Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 06:45 AM JST

PDB ID	:	7F0G
Title	:	Crystal Structure of EnPKS1
Authors	:	Huang, S.X.; Yan, Y.J.
Deposited on	:	2021-06-04
Resolution	:	2.67 Å(reported)

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

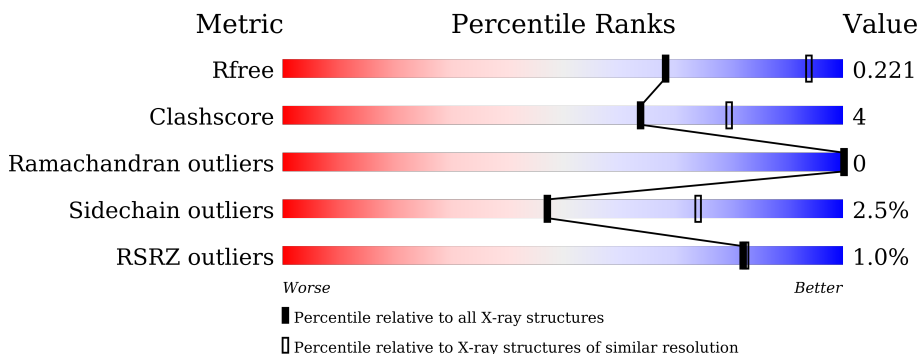|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.67 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.
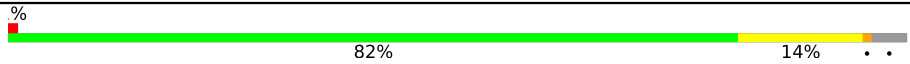
Metric	Percentile Ranks	Value
Rfree		0.221
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		2.5%
RSRZ outliers		1.0%

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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	393	85% 10% •
1	B	393	% 90% 9% •
1	C	393	% 87% 9% •
1	D	393	3% 90% 9% •
1	E	393	% 87% 9% •
1	F	393	85% 10% • •

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	393	82% 14%
1	H	393	87% 9%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 23815 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 EnPKS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2886	1835	499	538	14			
1	B	391	Total	C	N	O	S	0	0	0
			3002	1904	526	556	16			
1	C	380	Total	C	N	O	S	0	0	0
			2925	1858	511	542	14			
1	D	391	Total	C	N	O	S	0	0	0
			3002	1904	526	556	16			
1	E	378	Total	C	N	O	S	0	0	0
			2903	1846	503	540	14			
1	F	378	Total	C	N	O	S	0	0	0
			2903	1846	503	540	14			
1	G	379	Total	C	N	O	S	0	1	0
			2922	1857	510	541	14			
1	H	379	Total	C	N	O	S	0	1	0
			2922	1857	510	541	14			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total 49	O 49	0	0
3	B	44	Total 44	O 44	0	0
3	C	33	Total 33	O 33	0	0
3	D	40	Total 40	O 40	0	0
3	E	46	Total 46	O 46	0	0
3	F	47	Total 47	O 47	0	0
3	G	36	Total 36	O 36	0	0
3	H	50	Total 50	O 50	0	0

