	expression tag	UNP S0DUX5
H	-12	HIS	-	expression tag	UNP S0DUX5
H	-11	HIS	-	expression tag	UNP S0DUX5
H	-10	HIS	-	expression tag	UNP S0DUX5
H	-9	HIS	-	expression tag	UNP S0DUX5
H	-8	HIS	-	expression tag	UNP S0DUX5
H	-7	HIS	-	expression tag	UNP S0DUX5
H	-6	GLU	-	expression tag	UNP S0DUX5
H	-5	ASN	-	expression tag	UNP S0DUX5
H	-4	LEU	-	expression tag	UNP S0DUX5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	TYR	-	expression tag	UNP S0DUX5
H	-2	PHE	-	expression tag	UNP S0DUX5
H	-1	GLN	-	expression tag	UNP S0DUX5
H	0	SER	-	expression tag	UNP S0DUX5
H	1	ASN	-	expression tag	UNP S0DUX5

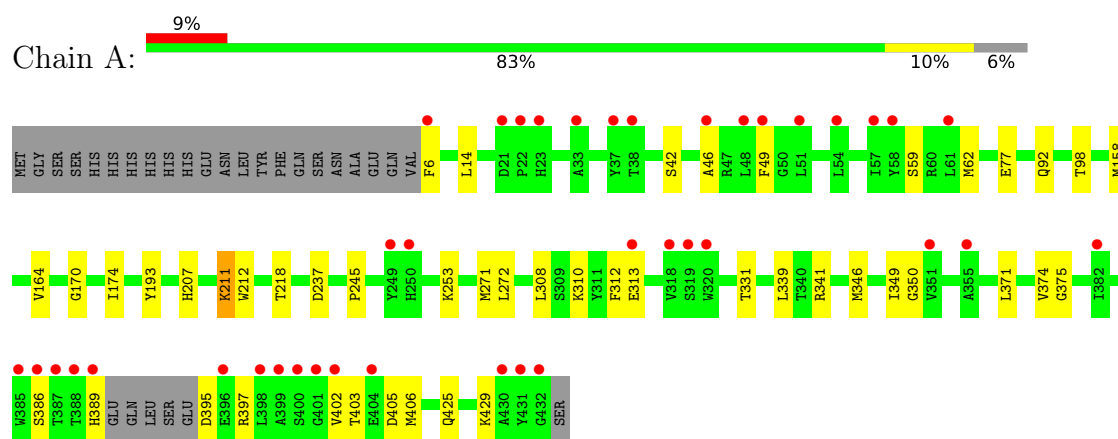
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	187	Total O 187 187	0	0
2	B	161	Total O 161 161	0	0
2	C	216	Total O 216 216	0	0
2	D	215	Total O 215 215	0	0
2	E	200	Total O 200 200	0	0
2	F	219	Total O 220 220	0	1
2	G	168	Total O 168 168	0	0
2	H	190	Total O 190 190	0	0

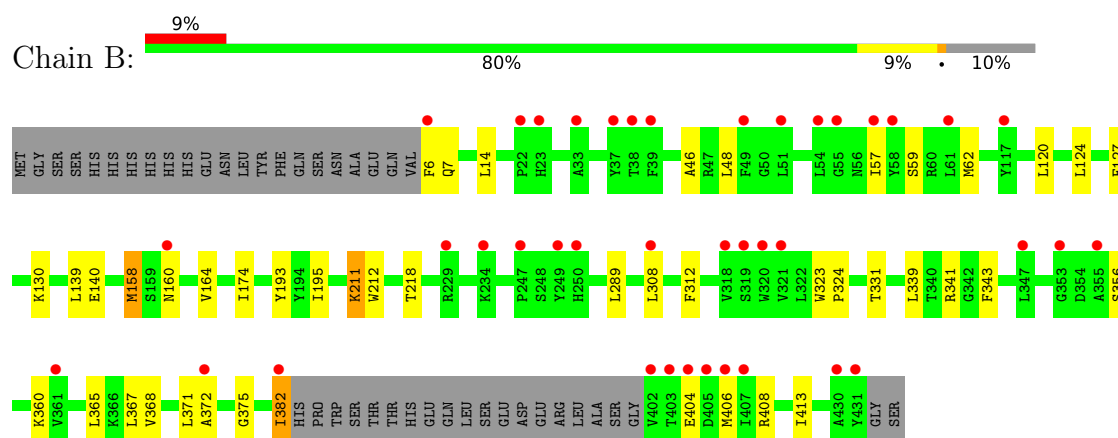
3 Residue-property plots [i](#)

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.

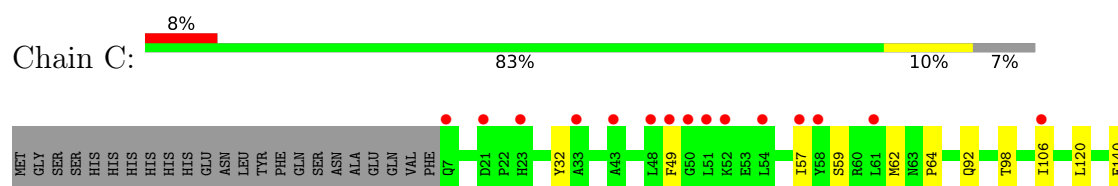
• Molecule 1: Sulfhydrylase FUB7

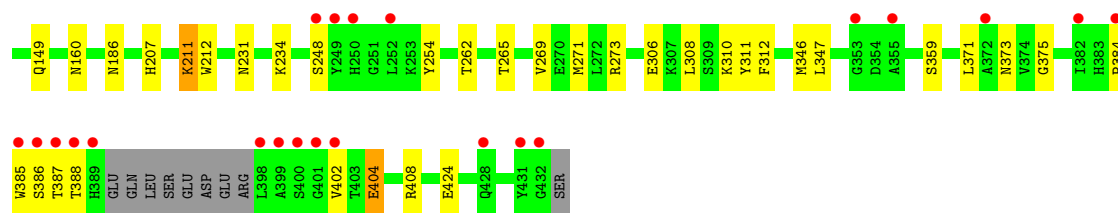


• Molecule 1: Sulfhydrylase FUB7

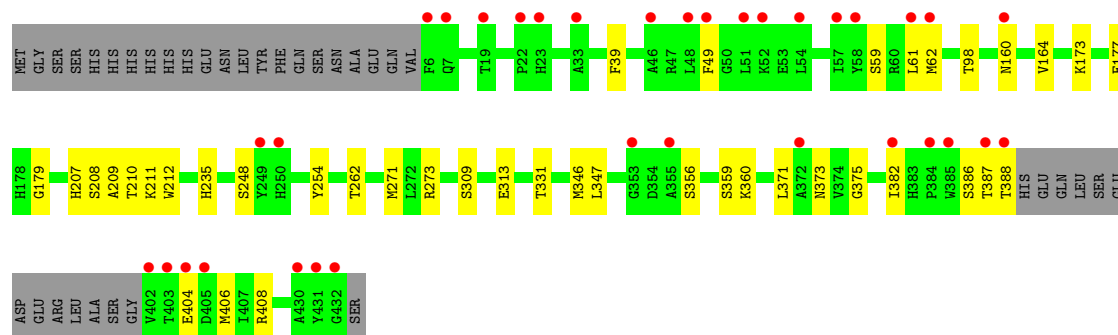
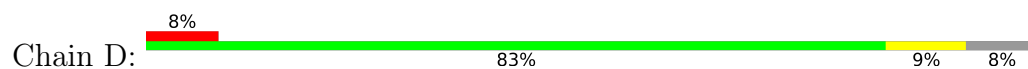