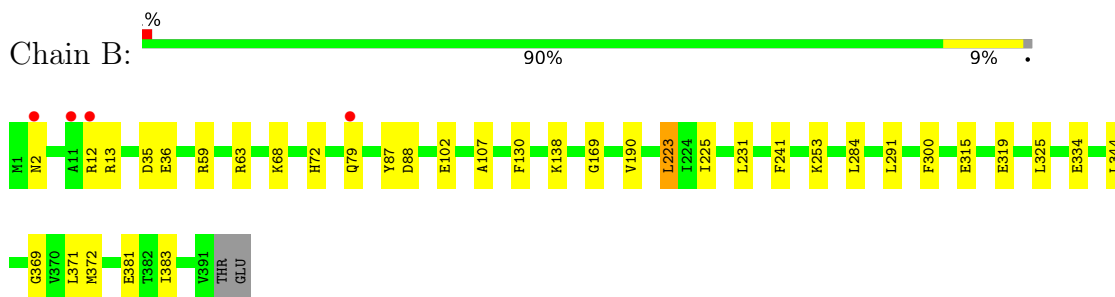# 3 Residue-property plots ⓘ

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.
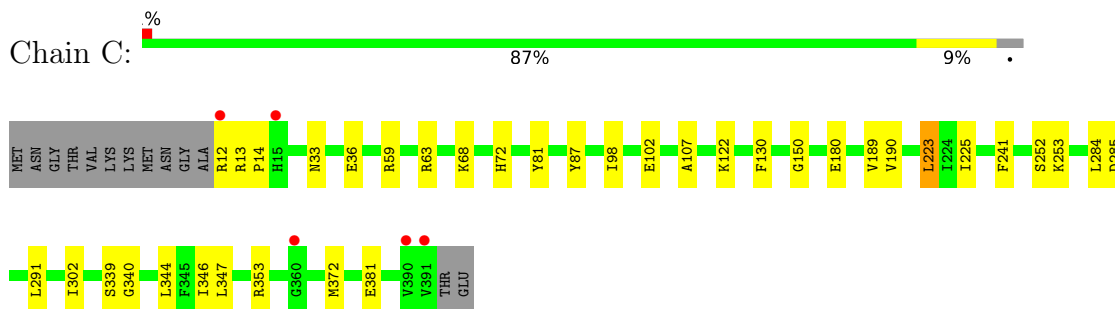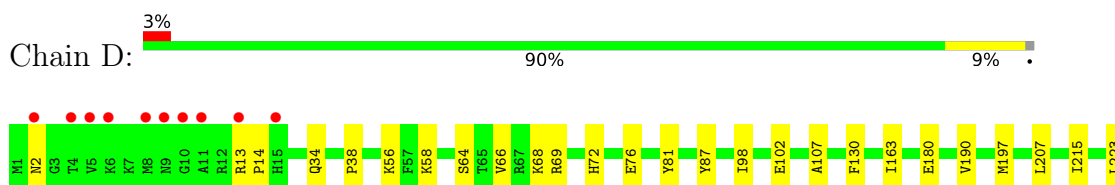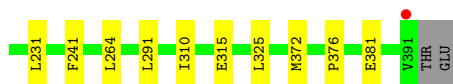
- Molecule 1: EnPKS1

Chain A:

- Molecule 1: EnPKS1

Chain B:

- Molecule 1: EnPKS1

Chain C:

- Molecule 1: EnPKS1

Chain D:

L231 F241 L264 L291 I310 E315 L325 M372 P376 E381 V391 THR GLU

• Molecule 1: EnPKS1

Chain E:

MET ASN GLY THR VAL LYS LYS MET ASN GLY ALA ARG P14 I20 D55 K56 R59 S64 K68 H72 E80 Y81 Y87 I98 A101 E102 A107 S112 E116 N123 F130 K138 P152 V155 V190 E204 I215

L223 I224 I225 L284 D285 S289 P290 E315 L325 E334 L344 M372 P376 E381 V391 THR GLU

• Molecule 1: EnPKS1

Chain F:

MET ASN GLY THR VAL LYS LYS MET ASN GLY ALA ARG P14 R43 H49 L50 T51 D55 K58 S64 K68 H72 Y81 Y87 I98 E102 A107 E116 N123 F130 G169 V183 V190 E204 T205 I215 L223 I224

I225 N250 K270 L291 I302 E315 L325 R329 E334 L344 F345 I346 R352 K356 L366 L371 M372 E381 T382 I383 V391 THR GLU

• Molecule 1: EnPKS1

Chain G:

MET ASN GLY THR VAL LYS LYS MET ASN GLY ALA ARG R13 P14 H15 P38 R43 L53 K58 E62 R63 S64 K68 H72 L73 T74 E75 E76 L77 L78 Y81 Y87 I98 E102 A107 A108 R109 F130 T133 K138 T162 I163 G164 C165

G169 V190 V196 M197 E204 L207 I211 I215 L223 I224 I225 K235 S252 K253 Q282 C283 L284 D285 N294 I302 E315 L325 S333 E334 Y335 G336 L344 F345 I346 K355 K356 W368 M372 P376 E381 T382 I383

R386 S389 V390 V391 THR GLU

• Molecule 1: EnPKS1

Chain H:

MET ASN GLY THR VAL LYS LYS MET ASN GLY ALA ARG R13 P14 H15 R43 T51 D55 K56 R59 R63 K68 H72 L73 Q79 Y87 E102 A107 F130 E137 T162 V190 F199 L207 L223 I224 I225 I237 K253

R258 I280 D285 W301 G307 I310 E315 L325 R329 E334 L344 R351 M372 P376 E381 R386 V391 THR GLU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	52.08Å 117.86Å 136.47Å 111.34° 90.62° 91.59°	Depositor
Resolution (Å)	23.07 – 2.67 66.49 – 2.67	Depositor EDS
% Data completeness (in resolution range)	94.3 (23.07-2.67) 89.8 (66.49-2.67)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.197 , 0.221 0.197 , 0.221	Depositor DCC
R_{free} test set	1969 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23815	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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

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	0.65	0/2941	0.79	0/3984
1	B	0.64	0/3059	0.79	1/4140 (0.0%)
1	C	0.65	0/2982	0.77	0/4039
1	D	0.64	0/3059	0.78	0/4140
1	E	0.64	0/2960	0.78	1/4010 (0.0%)
1	F	0.64	0/2960	0.80	0/4010
1	G	0.65	0/2982	0.77	0/4039
1	H	0.65	0/2982	0.79	1/4039 (0.0%)
All	All	0.65	0/23925	0.78	3/32401 (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	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	2
1	H	0	1
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	329	ARG	CG-CD-NE	-6.42	98.31	111.80
1	B	79	GLN	CB-CA-C	5.58	121.57	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	123	ASN	CB-CA-C	-5.21	99.97	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	87	TYR	Peptide
1	D	87	TYR	Peptide
1	E	87	TYR	Peptide
1	F	87	TYR	Peptide
1	G	163	ILE	Peptide
1	G	87	TYR	Peptide
1	H	87	TYR	Peptide