• Molecule 1: Sulfhydrylase FUB7

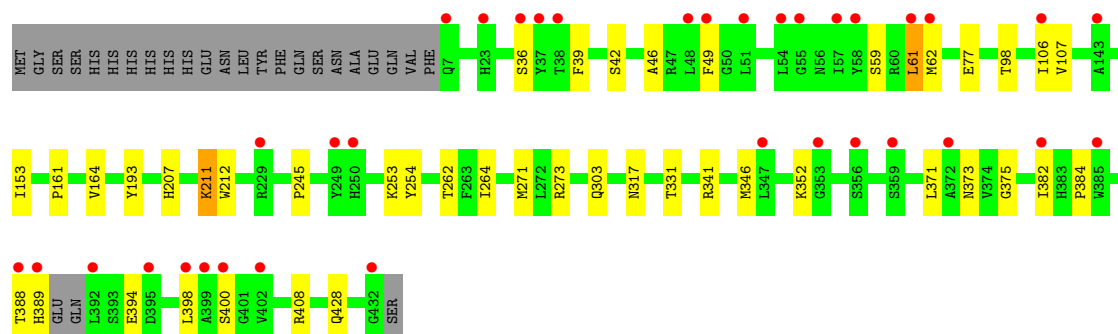
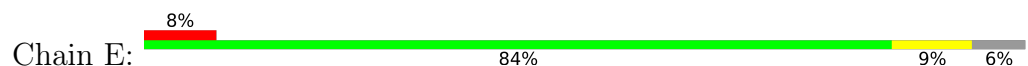




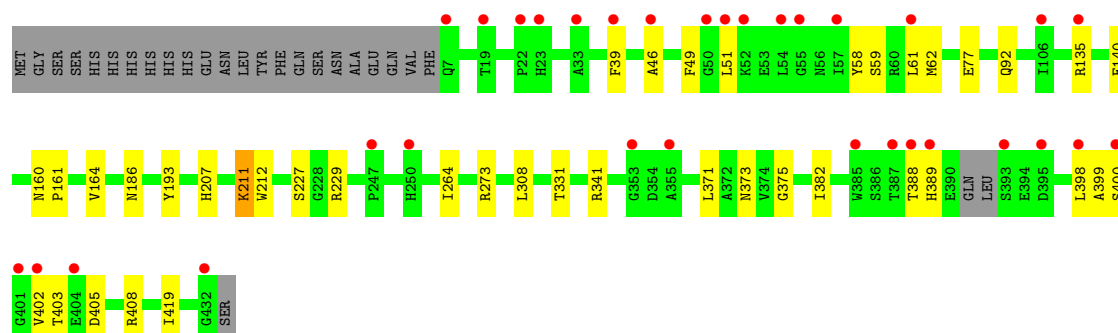
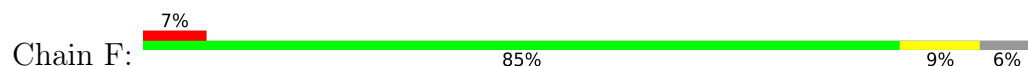
● Molecule 1: Sulfhydrylase FUB7



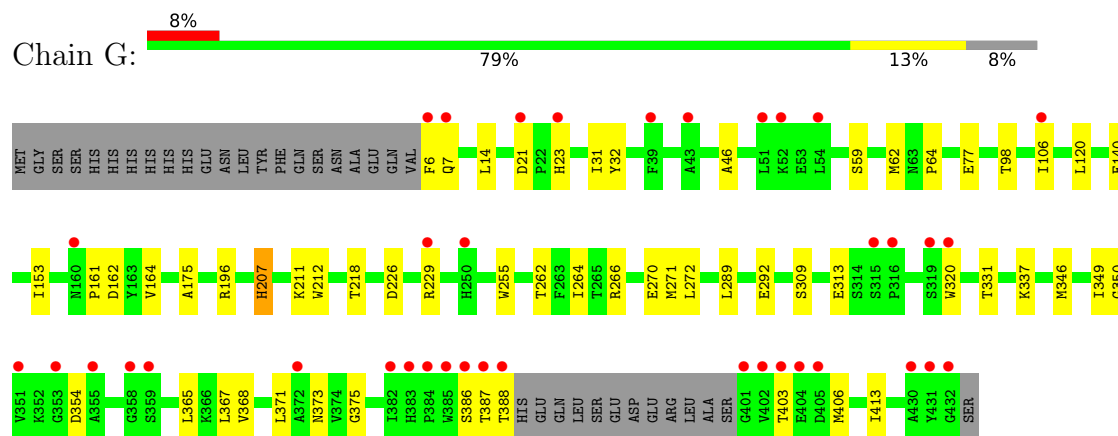
● Molecule 1: Sulfhydrylase FUB7



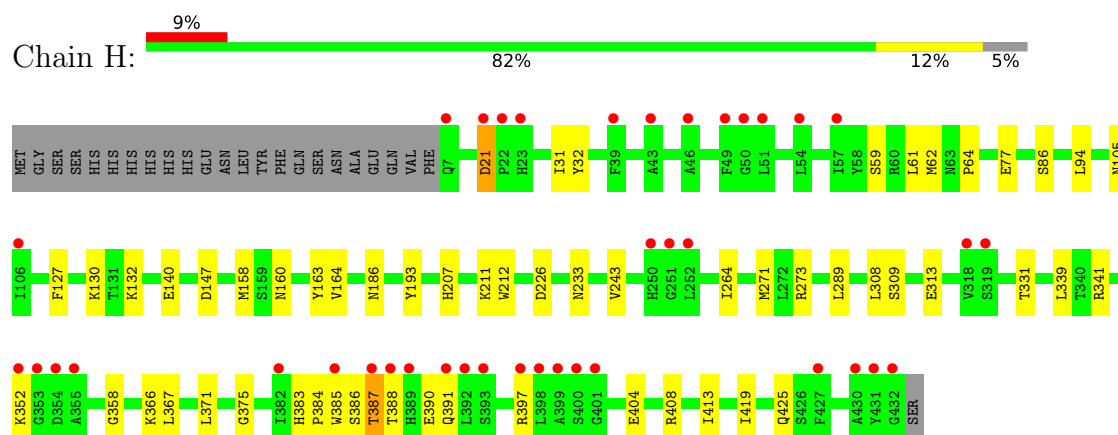
● Molecule 1: Sulfhydrylase FUB7



• Molecule 1: Sulfhydrylase FUB7



• Molecule 1: Sulfhydrylase FUB7



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.93Å 195.29Å 112.42Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	47.97 – 1.76 47.97 – 1.76	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.97-1.76) 98.9 (47.97-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.198 , 0.229 0.200 , 0.231	Depositor DCC
R_{free} test set	20084 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27419	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 25.76 % 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 2.9858e-03. 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: LLP