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	2886	0	2947	30	0
1	B	3002	0	3073	27	0
1	C	2925	0	2987	23	0
1	D	3002	0	3073	28	0
1	E	2903	0	2962	25	0
1	F	2903	0	2962	30	0
1	G	2922	0	2987	35	0
1	H	2922	0	2987	21	0
2	G	5	0	0	0	0
3	A	49	0	0	0	0
3	B	44	0	0	0	0
3	C	33	0	0	1	0
3	D	40	0	0	1	0
3	E	46	0	0	0	0
3	F	47	0	0	0	0
3	G	36	0	0	1	0
3	H	50	0	0	0	0
All	All	23815	0	23978	198	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 (198) 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:80:GLU:HG2	1:F:205:THR:HB	1.39	0.99
1:D:34:GLN:HE22	1:D:69:ARG:HH21	1.03	0.98
1:D:34:GLN:HG3	1:D:66:VAL:O	1.64	0.96
1:E:152:PRO:O	1:E:155:VAL:HG13	1.76	0.84
1:A:315:GLU:OE2	1:A:329:ARG:NH2	2.13	0.82
1:H:72:HIS:CE1	1:H:102:GLU:HG3	2.19	0.77
1:B:72:HIS:CE1	1:B:102:GLU:HG3	2.19	0.76
1:G:73:LEU:CD2	1:G:196:VAL:HG22	2.15	0.75
1:G:368:TRP:CZ3	1:G:386:ARG:HG3	2.21	0.74
1:D:34:GLN:HE22	1:D:69:ARG:NH2	1.83	0.73
1:B:13:ARG:HD3	1:D:13:ARG:HD3	1.74	0.68
1:G:38:PRO:HG2	1:G:58:LYS:HD2	1.75	0.67
1:B:223:LEU:CD1	1:B:225:ILE:HD11	2.27	0.65
1:G:207:LEU:O	1:G:211:ILE:HD12	1.98	0.64
1:H:223:LEU:CD1	1:H:225:ILE:HD11	2.28	0.64
1:F:223:LEU:CD1	1:F:225:ILE:HD11	2.29	0.63
1:G:43:ARG:HH22	1:G:75:GLU:CD	2.02	0.63
1:D:38:PRO:HG2	1:D:58:LYS:HD3	1.82	0.62
1:A:207:LEU:O	1:A:211:ILE:HD12	1.99	0.62
1:G:223:LEU:CD1	1:G:225:ILE:HD11	2.29	0.61
1:B:223:LEU:HD12	1:B:225:ILE:HD11	1.82	0.61
1:G:163:ILE:HB	1:G:164:GLY:HA2	1.82	0.60
1:F:223:LEU:HD12	1:F:225:ILE:HD11	1.85	0.59
1:C:339:SER:OG	1:C:340:GLY:N	2.36	0.59
1:D:38:PRO:HG2	1:D:58:LYS:CD	2.32	0.58
1:H:237:ILE:HG21	1:H:351:ARG:HD2	1.86	0.58
1:A:252:SER:O	1:A:253:LYS:HB2	2.04	0.58
1:A:223:LEU:HD13	1:A:225:ILE:HD11	1.85	0.58
1:F:329:ARG:HD2	1:H:51:THR:OG1	2.04	0.58
1:G:73:LEU:HD23	1:G:196:VAL:HG22	1.86	0.58
1:G:223:LEU:HD12	1:G:225:ILE:HD11	1.85	0.58
1:H:73:LEU:HD13	1:H:199:PHE:CD2	2.38	0.58
1:A:349:GLU:OE2	1:A:353:ARG:HG3	2.03	0.58
1:E:80:GLU:HG2	1:F:205:THR:CB	2.26	0.57
1:H:223:LEU:HD12	1:H:225:ILE:HD11	1.85	0.57
1:H:301:TRP:CZ3	1:H:372:MET:CE	2.87	0.57
1:A:43:ARG:NH2	1:B:319:GLU:OE1	2.32	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ILE:H	1:A:310:ILE:HD12	1.70	0.56
1:E:289:SER:OG	1:E:290:PRO:HD3	2.06	0.56
1:B:231:LEU:HD12	1:D:2:ASN:O	2.05	0.56
1:E:80:GLU:CG	1:F:205:THR:HB	2.25	0.56
1:G:107:ALA:HB1	1:G:190:VAL:HG11	1.88	0.56
1:A:223:LEU:CD1	1:A:225:ILE:HD11	2.36	0.55
1:E:223:LEU:CD1	1:E:225:ILE:HD11	2.36	0.55
1:H:107:ALA:HB1	1:H:190:VAL:HG11	1.89	0.55
1:D:310:ILE:HD12	1:D:310:ILE:H	1.72	0.55
1:A:113:ARG:NH2	1:B:36:GLU:HG2	2.22	0.55
1:A:289:SER:OG	1:A:290:PRO:HD3	2.06	0.55
1:A:53:LEU:HD13	1:A:204:GLU:HG3	1.90	0.54
1:E:223:LEU:HD13	1:E:225:ILE:HD11	1.90	0.54
1:B:107:ALA:HB1	1:B:190:VAL:HG11	1.90	0.54
1:F:250:ASN:O	1:F:250:ASN:OD1	2.27	0.53
1:D:107:ALA:HB1	1:D:190:VAL:HG11	1.90	0.53
1:C:107:ALA:HB1	1:C:190:VAL:HG11	1.91	0.52
1:D:34:GLN:NE2	1:D:69:ARG:HE	2.06	0.52
1:F:366:LEU:HD12	1:F:366:LEU:N	2.23	0.52
1:A:107:ALA:HB1	1:A:190:VAL:HG11	1.91	0.52
1:E:112:SER:O	1:E:116:GLU:HG2	2.09	0.52
1:D:223:LEU:HD23	1:D:223:LEU:N	2.25	0.52
1:F:107:ALA:HB1	1:F:190:VAL:HG11	1.91	0.51
1:C:223:LEU:HD21	1:C:344:LEU:HD13	1.91	0.51
1:G:73:LEU:HD22	1:G:196:VAL:HG22	1.92	0.51
1:H:59:ARG:O	1:H:63:ARG:HD3	2.11	0.51
1:B:300:PHE:CE1	1:B:369:GLY:HA3	2.47	0.50
1:D:197:MET:HG2	1:D:264:LEU:HB2	1.93	0.50
1:C:302:ILE:CD1	1:C:347:LEU:HD23	2.42	0.50
1:F:169:GLY:HA2	1:F:383:ILE:CD1	2.42	0.50
1:G:368:TRP:CE3	1:G:386:ARG:HG3	2.45	0.50
1:E:107:ALA:HB1	1:E:190:VAL:HG11	1.92	0.50
1:G:169:GLY:HA2	1:G:383:ILE:CD1	2.42	0.50
1:A:20:ILE:HG12	1:A:225:ILE:CD1	2.42	0.49
1:B:169:GLY:HA2	1:B:383:ILE:CD1	2.42	0.49
1:H:307:GLY:O	1:H:310:ILE:HG22	2.13	0.49
1:E:101:ALA:HB2	1:F:50:LEU:HD21	1.95	0.49
1:A:321:LYS:HB3	1:A:322:PRO:CD	2.42	0.49
1:C:14:PRO:HD2	1:C:180:GLU:O	2.13	0.48
1:A:68:LYS:HE2	1:A:334:GLU:OE1	2.13	0.48
1:E:20:ILE:HG12	1:E:225:ILE:CD1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:223:LEU:HD21	1:H:344:LEU:HD22	1.96	0.48
1:C:241:PHE:CE2	1:C:291:LEU:HD21	2.49	0.48
1:F:49:HIS:H	1:F:49:HIS:CD2	2.29	0.48
1:F:68:LYS:HE3	1:F:68:LYS:HB2	1.68	0.48
1:H:56:LYS:HE3	1:H:207:LEU:HD21	1.96	0.48
1:B:68:LYS:HE3	1:B:68:LYS:HB2	1.68	0.48
1:A:138:LYS:HD2	1:H:376:PRO:HG2	1.95	0.48
1:E:68:LYS:HE3	1:E:68:LYS:HB2	1.67	0.48
1:G:133:THR:O	1:G:197:MET:HE1	2.14	0.47
1:D:241:PHE:CE2	1:D:291:LEU:HD11	2.49	0.47
1:C:68:LYS:HE3	1:C:68:LYS:HB2	1.68	0.47
1:D:72:HIS:CD2	1:D:102:GLU:HG2	2.49	0.47
1:G:355:LYS:HB2	1:G:355:LYS:HE2	1.62	0.47
1:G:315:GLU:HG3	1:G:325:LEU:HD22	1.96	0.47
1:B:223:LEU:HD12	1:B:225:ILE:CD1	2.45	0.47
1:H:280:ILE:HD11	1:H:372:MET:CE	2.44	0.47
1:B:372:MET:HA	1:B:381:GLU:O	2.14	0.47
1:C:252:SER:O	1:C:253:LYS:HG2	2.15	0.47
1:C:372:MET:HA	1:C:381:GLU:O	2.15	0.47
1:E:372:MET:HA	1:E:381:GLU:O	2.15	0.47
1:C:33:ASN:HB2	1:C:36:GLU:OE1	2.15	0.47
1:F:372:MET:HA	1:F:381:GLU:O	2.15	0.47
1:E:68:LYS:HE2	1:E:334:GLU:OE1	2.15	0.47
1:G:372:MET:HA	1:G:381:GLU:O	2.15	0.47
1:F:270:LYS:HE2	1:F:270:LYS:HB3	1.62	0.46
1:B:2:ASN:O	1:D:231:LEU:HD12	2.14	0.46