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	0.42	0/3313	0.59	0/4498
1	B	0.46	0/3192	0.66	1/4332 (0.0%)
1	C	0.48	0/3273	0.66	0/4445
1	D	0.53	2/3251 (0.1%)	0.69	1/4415 (0.0%)
1	E	0.43	0/3324	0.60	0/4513
1	F	0.44	0/3325	0.62	0/4514
1	G	0.43	1/3266 (0.0%)	0.59	0/4435
1	H	0.41	0/3343	0.62	0/4540
All	All	0.45	3/26287 (0.0%)	0.63	2/35692 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	ALA	C-O	-5.74	1.16	1.24
1	G	207	HIS	C-O	-5.33	1.17	1.23
1	D	207	HIS	C-O	-5.05	1.17	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	372	ALA	N-CA-C	10.48	122.28	111.07
1	D	208	SER	N-CA-C	-5.45	99.63	108.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	211	LLP	Mainchain

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	3259	0	3173	31	0
1	B	3143	0	3073	28	0
1	C	3220	0	3141	27	0
1	D	3198	0	3119	21	0
1	E	3271	0	3186	27	0
1	F	3272	0	3181	24	0
1	G	3210	0	3136	41	0
1	H	3289	0	3201	40	0
2	A	187	0	0	0	0
2	B	161	0	0	1	0
2	C	216	0	0	1	0
2	D	215	0	0	0	0
2	E	200	0	0	1	0
2	F	220	0	0	0	0
2	G	168	0	0	2	0
2	H	190	0	0	1	0
All	All	27419	0	25210	216	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 4.