1:H:68:LYS:HB2	1:H:68:LYS:HE3	1.68	0.46
1:F:14:PRO:HG3	1:F:183:VAL:HA	1.96	0.46
1:D:372:MET:HA	1:D:381:GLU:O	2.15	0.46
1:F:223:LEU:HD21	1:F:344:LEU:HD22	1.97	0.46
1:A:137:GLU:OE1	1:H:258:ARG:NH1	2.45	0.46
1:H:223:LEU:HD12	1:H:225:ILE:CD1	2.46	0.46
1:H:372:MET:HA	1:H:381:GLU:O	2.15	0.46
1:B:241:PHE:CE2	1:B:291:LEU:HD21	2.51	0.45
1:E:72:HIS:CD2	1:E:102:GLU:HG2	2.51	0.45
1:G:169:GLY:O	1:G:383:ILE:HD11	2.17	0.45
1:C:302:ILE:HD13	1:C:347:LEU:HD23	1.98	0.45
1:F:72:HIS:CD2	1:F:102:GLU:HG2	2.51	0.45
1:B:223:LEU:HD21	1:B:344:LEU:HD22	1.99	0.45
1:A:203:SER:HA	1:G:62:GLU:OE1	2.16	0.45
1:C:302:ILE:HD13	1:C:347:LEU:CD2	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:68:LYS:HE3	1:G:68:LYS:HB2	1.68	0.44
1:E:64:SER:HB2	1:E:215:ILE:HD13	1.99	0.44
1:C:302:ILE:CD1	1:C:347:LEU:CD2	2.95	0.44
1:F:371:LEU:HD22	1:F:383:ILE:HD12	1.99	0.44
1:G:64:SER:HB2	1:G:215:ILE:HD13	2.00	0.44
1:G:73:LEU:HD12	1:G:78:LEU:HG	1.99	0.44
1:C:72:HIS:CD2	1:C:102:GLU:HG2	2.53	0.44
1:A:258:ARG:NE	1:H:137:GLU:OE1	2.49	0.44
1:G:72:HIS:CD2	1:G:102:GLU:HG2	2.53	0.44
1:G:223:LEU:HD21	1:G:344:LEU:HD22	2.00	0.44
1:A:310:ILE:HD12	1:A:310:ILE:N	2.33	0.44
1:E:315:GLU:HG3	1:E:325:LEU:HD22	1.99	0.44
1:F:352:ARG:O	1:F:356:LYS:HG3	2.17	0.44
1:G:109[B]:ARG:NH1	3:G:505:HOH:O	2.50	0.44
1:G:223:LEU:HD12	1:G:225:ILE:CD1	2.47	0.44
1:E:55:ASP:O	1:E:59:ARG:HG3	2.18	0.43
1:F:315:GLU:HG3	1:F:325:LEU:HD22	2.00	0.43
1:G:207:LEU:HD22	1:G:207:LEU:HA	1.82	0.43
1:F:64:SER:HB2	1:F:215:ILE:HD13	2.00	0.43
1:A:223:LEU:HD21	1:A:344:LEU:HD22	2.00	0.43
1:E:223:LEU:HD21	1:E:344:LEU:HD22	2.01	0.43
1:D:58:LYS:HD2	1:D:58:LYS:HA	1.68	0.43
1:F:315:GLU:OE2	1:F:329:ARG:NH1	2.45	0.43
1:D:163:ILE:HG12	3:D:414:HOH:O	2.18	0.43
1:E:56:LYS:HA	1:E:59:ARG:NH1	2.34	0.43
1:A:372:MET:HA	1:A:381:GLU:O	2.18	0.43
1:D:315:GLU:HG3	1:D:325:LEU:HD22	2.01	0.42
1:E:376:PRO:HG2	1:G:138:LYS:HD2	2.02	0.42
1:F:223:LEU:HD12	1:F:225:ILE:CD1	2.47	0.42
1:C:102:GLU:CD	3:C:416:HOH:O	2.56	0.42
1:G:53:LEU:HD13	1:G:204:GLU:HG3	2.01	0.42
1:G:68:LYS:HE3	1:G:334:GLU:O	2.19	0.42
1:A:68:LYS:HE3	1:A:68:LYS:HB2	1.68	0.42
1:C:122:LYS:HE3	1:C:150:GLY:O	2.19	0.42
1:E:81:TYR:CD2	1:E:98:ILE:HD11	2.54	0.42
1:B:138:LYS:HD2	1:D:376:PRO:HG2	2.01	0.42
1:B:315:GLU:HG3	1:B:325:LEU:HD22	2.02	0.42
1:C:72:HIS:NE2	1:C:102:GLU:HG2	2.34	0.42
1:C:81:TYR:CD2	1:C:98:ILE:HD11	2.55	0.42
1:F:81:TYR:CD2	1:F:98:ILE:HD11	2.55	0.42
1:G:356:LYS:HA	1:G:356:LYS:HD3	1.74	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:ILE:HD12	1:D:310:ILE:N	2.33	0.42
1:D:64:SER:HB2	1:D:215:ILE:HD13	2.02	0.42
1:E:81:TYR:OH	1:F:205:THR:CG2	2.68	0.41
1:E:138:LYS:HD2	1:G:376:PRO:HG2	2.01	0.41
1:G:81:TYR:CD2	1:G:98:ILE:HD11	2.55	0.41
1:D:68:LYS:HE3	1:D:68:LYS:HB2	1.68	0.41
1:G:68:LYS:HE2	1:G:334:GLU:OE1	2.21	0.41
1:A:17:LEU:HD13	1:A:241:PHE:HA	2.01	0.41
1:B:68:LYS:HE3	1:B:334:GLU:O	2.20	0.41
1:C:59:ARG:O	1:C:63:ARG:HG2	2.20	0.41
1:D:34:GLN:HG3	1:D:66:VAL:C	2.36	0.41
1:F:55:ASP:HA	1:F:58:LYS:HE2	2.03	0.41
1:H:315:GLU:HG3	1:H:325:LEU:HD22	2.03	0.41
1:B:87:TYR:H	1:C:63:ARG:HH21	1.69	0.41
1:D:38:PRO:HG2	1:D:58:LYS:HD2	2.02	0.41
1:D:81:TYR:CD2	1:D:98:ILE:HD11	2.56	0.41
1:F:169:GLY:HA2	1:F:383:ILE:HD11	2.01	0.41
1:F:302:ILE:HG23	1:F:346:ILE:CG2	2.51	0.41
1:A:349:GLU:OE2	1:A:353:ARG:CG	2.68	0.41
1:B:371:LEU:HD22	1:B:383:ILE:HD12	2.03	0.41
1:C:72:HIS:CE1	1:C:102:GLU:HG2	2.56	0.41
1:C:189:VAL:HG21	1:C:225:ILE:HD13	2.03	0.41
1:C:302:ILE:HG23	1:C:346:ILE:CG2	2.51	0.41
1:F:291:LEU:HD22	1:F:291:LEU:N	2.36	0.41
1:H:68:LYS:HE3	1:H:334:GLU:O	2.21	0.41
1:B:13:ARG:HH11	1:B:13:ARG:HD2	1.77	0.41
1:B:72:HIS:NE2	1:B:102:GLU:HG3	2.36	0.41
1:A:72:HIS:CD2	1:A:102:GLU:HG2	2.56	0.40
1:A:113:ARG:HH22	1:B:36:GLU:HG2	1.85	0.40
1:A:321:LYS:HB3	1:A:322:PRO:HD2	2.03	0.40
1:B:169:GLY:O	1:B:383:ILE:HD11	2.20	0.40
1:D:56:LYS:CE	1:D:207:LEU:HD13	2.51	0.40
1:A:81:TYR:CD2	1:A:98:ILE:HD11	2.55	0.40
1:E:68:LYS:HE3	1:E:334:GLU:O	2.21	0.40
1:A:109:ARG:HE	1:B:35:ASP:CG	2.25	0.40
1:B:169:GLY:HA2	1:B:383:ILE:HD11	2.04	0.40
1:D:14:PRO:HD2	1:D:180:GLU:O	2.21	0.40
1:G:302:ILE:HG23	1:G:346:ILE:CG2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/393 (95%)	363 (97%)	11 (3%)	0	100	100
1	B	389/393 (99%)	377 (97%)	12 (3%)	0	100	100
1	C	378/393 (96%)	366 (97%)	12 (3%)	0	100	100
1	D	389/393 (99%)	378 (97%)	11 (3%)	0	100	100
1	E	376/393 (96%)	364 (97%)	12 (3%)	0	100	100
1	F	376/393 (96%)	366 (97%)	10 (3%)	0	100	100
1	G	378/393 (96%)	370 (98%)	8 (2%)	0	100	100
1	H	378/393 (96%)	369 (98%)	9 (2%)	0	100	100
All	All	3038/3144 (97%)	2953 (97%)	85 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/329 (96%)	310 (98%)	5 (2%)	62	83
1	B	327/329 (99%)	319 (98%)	8 (2%)	49	75
1	C	319/329 (97%)	312 (98%)	7 (2%)	52	77
1	D	327/329 (99%)	325 (99%)	2 (1%)	86	94
1	E	317/329 (96%)	312 (98%)	5 (2%)	62	83
1	F	317/329 (96%)	308 (97%)	9 (3%)	43	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	319/329 (97%)	303 (95%)	16 (5%)	24	47
1	H	319/329 (97%)	307 (96%)	12 (4%)	33	59
All	All	2560/2632 (97%)	2496 (98%)	64 (2%)	47	74