All (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:THR:HG23	1:E:389:HIS:HD2	1.28	0.98
1:E:388:THR:HG23	1:E:389:HIS:CD2	2.13	0.83
1:D:61:LEU:HD11	1:D:273:ARG:HB2	1.67	0.75
1:G:309:SER:O	1:G:313:GLU:HG2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:SER:HB3	1:C:273:ARG:HH12	1.58	0.67
1:C:384:PRO:HB2	1:C:402:VAL:HG11	1.78	0.65
1:G:266:ARG:NH1	1:G:270:GLU:OE1	2.29	0.65
1:E:59:SER:HA	1:E:62:MET:O	1.97	0.65
1:B:158:MET:HE2	1:B:195:ILE:HD11	1.77	0.65
1:A:389:HIS:HB3	1:A:397:ARG:HG2	1.79	0.63
1:C:385:TRP:CE2	1:C:404:GLU:HB2	2.33	0.63
1:A:245:PRO:HG3	1:A:253:LYS:HE2	1.80	0.62
1:D:59:SER:HA	1:D:62:MET:O	2.00	0.62
1:H:384:PRO:HA	1:H:387:THR:HG23	1.81	0.62
1:F:39:PHE:HZ	1:F:49:PHE:HE2	1.47	0.61
1:G:164:VAL:HG13	1:G:331:THR:HG21	1.85	0.59
1:D:387:THR:O	1:D:388:THR:HB	2.03	0.58
1:F:59:SER:HA	1:F:62:MET:O	2.04	0.58
1:A:14:LEU:HD11	1:H:413:ILE:HG13	1.86	0.56
1:G:59:SER:HA	1:G:62:MET:O	2.05	0.56
1:G:212:TRP:CE2	1:G:375:GLY:HA2	2.41	0.56
1:H:308:LEU:HD11	1:H:419:ILE:HG21	1.86	0.55
1:B:367:LEU:HD13	1:G:6:PHE:CZ	2.41	0.55
1:B:382:ILE:HD11	1:B:408:ARG:NE	2.21	0.55
1:F:77:GLU:OE2	1:F:207:HIS:NE2	2.35	0.55
1:H:59:SER:HA	1:H:62:MET:O	2.07	0.54
1:H:140:GLU:CD	1:H:140:GLU:H	2.16	0.54
1:C:231:ASN:CG	1:C:234:LYS:HG2	2.33	0.54
1:H:212:TRP:CE2	1:H:375:GLY:HA2	2.43	0.54
1:D:173:LYS:NZ	1:D:177:GLU:OE1	2.37	0.54
1:D:386:SER:O	1:F:46:ALA:HB2	2.08	0.54
1:A:212:TRP:CE2	1:A:375:GLY:HA2	2.43	0.53
1:H:309:SER:O	1:H:313:GLU:HG2	2.08	0.53
1:H:387:THR:OG1	1:H:388:THR:N	2.41	0.53
1:B:139:LEU:HB3	1:B:174:ILE:HD11	1.91	0.53
1:A:158:MET:CE	1:A:339:LEU:HD21	2.38	0.53
1:F:389:HIS:CG	1:F:402:VAL:HG21	2.43	0.53
1:E:245:PRO:HD3	1:E:253:LYS:HE3	1.91	0.53
1:H:77:GLU:OE2	1:H:207:HIS:NE2	2.40	0.53
1:E:77:GLU:OE2	1:E:207:HIS:NE2	2.38	0.53
1:F:227:SER:HB2	1:F:229:ARG:HD2	1.91	0.52
1:C:106:ILE:HD11	1:C:120:LEU:HD22	1.90	0.52
1:C:212:TRP:CE2	1:C:375:GLY:HA2	2.45	0.52
1:C:306:GLU:OE2	1:C:310:LYS:HE3	2.09	0.52
1:G:153:ILE:HD12	1:G:175:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:337:LYS:HE2	2:G:501:HOH:O	2.10	0.51
1:A:6:PHE:CZ	1:H:367:LEU:HD13	2.45	0.51
1:D:212:TRP:CE2	1:D:375:GLY:HA2	2.45	0.51
1:E:254:TYR:HB3	1:E:262:THR:HG23	1.93	0.51
1:G:161:PRO:HG2	1:G:406:MET:HE1	1.93	0.50
1:H:186:ASN:HB3	1:H:207:HIS:CE1	2.46	0.50
1:B:339:LEU:HD23	1:B:343:PHE:HA	1.93	0.50
1:H:390:GLU:O	1:H:397:ARG:NH1	2.45	0.50
1:H:132:LYS:NZ	1:H:147:ASP:OD2	2.32	0.50
1:C:386:SER:O	1:E:46:ALA:HB2	2.12	0.50
1:E:382:ILE:O	1:E:384:PRO:HD3	2.12	0.50
1:A:218:THR:HG21	1:H:289:LEU:HD21	1.94	0.50
1:G:365:LEU:HD13	1:G:368:VAL:HB	1.94	0.50
1:F:61:LEU:HD21	1:F:273:ARG:HB2	1.94	0.50
1:E:382:ILE:HD11	1:E:408:ARG:CZ	2.42	0.49
1:H:383:HIS:O	1:H:387:THR:HG22	2.11	0.49
1:G:371:LEU:HD12	1:G:373:ASN:H	1.77	0.49
1:D:98:THR:OG1	1:D:271:MET:HG3	2.11	0.49
1:F:140:GLU:H	1:F:140:GLU:CD	2.20	0.49
1:E:212:TRP:CE2	1:E:375:GLY:HA2	2.48	0.49
1:D:164:VAL:HG13	1:D:331:THR:HG21	1.95	0.49
1:H:130:LYS:HE2	2:H:680:HOH:O	2.12	0.49
1:A:164:VAL:HG13	1:A:331:THR:HG21	1.95	0.49
1:A:350:GLY:HA2	1:A:405:ASP:O	2.12	0.49
1:C:308:LEU:HG	1:C:312:PHE:CE2	2.48	0.49
1:F:186:ASN:HB3	1:F:207:HIS:CE1	2.48	0.49
1:B:382:ILE:HD11	1:B:408:ARG:CZ	2.43	0.48
1:C:371:LEU:HD12	1:C:373:ASN:H	1.79	0.48
1:G:349:ILE:O	1:G:406:MET:HA	2.13	0.48
1:H:226:ASP:HB2	1:H:264:ILE:HB	1.95	0.48
1:A:386:SER:O	1:G:46:ALA:HB2	2.13	0.48
1:A:98:THR:OG1	1:A:271:MET:HG3	2.13	0.48
1:F:161:PRO:HD2	1:F:400:SER:HB3	1.96	0.48
1:F:382:ILE:HD13	1:F:388:THR:HG23	1.96	0.48
1:B:193:TYR:CE2	1:B:341:ARG:HG2	2.48	0.48
1:B:413:ILE:HG13	1:G:14:LEU:HD11	1.96	0.48
1:A:77:GLU:OE2	1:A:207:HIS:NE2	2.43	0.48
1:D:387:THR:OG1	1:D:388:THR:N	2.41	0.48
1:A:42:SER:O	1:G:387:THR:HG22	2.13	0.48
1:B:218:THR:HG21	1:G:289:LEU:HD21	1.95	0.48
1:E:193:TYR:CE2	1:E:341:ARG:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ALA:HB2	1:H:386:SER:O	2.14	0.48
1:G:98:THR:OG1	1:G:271:MET:HG3	2.14	0.48
1:D:254:TYR:HB3	1:D:262:THR:HG23	1.95	0.47
1:G:162:ASP:OD1	1:G:162:ASP:N	2.47	0.47
1:A:310:LYS:HA	1:A:313:GLU:HG2	1.96	0.47
1:G:140:GLU:CD	1:G:140:GLU:H	2.21	0.47
1:C:254:TYR:HB3	1:C:262:THR:HG23	1.96	0.47
1:H:352:LYS:HD2	1:H:352:LYS:HA	1.59	0.47
1:E:39:PHE:HZ	1:E:49:PHE:HE2	1.62	0.47
1:A:46:ALA:HB2	1:G:386:SER:O	2.14	0.47
1:B:212:TRP:CE2	1:B:375:GLY:HA2	2.49	0.47
1:F:212:TRP:CE2	1:F:375:GLY:HA2	2.50	0.47
1:H:366:LYS:HE2	1:H:425:GLN:CD	2.40	0.47
1:C:92:GLN:OE1	1:C:211:LLP:H6	2.15	0.47
1:D:248:SER:HB3	1:D:273:ARG:HH22	1.79	0.47
1:C:57:ILE:HG22	1:C:62:MET:SD	2.55	0.46
1:B:308:LEU:HG	1:B:312:PHE:CE2	2.50	0.46
1:C:59:SER:HA	1:C:62:MET:O	2.15	0.46
1:A:158:MET:HE2	1:A:339:LEU:HD21	1.97	0.46
1:A:403:THR:OG1	1:A:405:ASP:OD1	2.29	0.46
1:F:308:LEU:HD11	1:F:419:ILE:HG21	1.97	0.46
1:E:371:LEU:HD12	1:E:373:ASN:H	1.81	0.46
1:H:193:TYR:CE2	1:H:341:ARG:HG2	2.51	0.46
1:B:59:SER:HA	1:B:62:MET:O	2.14	0.46
1:C:49:PHE:CE1	1:C:57:ILE:HD11	2.50	0.46
1:C:387:THR:OG1	1:C:388:THR:N	2.49	0.46
1:H:158:MET:CE	1:H:339:LEU:HD21	2.46	0.46
1:B:164:VAL:HG13	1:B:331:THR:HG21	1.97	0.46
1:B:140:GLU:CD	1:B:140:GLU:H	2.24	0.46
1:F:371:LEU:HD12	1:F:373:ASN:H	1.81	0.46
1:H:32:TYR:CD2	1:H:64:PRO:HB2	2.51	0.46
1:H:383:HIS:CE1	1:H:385:TRP:HB3	2.51	0.46
1:G:226:ASP:HB2	1:G:264:ILE:HB	1.98	0.45
1:A:92:GLN:OE1	1:A:211:LLP:H6	2.16	0.45
1:B:14:LEU:HD11	1:G:413:ILE:HG13	1.97	0.45
1:B:289:LEU:HD21	1:G:218:THR:HG21	1.97	0.45
1:G:196[B]:ARG:NH2	2:G:506:HOH:O	2.49	0.45
1:B:120:LEU:HD23	1:B:124:LEU:HD12	1.98	0.45
1:B:356:SER:HB3	1:B:360:LYS:HE3	1.99	0.45
1:C:265:THR:O	1:C:269:VAL:HG22	2.17	0.45
1:H:21:ASP:OD1	1:H:21:ASP:N	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:366:LYS:HE3	1:H:366:LYS:HB2	1.78	0.45
1:E:317:ASN:HA	1:E:352:LYS:HD3	1.99	0.45
1:H:358:GLY:HA3	1:H:383:HIS:CD2	2.52	0.44
1:E:61:LEU:HD11	1:E:273:ARG:CA	2.47	0.44
1:E:98:THR:OG1	1:E:271:MET:HG3	2.18	0.44
1:F:193:TYR:CE2	1:F:341:ARG:HG2	2.52	0.44
1:B:127:PHE:HB3	1:H:127:PHE:HB3	1.98	0.44
1:F:164:VAL:HG13	1:F:331:THR:HG21	1.98	0.44
1:B:48:LEU:HB3	1:B:57:ILE:HG12	2.00	0.44
1:G:106:ILE:HD11	1:G:120:LEU:HD22	1.99	0.44
1:A:49:PHE:CE1	1:G:388:THR:HG22	2.52	0.44
1:A:389:HIS:CD2	1:A:402:VAL:HG21	2.52	0.44
1:B:158:MET:HE2	1:B:158:MET:HB2	1.84	0.44
1:D:39:PHE:HZ	1:D:49:PHE:HE2	1.65	0.44
1:F:398:LEU:HD23	1:F:398:LEU:HA	1.88	0.44
1:G:272:LEU:HD23	1:G:272:LEU:HA	1.89	0.44
1:H:61:LEU:HD11	1:H:273:ARG:HB2	1.99	0.44
1:B:130:LYS:HB2	1:B:130:LYS:HE2	1.63	0.43
1:C:160:ASN:OD1	1:C:408:ARG:HD2	2.18	0.43
1:C:98:THR:OG1	1:C:271:MET:HG3	2.18	0.43
1:D:356:SER:O	1:D:360:LYS:HG3	2.17	0.43
1:B:323:TRP:CD1	1:B:324:PRO:HD2	2.53	0.43
1:G:23:HIS:ND1	1:H:21:ASP:HB3	2.34	0.43
1:H:160:ASN:OD1	1:H:408:ARG:HD2	2.19	0.43
1:E:61:LEU:HD11	1:E:273:ARG:HB2	1.99	0.43
1:D:371:LEU:HD12	1:D:373:ASN:H	1.84	0.43
1:G:212:TRP:NE1	1:G:375:GLY:HA2	2.33	0.43
1:H:158:MET:HE1	1:H:339:LEU:HD21	2.00	0.43
1:F:135:ARG:HH21	1:F:399:ALA:HB2	1.84	0.43
1:E:398:LEU:HD13	1:E:398:LEU:HA	1.91	0.42
1:G:354:ASP:OD1	1:G:354:ASP:N	2.46	0.42
1:C:186:ASN:HB3	1:C:207:HIS:CE1	2.54	0.42
1:D:179:GLY:HA2	1:D:235:HIS:CD2	2.54	0.42
1:A:59:SER:HA	1:A:62:MET:O	2.19	0.42
1:D:309:SER:O	1:D:313:GLU:HG2	2.19	0.42
1:D:346:MET:HE3	1:D:346:MET:HB3	1.92	0.42
1:G:14:LEU:HD23	1:G:292:GLU:HG2	2.00	0.42
1:H:158:MET:HG2	1:H:163:TYR:HA	2.01	0.42
1:A:346:MET:HE3	1:A:346:MET:HB3	1.84	0.42
1:E:264:ILE:HD12	1:E:264:ILE:HA	1.95	0.42
1:G:6:PHE:N	1:G:6:PHE:CD1	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:ASP:OD1	1:G:21:ASP:N	2.52	0.42
1:B:6:PHE:CE1	1:G:367:LEU:HD13	2.54	0.42
1:F:403:THR:OG1	1:F:405:ASP:OD1	2.36	0.42
1:G:32:TYR:CD2	1:G:64:PRO:HB2	2.54	0.42
1:G:320:TRP:CE2	1:G:350:GLY:HA3	2.55	0.42
1:H:385:TRP:CG	1:H:404:GLU:HA	2.54	0.42
1:D:212:TRP:NE1	1:D:375:GLY:HA2	2.35	0.42
1:E:164:VAL:HG13	1:E:331:THR:HG21	2.01	0.42
1:F:264:ILE:HD12	1:F:264:ILE:HA	1.98	0.42
1:A:46:ALA:HB2	1:G:387:THR:HA	2.02	0.41
1:B:365:LEU:HD13	1:B:368:VAL:HB	2.02	0.41
1:A:170:GLY:O	1:A:174:ILE:HG12	2.20	0.41
1:G:77:GLU:OE2	1:G:207:HIS:NE2	2.51	0.41
1:F:92:GLN:OE1	1:F:211:LLP:H6	2.21	0.41
1:C:32:TYR:CD2	1:C:64:PRO:HB2	2.56	0.41
1:C:160:ASN:ND2	2:C:502:HOH:O	2.42	0.41
1:F:39:PHE:CZ	1:F:49:PHE:HE2	2.33	0.41
1:C:373:ASN:HB2	1:E:36:SER:OG	2.20	0.41
1:E:107:VAL:O	1:E:153:ILE:HA	2.20	0.41
1:G:31:ILE:HB	1:H:31:ILE:HB	2.03	0.41
1:H:130:LYS:HE2	1:H:130:LYS:HB2	1.96	0.41
1:A:425:GLN:OE1	1:A:429:LYS:HE2	2.20	0.41
1:B:211:LLP:H	1:B:211:LLP:HG3	1.69	0.41
1:C:387:THR:HG22	1:E:42:SER:O	2.21	0.41
1:D:210:THR:HG21	1:F:58:TYR:OH	2.21	0.41
1:E:212:TRP:NE1	1:E:375:GLY:HA2	2.36	0.41
1:G:346:MET:HE3	1:G:346:MET:HB3	1.91	0.41
1:H:94:LEU:HG	1:H:271:MET:HB3	2.03	0.41
1:A:237:ASP:N	1:A:237:ASP:OD1	2.53	0.41
1:E:62:MET:HB2	2:E:671:HOH:O	2.20	0.41
1:F:160:ASN:OD1	1:F:408:ARG:HD2	2.21	0.41
1:G:255:TRP:HA	1:G:262:THR:OG1	2.21	0.41
1:H:164:VAL:HG13	1:H:331:THR:HG21	2.02	0.41
1:H:233:ASN:HA	1:H:243:VAL:HG11	2.03	0.41
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.85	0.40
1:H:105:ASN:HA	1:H:130:LYS:O	2.21	0.40
1:A:349:ILE:O	1:A:406:MET:HA	2.20	0.40
1:A:193:TYR:CZ	1:A:341:ARG:HD2	2.56	0.40
1:A:308:LEU:HG	1:A:312:PHE:CE2	2.56	0.40
1:D:347:LEU:HD12	1:D:347:LEU:C	2.47	0.40
1:A:211:LLP:HD3	1:A:374:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:MET:HA	2:B:594:HOH:O	2.21	0.40
1:C:347:LEU:C	1:C:347:LEU:HD12	2.46	0.40
1:D:382:ILE:HG22	1:D:408:ARG:HB3	2.03	0.40
1:E:346:MET:HE3	1:E:346:MET:HB3	1.79	0.40
1:C:311:TYR:OH	1:C:424:GLU:OE2	2.32	0.40
1:C:346:MET:HE3	1:C:346:MET:HB3	1.98	0.40
1:E:161:PRO:HD2	1:E:400:SER:HB3	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	417/450 (93%)	406 (97%)	11 (3%)	0	100	100
1	B	402/450 (89%)	393 (98%)	9 (2%)	0	100	100
1	C	413/450 (92%)	405 (98%)	8 (2%)	0	100	100
1	D	409/450 (91%)	400 (98%)	9 (2%)	0	100	100
1	E	419/450 (93%)	405 (97%)	14 (3%)	0	100	100
1	F	419/450 (93%)	408 (97%)	11 (3%)	0	100	100
1	G	411/450 (91%)	405 (98%)	6 (2%)	0	100	100
1	H	423/450 (94%)	414 (98%)	9 (2%)	0	100	100
All	All	3313/3600 (92%)	3236 (98%)	77 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/365 (93%)	337 (99%)	2 (1%)	78	71
1	B	327/365 (90%)	320 (98%)	7 (2%)	47	27
1	C	335/365 (92%)	331 (99%)	4 (1%)	63	49
1	D	333/365 (91%)	329 (99%)	4 (1%)	63	49
1	E	341/365 (93%)	336 (98%)	5 (2%)	57	41
1	F	341/365 (93%)	340 (100%)	1 (0%)	86	83
1	G	334/365 (92%)	331 (99%)	3 (1%)	70	60
1	H	343/365 (94%)	338 (98%)	5 (2%)	57	41
All	All	2693/2920 (92%)	2662 (99%)	31 (1%)	63	49

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	LEU
1	A	395	ASP
1	B	7	GLN
1	B	158	MET
1	B	160	ASN
1	B	371	LEU
1	B	382	ILE
1	B	404	GLU
1	B	406	MET
1	C	140	GLU
1	C	149	GLN
1	C	359	SER
1	C	404	GLU
1	D	160	ASN
1	D	359	SER
1	D	404	GLU
1	D	406	MET
1	E	61	LEU
1	E	106	ILE
1	E	303	GLN
1	E	394	GLU
1	E	428	GLN
1	F	51	LEU

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Mol	Chain	Res	Type
1	G	7	GLN
1	G	229	ARG
1	G	403	THR
1	H	21	ASP
1	H	86	SER
1	H	371	LEU
1	H	387	THR
1	H	391	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	373	ASN
1	B	121	ASN
1	B	235	HIS
1	B	250	HIS
1	B	303	GLN
1	B	334	GLN
1	C	105	ASN
1	C	303	GLN
1	D	105	ASN
1	E	235	HIS
1	E	389	HIS
1	F	235	HIS
1	G	303	GLN
1	H	235	HIS
1	H	303	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	G	211	1	23,24,25	2.07	5 (21%)	25,32,34	1.41	4 (16%)
1	LLP	A	211	1	23,24,25	1.98	5 (21%)	25,32,34	1.40	5 (20%)
1	LLP	F	211	1	23,24,25	1.80	5 (21%)	25,32,34	1.45	4 (16%)
1	LLP	D	211	1	23,24,25	1.83	6 (26%)	25,32,34	1.40	4 (16%)
1	LLP	C	211	1	23,24,25	2.14	7 (30%)	25,32,34	1.47	5 (20%)
1	LLP	E	211	1	23,24,25	1.60	4 (17%)	25,32,34	1.58	5 (20%)
1	LLP	H	211	1	23,24,25	1.81	5 (21%)	25,32,34	1.57	6 (24%)
1	LLP	B	211	1	23,24,25	2.04	6 (26%)	25,32,34	1.42	5 (20%)

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
1	LLP	G	211	1	-	4/16/17/19	0/1/1/1
1	LLP	A	211	1	-	4/16/17/19	0/1/1/1
1	LLP	F	211	1	-	4/16/17/19	0/1/1/1
1	LLP	D	211	1	-	4/16/17/19	0/1/1/1
1	LLP	C	211	1	-	4/16/17/19	0/1/1/1
1	LLP	E	211	1	-	4/16/17/19	0/1/1/1
1	LLP	H	211	1	-	4/16/17/19	0/1/1/1
1	LLP	B	211	1	-	5/16/17/19	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	211	LLP	P-OP4	6.17	1.79	1.60
1	A	211	LLP	P-OP4	6.00	1.79	1.60
1	B	211	LLP	P-OP4	5.63	1.78	1.60
1	H	211	LLP	P-OP4	5.01	1.76	1.60
1	D	211	LLP	P-OP4	4.89	1.75	1.60
1	C	211	LLP	CB-CA	4.57	1.60	1.53
1	C	211	LLP	P-OP4	4.55	1.74	1.60
1	C	211	LLP	C6-C5	4.41	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	211	LLP	P-OP4	4.19	1.73	1.60
1	E	211	LLP	P-OP4	3.83	1.72	1.60
1	B	211	LLP	C6-C5	3.82	1.45	1.37
1	F	211	LLP	CB-CA	3.69	1.59	1.53
1	G	211	LLP	OP4-C5'	-3.48	1.32	1.44
1	H	211	LLP	OP4-C5'	-3.40	1.32	1.44
1	G	211	LLP	CD-CE	3.37	1.63	1.51
1	E	211	LLP	CD-CE	3.33	1.62	1.51
1	F	211	LLP	C3-C2	3.32	1.44	1.41
1	A	211	LLP	OP4-C5'	-3.17	1.33	1.44
1	D	211	LLP	CD-CE	3.06	1.62	1.51
1	D	211	LLP	CB-CA	3.05	1.58	1.53
1	F	211	LLP	OP4-C5'	-3.00	1.33	1.44
1	B	211	LLP	OP4-C5'	-2.98	1.33	1.44
1	E	211	LLP	OP4-C5'	-2.98	1.33	1.44
1	C	211	LLP	CD-CE	2.94	1.61	1.51
1	C	211	LLP	OP4-C5'	-2.93	1.34	1.44
1	G	211	LLP	C6-C5	2.90	1.43	1.37
1	A	211	LLP	CB-CA	2.88	1.57	1.53
1	H	211	LLP	C2-N1	2.83	1.38	1.33
1	B	211	LLP	C4-C5	-2.77	1.38	1.42
1	A	211	LLP	CD-CE	2.72	1.60	1.51
1	B	211	LLP	CB-CA	2.70	1.57	1.53
1	D	211	LLP	OP4-C5'	-2.60	1.35	1.44
1	A	211	LLP	C6-C5	2.60	1.42	1.37
1	D	211	LLP	CG-CB	2.54	1.62	1.52
1	B	211	LLP	C2-N1	2.52	1.38	1.33
1	D	211	LLP	C6-C5	2.46	1.42	1.37
1	G	211	LLP	CB-CA	2.42	1.57	1.53
1	C	211	LLP	C4-C5	-2.36	1.38	1.42
1	H	211	LLP	CD-CE	2.29	1.59	1.51
1	F	211	LLP	C6-C5	2.22	1.42	1.37
1	C	211	LLP	CG-CB	2.19	1.61	1.52
1	E	211	LLP	C6-C5	2.12	1.41	1.37
1	H	211	LLP	C6-C5	2.12	1.41	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	211	LLP	OP4-P-OP1	-4.58	94.07	106.44
1	C	211	LLP	OP3-P-OP2	3.48	120.83	107.80
1	D	211	LLP	OP4-P-OP1	-3.43	97.16	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	211	LLP	OP4-P-OP1	-3.41	97.21	106.44
1	H	211	LLP	OP3-P-OP2	3.21	119.84	107.80
1	B	211	LLP	OP3-P-OP2	3.14	119.59	107.80
1	E	211	LLP	C5'-C5-C6	-3.12	114.28	119.36
1	A	211	LLP	OP3-P-OP2	3.06	119.26	107.80
1	G	211	LLP	C5'-C5-C6	-3.00	114.46	119.36
1	H	211	LLP	OP4-P-OP1	-3.00	98.32	106.44
1	G	211	LLP	OP3-P-OP2	2.99	119.03	107.80
1	H	211	LLP	C5'-C5-C6	-2.99	114.49	119.36
1	C	211	LLP	OP3-P-OP4	-2.98	98.91	106.67
1	F	211	LLP	C5'-C5-C6	-2.97	114.53	119.36
1	D	211	LLP	OP3-P-OP2	2.95	118.88	107.80
1	A	211	LLP	OP4-P-OP1	-2.94	98.49	106.44
1	D	211	LLP	C5'-C5-C6	-2.75	114.88	119.36
1	H	211	LLP	OP2-P-OP4	-2.67	99.71	106.67
1	C	211	LLP	OP2-P-OP4	-2.64	99.80	106.67
1	H	211	LLP	OP3-P-OP4	-2.63	99.80	106.67
1	B	211	LLP	C5'-C5-C6	-2.60	115.12	119.36
1	A	211	LLP	OP3-P-OP4	-2.59	99.91	106.67
1	E	211	LLP	OP3-P-OP2	2.55	117.36	107.80
1	B	211	LLP	OP4-P-OP1	-2.36	100.07	106.44
1	A	211	LLP	C4-C4'-NZ	-2.35	113.22	124.04
1	B	211	LLP	OP3-P-OP4	-2.33	100.59	106.67
1	G	211	LLP	OP4-P-OP1	-2.32	100.17	106.44
1	B	211	LLP	C4-C4'-NZ	-2.32	113.34	124.04
1	F	211	LLP	C4-C4'-NZ	-2.31	113.39	124.04
1	C	211	LLP	OP4-P-OP1	-2.31	100.21	106.44
1	E	211	LLP	C4-C4'-NZ	-2.31	113.40	124.04
1	C	211	LLP	C4-C4'-NZ	-2.29	113.47	124.04
1	D	211	LLP	C4-C4'-NZ	-2.29	113.49	124.04
1	G	211	LLP	C4-C4'-NZ	-2.26	113.63	124.04
1	A	211	LLP	C5'-C5-C6	-2.24	115.71	119.36
1	H	211	LLP	C4-C4'-NZ	-2.24	113.71	124.04
1	F	211	LLP	OP3-P-OP2	2.08	115.60	107.80
1	E	211	LLP	OP3-P-OP4	-2.03	101.37	106.67

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	211	LLP	O-C-CA-CB
1	B	211	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	C	211	LLP	O-C-CA-CB
1	D	211	LLP	O-C-CA-CB
1	E	211	LLP	O-C-CA-CB
1	F	211	LLP	O-C-CA-CB
1	G	211	LLP	O-C-CA-CB
1	H	211	LLP	O-C-CA-CB
1	A	211	LLP	CG-CD-CE-NZ
1	E	211	LLP	CG-CD-CE-NZ
1	F	211	LLP	CG-CD-CE-NZ
1	H	211	LLP	CG-CD-CE-NZ
1	C	211	LLP	CG-CD-CE-NZ
1	D	211	LLP	CG-CD-CE-NZ
1	G	211	LLP	CG-CD-CE-NZ
1	B	211	LLP	CG-CD-CE-NZ
1	B	211	LLP	CD-CE-NZ-C4'
1	D	211	LLP	CD-CE-NZ-C4'
1	C	211	LLP	CD-CE-NZ-C4'
1	G	211	LLP	CD-CE-NZ-C4'
1	A	211	LLP	C3-C4-C4'-NZ
1	B	211	LLP	C3-C4-C4'-NZ
1	C	211	LLP	C3-C4-C4'-NZ
1	D	211	LLP	C3-C4-C4'-NZ
1	A	211	LLP	CD-CE-NZ-C4'
1	F	211	LLP	CD-CE-NZ-C4'
1	H	211	LLP	CD-CE-NZ-C4'
1	F	211	LLP	C3-C4-C4'-NZ
1	G	211	LLP	C3-C4-C4'-NZ
1	H	211	LLP	C3-C4-C4'-NZ
1	E	211	LLP	C3-C4-C4'-NZ
1	E	211	LLP	CD-CE-NZ-C4'
1	B	211	LLP	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	211	LLP	2	0
1	F	211	LLP	1	0
1	C	211	LLP	1	0
1	B	211	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	421/450 (93%)	0.57	39 (9%)	14	17	23, 35, 59, 76	1 (0%)
1	B	406/450 (90%)	0.61	40 (9%)	13	15	23, 35, 59, 74	1 (0%)
1	C	417/450 (92%)	0.40	37 (8%)	15	18	20, 30, 57, 72	1 (0%)
1	D	413/450 (91%)	0.40	34 (8%)	17	21	20, 30, 53, 75	1 (0%)
1	E	423/450 (94%)	0.53	35 (8%)	17	20	20, 33, 56, 77	1 (0%)
1	F	423/450 (94%)	0.39	32 (7%)	20	23	21, 32, 54, 69	2 (0%)
1	G	414/450 (92%)	0.66	38 (9%)	14	17	20, 36, 61, 75	2 (0%)
1	H	425/450 (94%)	0.58	39 (9%)	14	17	23, 35, 60, 77	1 (0%)
All	All	3342/3600 (92%)	0.52	294 (8%)	15	19	20, 33, 58, 77	10 (0%)

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	385	TRP	8.0
1	E	54	LEU	7.6
1	C	398	LEU	6.8
1	B	54	LEU	6.5
1	D	6	PHE	6.1
1	D	54	LEU	6.0
1	H	54	LEU	5.8
1	F	54	LEU	5.7
1	A	54	LEU	5.7
1	C	385	TRP	5.6
1	B	372	ALA	5.5
1	G	54	LEU	5.3
1	D	388	THR	5.3
1	C	54	LEU	5.1
1	G	402	VAL	5.0
1	B	6	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	H	392	LEU	4.7
1	B	402	VAL	4.7
1	D	402	VAL	4.6
1	G	6	PHE	4.6
1	A	385	TRP	4.5
1	D	385	TRP	4.5
1	B	403	THR	4.5
1	G	401	GLY	4.5
1	E	400	SER	4.4
1	A	432	GLY	4.4
1	E	385	TRP	4.3
1	B	382	ILE	4.2
1	F	400	SER	4.1
1	A	355	ALA	4.1
1	A	6	PHE	4.1
1	C	402	VAL	4.1
1	G	250	HIS	4.1
1	G	372	ALA	4.1
1	A	398	LEU	4.1
1	G	51	LEU	4.1
1	H	23	HIS	4.1
1	D	432	GLY	4.0
1	E	432	GLY	4.0
1	D	61	LEU	4.0
1	G	403	THR	4.0
1	C	432	GLY	4.0
1	D	57	ILE	3.9
1	D	51	LEU	3.9
1	F	432	GLY	3.9
1	D	23	HIS	3.9
1	H	385	TRP	3.9
1	G	388	THR	3.8
1	E	51	LEU	3.8
1	B	23	HIS	3.8
1	E	398	LEU	3.8
1	E	23	HIS	3.8
1	A	399	ALA	3.7
1	E	61	LEU	3.7
1	H	398	LEU	3.7
1	F	393	SER	3.7
1	D	382	ILE	3.6
1	E	49	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	400	SER	3.6
1	D	250	HIS	3.6
1	H	352	LYS	3.5
1	G	386	SER	3.5
1	F	23	HIS	3.5
1	H	51	LEU	3.4
1	D	355	ALA	3.4
1	C	57	ILE	3.4
1	C	61	LEU	3.4
1	C	401	GLY	3.4
1	E	57	ILE	3.4
1	G	432	GLY	3.4
1	C	50	GLY	3.3
1	H	251	GLY	3.3
1	D	58	TYR	3.3
1	C	355	ALA	3.3
1	G	387	THR	3.3
1	G	382	ILE	3.3
1	A	23	HIS	3.3
1	E	250	HIS	3.2
1	E	389	HIS	3.2
1	B	51	LEU	3.2
1	F	51	LEU	3.2
1	C	23	HIS	3.2
1	H	399	ALA	3.2
1	F	7	GLN	3.1
1	C	49	PHE	3.1
1	C	388	THR	3.1
1	B	431	TYR	3.1
1	G	383	HIS	3.1
1	H	22	PRO	3.1
1	E	392	LEU	3.1
1	G	384	PRO	3.0
1	B	57	ILE	3.0
1	D	49	PHE	3.0
1	C	249	TYR	3.0
1	C	399	ALA	3.0
1	C	386	SER	3.0
1	C	389	HIS	3.0
1	C	58	TYR	3.0
1	A	400	SER	3.0
1	A	33	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	250	HIS	3.0
1	D	7	GLN	3.0
1	H	21	ASP	2.9
1	B	250	HIS	2.9
1	G	23	HIS	2.9
1	C	387	THR	2.9
1	B	33	ALA	2.9
1	B	355	ALA	2.9
1	F	395	ASP	2.9
1	A	250	HIS	2.9
1	F	387	THR	2.9
1	F	46	ALA	2.9
1	H	355	ALA	2.9
1	C	51	LEU	2.9
1	A	21	ASP	2.9
1	H	387	THR	2.9
1	D	249	TYR	2.9
1	B	405	ASP	2.9
1	H	250	HIS	2.9
1	B	49	PHE	2.8
1	F	388	THR	2.8
1	C	400	SER	2.8
1	E	382	ILE	2.8
1	C	384	PRO	2.8
1	A	387	THR	2.8
1	H	391	GLN	2.8
1	A	38	THR	2.8
1	D	387	THR	2.8
1	H	432	GLY	2.8
1	F	22	PRO	2.7
1	F	250	HIS	2.7
1	B	353	GLY	2.7
1	A	386	SER	2.7
1	C	248	SER	2.7
1	D	384	PRO	2.7
1	F	385	TRP	2.7
1	H	431	TYR	2.7
1	C	382	ILE	2.7
1	B	61	LEU	2.6
1	E	37	TYR	2.6
1	E	58	TYR	2.6
1	G	355	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	353	GLY	2.6
1	A	404	GLU	2.6
1	E	38	THR	2.6
1	E	48	LEU	2.6
1	A	431	TYR	2.6
1	B	37	TYR	2.6
1	F	106	ILE	2.6
1	B	430	ALA	2.6
1	F	135	ARG	2.6
1	C	7	GLN	2.5
1	B	117	TYR	2.5
1	B	249	TYR	2.5
1	E	249	TYR	2.5
1	E	402	VAL	2.5
1	B	407	ILE	2.5
1	A	430	ALA	2.5
1	C	372	ALA	2.5
1	D	372	ALA	2.5
1	D	353	GLY	2.5
1	F	55	GLY	2.5
1	G	320	TRP	2.5
1	G	319	SER	2.5
1	G	229	ARG	2.5
1	B	39	PHE	2.5
1	A	46	ALA	2.5
1	A	318	VAL	2.5
1	E	55	GLY	2.5
1	F	52	LYS	2.5
1	G	315	SER	2.5
1	F	398	LEU	2.4
1	F	404	GLU	2.4
1	A	22	PRO	2.4
1	B	406	MET	2.4
1	G	358	GLY	2.4
1	B	318	VAL	2.4
1	E	356	SER	2.4
1	G	106	ILE	2.4
1	H	106	ILE	2.4
1	G	21	ASP	2.4
1	B	404	GLU	2.4
1	A	61	LEU	2.4
1	F	247	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	355	ALA	2.4
1	H	43	ALA	2.4
1	H	393	SER	2.4
1	D	404	GLU	2.4
1	G	404	GLU	2.4
1	G	353	GLY	2.4
1	B	22	PRO	2.4
1	E	36	SER	2.4
1	A	48	LEU	2.4
1	C	48	LEU	2.4
1	G	430	ALA	2.4
1	A	58	TYR	2.4
1	C	431	TYR	2.4
1	D	431	TYR	2.4
1	G	431	TYR	2.4
1	E	106	ILE	2.4
1	F	57	ILE	2.4
1	D	48	LEU	2.3
1	D	403	THR	2.3
1	D	52	LYS	2.3
1	A	37	TYR	2.3
1	A	57	ILE	2.3
1	A	382	ILE	2.3
1	A	388	THR	2.3
1	D	62	MET	2.3
1	H	430	ALA	2.3
1	A	51	LEU	2.3
1	F	389	HIS	2.3
1	H	39	PHE	2.3
1	H	57	ILE	2.3
1	B	38	THR	2.3
1	D	19	THR	2.3
1	D	430	ALA	2.3
1	C	252	LEU	2.3
1	B	319	SER	2.3
1	G	39	PHE	2.3
1	A	249	TYR	2.3
1	B	58	TYR	2.3
1	C	52	LYS	2.3
1	G	52	LYS	2.3
1	A	401	GLY	2.3
1	B	55	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	21	ASP	2.3
1	E	353	GLY	2.3
1	F	401	GLY	2.3
1	H	382	ILE	2.3
1	H	7	GLN	2.2
1	H	388	THR	2.2
1	A	396	GLU	2.2
1	G	43	ALA	2.2
1	G	160	ASN	2.2
1	B	347	LEU	2.2
1	F	50	GLY	2.2
1	H	50	GLY	2.2
1	E	7	GLN	2.2
1	G	316	PRO	2.2
1	A	319	SER	2.2
1	G	359	SER	2.2
1	E	347	LEU	2.2
1	H	353	GLY	2.2
1	H	401	GLY	2.2
1	A	402	VAL	2.2
1	E	359	SER	2.2
1	D	33	ALA	2.2
1	E	62	MET	2.2
1	E	143	ALA	2.2
1	H	46	ALA	2.2
1	A	320	TRP	2.2
1	B	320	TRP	2.2
1	B	308	LEU	2.2
1	A	49	PHE	2.2
1	F	39	PHE	2.2
1	E	395	ASP	2.1
1	F	402	VAL	2.1
1	C	428	GLN	2.1
1	H	389	HIS	2.1
1	A	313	GLU	2.1
1	H	397	ARG	2.1
1	A	351	VAL	2.1
1	B	361	VAL	2.1
1	B	234	LYS	2.1
1	F	61	LEU	2.1
1	H	319	SER	2.1
1	E	388	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	19	THR	2.1
1	H	49	PHE	2.1
1	C	43	ALA	2.1
1	F	33	ALA	2.1
1	D	160	ASN	2.1
1	H	354	ASP	2.1
1	B	247	PRO	2.1
1	D	22	PRO	2.1
1	A	389	HIS	2.1
1	C	106	ILE	2.1
1	F	353	GLY	2.0
1	C	33	ALA	2.0
1	B	321	VAL	2.0
1	D	405	ASP	2.0
1	G	351	VAL	2.0
1	G	405	ASP	2.0
1	E	229	ARG	2.0
1	H	318	VAL	2.0
1	H	252	LEU	2.0
1	B	160	ASN	2.0
1	G	7	GLN	2.0
1	B	229	ARG	2.0
1	H	427	PHE	2.0
1	D	46	ALA	2.0
1	E	372	ALA	2.0
1	E	399	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	G	211	24/25	0.96	0.08	23,32,34,38	0
1	LLP	B	211	24/25	0.97	0.07	24,29,33,37	0
1	LLP	C	211	24/25	0.97	0.06	19,25,31,33	0
1	LLP	A	211	24/25	0.97	0.06	25,29,34,36	0
1	LLP	H	211	24/25	0.97	0.07	23,31,36,37	0
1	LLP	F	211	24/25	0.98	0.06	23,27,31,34	0
1	LLP	D	211	24/25	0.98	0.06	19,24,30,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	E	211	24/25	0.98	0.06	23,27,31,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.