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASP
1	A	130	PHE
1	A	223	LEU
1	A	284	LEU
1	A	386	ARG
1	B	12	ARG
1	B	59	ARG
1	B	63	ARG
1	B	88	ASP
1	B	130	PHE
1	B	223	LEU
1	B	253	LYS
1	B	284	LEU
1	C	12	ARG
1	C	13	ARG
1	C	130	PHE
1	C	223	LEU
1	C	284	LEU
1	C	285	ASP
1	C	353	ARG
1	D	76	GLU
1	D	130	PHE
1	E	130	PHE
1	E	204	GLU
1	E	223	LEU
1	E	284	LEU
1	E	285	ASP
1	F	43	ARG
1	F	51	THR
1	F	116	GLU
1	F	123	ASN
1	F	130	PHE
1	F	204	GLU
1	F	223	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	270	LYS
1	F	334	GLU
1	G	63	ARG
1	G	73	LEU
1	G	76	GLU
1	G	130	PHE
1	G	162	THR
1	G	165	CYS
1	G	207	LEU
1	G	223	LEU
1	G	235	LYS
1	G	252	SER
1	G	253	LYS
1	G	282	GLN
1	G	284	LEU
1	G	285	ASP
1	G	294	ASN
1	G	333	SER
1	H	43	ARG
1	H	51	THR
1	H	55	ASP
1	H	63	ARG
1	H	79	GLN
1	H	130	PHE
1	H	162	THR
1	H	223	LEU
1	H	253	LYS
1	H	285	ASP
1	H	351	ARG
1	H	386	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	B	72	HIS
1	C	30	ASN
1	D	34	GLN
1	D	49	HIS
1	D	123	ASN
1	D	279	ASN
1	E	49	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	49	HIS
1	F	79	GLN
1	F	250	ASN
1	G	30	ASN
1	H	147	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	G	401	-	4,4,4	0.34	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	376/393 (95%)	-0.15	1 (0%)	94	95	16, 27, 41, 88	0
1	B	391/393 (99%)	-0.12	4 (1%)	82	82	17, 27, 48, 74	0
1	C	380/393 (96%)	0.05	5 (1%)	77	78	19, 30, 51, 83	0
1	D	391/393 (99%)	-0.07	11 (2%)	53	52	17, 27, 53, 79	0
1	E	378/393 (96%)	-0.07	2 (0%)	91	92	19, 29, 46, 84	0
1	F	378/393 (96%)	-0.09	1 (0%)	94	95	18, 28, 44, 75	0
1	G	379/393 (96%)	0.01	5 (1%)	77	78	18, 29, 48, 79	0
1	H	379/393 (96%)	-0.12	3 (0%)	86	86	16, 26, 43, 88	0
All	All	3052/3144 (97%)	-0.07	32 (1%)	82	82	16, 28, 47, 88	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	13	ARG	4.4
1	E	391	VAL	4.1
1	C	15	HIS	3.7
1	C	390	VAL	3.7
1	G	391	VAL	3.7
1	B	12	ARG	3.4
1	C	360	GLY	3.3
1	A	391	VAL	3.3
1	B	11	ALA	3.2
1	D	391	VAL	3.2
1	H	15	HIS	3.1
1	H	391	VAL	2.9
1	G	15	HIS	2.8
1	G	336	GLY	2.8
1	F	14	PRO	2.7
1	C	391	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	5	VAL	2.6
1	D	9	ASN	2.6
1	D	4	THR	2.5
1	D	11	ALA	2.4
1	D	2	ASN	2.3
1	D	15	HIS	2.3
1	B	79	GLN	2.3
1	C	12	ARG	2.3
1	G	164	GLY	2.2
1	D	10	GLY	2.2
1	D	13	ARG	2.2
1	D	8	MET	2.1
1	D	6	LYS	2.1
1	B	2	ASN	2.1
1	G	389	SER	2.1
1	E	14	PRO	2.1

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
2	SO4	G	401	5/5	0.84	0.46	84,89,93,96	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK