



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2021 – 04:03 PM EDT

PDB ID : 7SA7
Title : Crystal structure of the apo SH2 domains of Syk
Authors : Hobbs, H.T.; Badroos, J.; Gee, C.L.; Kuriyan, J.
Deposited on : 2021-09-22
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

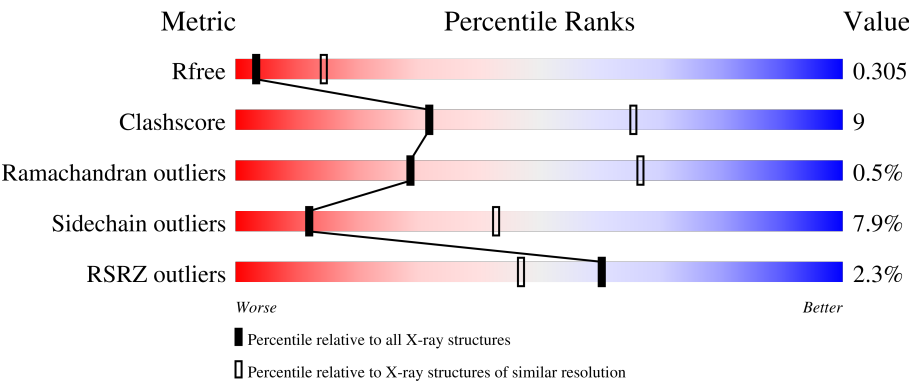
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	267	<div><div></div><div>63%19%•17%</div></div>
1	B	267	<div><div>%</div><div>65%21%•12%</div></div>
1	C	267	<div><div>4%</div><div>63%17%•18%</div></div>
1	D	267	<div><div>4%</div><div>58%27%6%9%</div></div>
1	E	267	<div><div>%</div><div>72%21%•5%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	267	<div><div></div><div>2%</div><div>74%</div><div>18%</div><div>• 5%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11300 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 Tyrosine-protein kinase SYK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1734	1099	312	317	6			
1	B	236	Total	C	N	O	S	0	0	0
			1872	1191	335	340	6			
1	C	218	Total	C	N	O	S	0	0	0
			1719	1091	309	313	6			
1	D	244	Total	C	N	O	S	0	0	0
			1941	1231	347	357	6			
1	E	254	Total	C	N	O	S	0	0	0
			2014	1280	360	368	6			
1	F	254	Total	C	N	O	S	0	0	0
			2016	1279	360	371	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP P43405
A	4	PRO	-	expression tag	UNP P43405
A	5	HIS	-	expression tag	UNP P43405
B	3	GLY	-	expression tag	UNP P43405
B	4	PRO	-	expression tag	UNP P43405
B	5	HIS	-	expression tag	UNP P43405
C	3	GLY	-	expression tag	UNP P43405
C	4	PRO	-	expression tag	UNP P43405
C	5	HIS	-	expression tag	UNP P43405
D	3	GLY	-	expression tag	UNP P43405
D	4	PRO	-	expression tag	UNP P43405
D	5	HIS	-	expression tag	UNP P43405
E	3	GLY	-	expression tag	UNP P43405
E	4	PRO	-	expression tag	UNP P43405
E	5	HIS	-	expression tag	UNP P43405
F	3	GLY	-	expression tag	UNP P43405
F	4	PRO	-	expression tag	UNP P43405

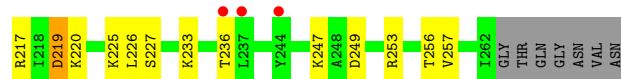
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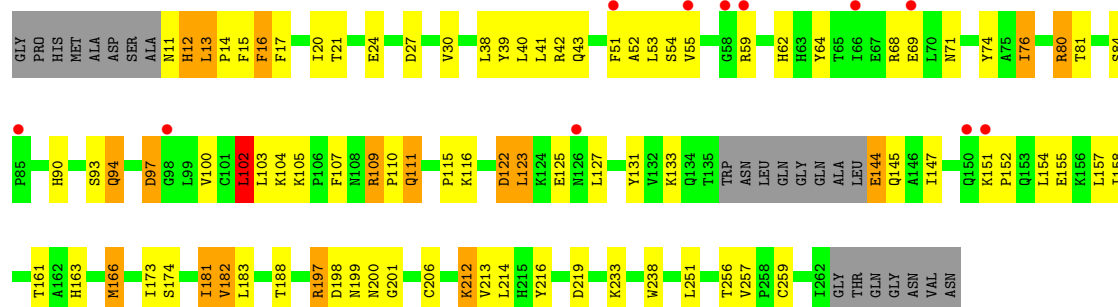
Chain	Residue	Modelled	Actual	Comment	Reference
F	5	HIS	-	expression tag	UNP P43405

- Molecule 2 is water.

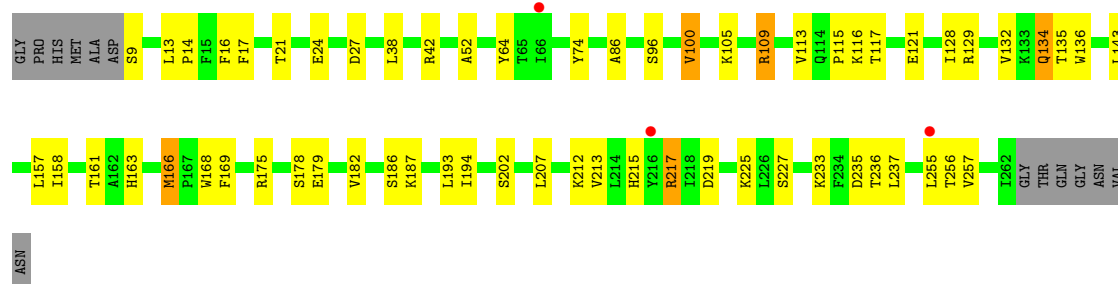
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	O 1	0	0
2	B	1	Total 1	O 1	0	0
2	F	2	Total 2	O 2	0	0



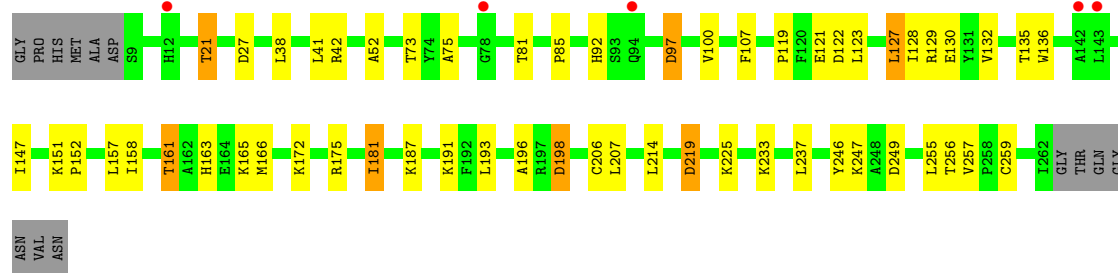
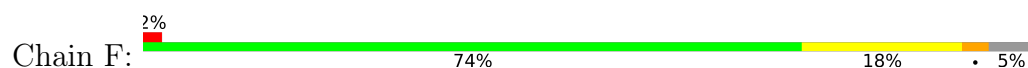
• Molecule 1: Tyrosine-protein kinase SYK



• Molecule 1: Tyrosine-protein kinase SYK



• Molecule 1: Tyrosine-protein kinase SYK



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.88Å 153.88Å 85.47Å 90.00° 91.05° 90.00°	Depositor
Resolution (Å)	45.78 – 3.20 48.31 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.78-3.20) 94.7 (48.31-3.20)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.270 , 0.304 0.269 , 0.305	Depositor DCC
R_{free} test set	1588 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11300	wwPDB-VP
Average B, all atoms (Å ²)	77.0	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.*

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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/1776	0.52	0/2399
1	B	0.26	0/1916	0.46	0/2586
1	C	0.25	0/1759	0.46	0/2374
1	D	0.25	0/1985	0.50	2/2678 (0.1%)
1	E	0.24	0/2061	0.46	0/2784
1	F	0.25	0/2063	0.45	0/2788
All	All	0.25	0/11560	0.47	2/15609 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	LEU	CA-CB-CG	5.40	127.71	115.30
1	D	59	ARG	NE-CZ-NH1	-5.24	117.68	120.30

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	1734	0	1682	26	1
1	B	1872	0	1841	38	1
1	C	1719	0	1688	23	2
1	D	1941	0	1909	56	1
1	E	2014	0	1985	31	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2016	0	1980	28	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	F	2	0	0	0	0
All	All	11300	0	11085	200	4

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 9.

All (200) 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:D:80:ARG:NH2	1:D:97:ASP:OD2	2.09	0.86
1:B:42:ARG:NH1	1:B:54:SER:OG	2.15	0.80
1:C:217:ARG:NH1	1:C:219:ASP:OD2	2.18	0.77
1:F:128:ILE:HG22	1:F:158:ILE:HG13	1.66	0.76
1:B:15:PHE:HD2	1:B:15:PHE:H	1.34	0.75
1:C:170:HIS:HB2	1:C:173:ILE:HD11	1.67	0.74
1:D:42:ARG:NH1	1:D:54:SER:OG	2.21	0.73
1:E:16:PHE:O	1:E:109:ARG:NH1	2.22	0.73
1:A:75:ALA:HB2	1:A:81:THR:HA	1.72	0.72
1:A:76:ILE:HG13	1:A:88:LEU:HD11	1.76	0.68
1:A:199:ASN:HB2	1:A:202:SER:HB3	1.75	0.68
1:D:17:PHE:HB3	1:D:20:ILE:HD12	1.75	0.68
1:D:122:ASP:N	1:D:122:ASP:OD1	2.25	0.68
1:F:130:GLU:OE1	1:F:165:LYS:NZ	2.27	0.68
1:D:16:PHE:HE2	1:D:41:LEU:HD22	1.59	0.67
1:E:128:ILE:HG22	1:E:158:ILE:HG13	1.76	0.66
1:B:16:PHE:O	1:B:109:ARG:NH1	2.29	0.66
1:D:20:ILE:HG23	1:D:24:GLU:HB3	1.78	0.65
1:C:187:LYS:HG3	1:C:208:LEU:HD21	1.77	0.65
1:F:219:ASP:N	1:F:219:ASP:OD1	2.28	0.64
1:B:179:GLU:HG3	1:B:213:VAL:HG11	1.79	0.63
1:D:127:LEU:HD21	1:D:154:LEU:HD23	1.79	0.63
1:E:202:SER:OG	1:E:217:ARG:NH1	2.31	0.63
1:C:19:ASN:N	1:C:116:LYS:O	2.32	0.62
1:A:30:VAL:HA	1:A:34:MET:HG2	1.82	0.61
1:E:9:SER:N	1:E:74:TYR:HH	1.98	0.61
1:A:17:PHE:O	1:A:115:PRO:HA	2.00	0.61
1:D:13:LEU:HD12	1:D:14:PRO:HD3	1.82	0.61
1:E:175:ARG:NH2	1:E:179:GLU:OE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:VAL:HG12	1:D:183:LEU:HD12	1.82	0.60
1:D:102:LEU:H	1:D:102:LEU:HD22	1.68	0.59
1:D:53:LEU:HD11	1:D:103:LEU:HD21	1.84	0.59
1:D:93:SER:OG	1:D:94:GLN:OE1	2.11	0.58
1:D:55:VAL:HG23	1:D:62:HIS:HB2	1.84	0.58
1:A:17:PHE:HE2	1:A:40:LEU:HD22	1.68	0.58
1:A:37:GLY:HA3	1:A:104:LYS:HD2	1.86	0.58
1:B:150:GLN:HB3	1:B:154:LEU:HG	1.86	0.58
1:F:161:THR:O	1:F:161:THR:OG1	2.22	0.58
1:B:75:ALA:HB2	1:B:81:THR:HA	1.85	0.57
1:F:157:LEU:O	1:F:161:THR:HG23	2.04	0.57
1:B:21:THR:HG21	1:B:246:TYR:CE1	2.40	0.57
1:A:119:PRO:HA	1:A:122:ASP:HB2	1.87	0.56
1:D:76:ILE:HD13	1:D:76:ILE:H	1.69	0.56
1:B:210:GLU:OE2	1:B:253:ARG:NH2	2.38	0.56
1:F:163:HIS:HA	1:F:166:MET:HG3	1.86	0.56
1:D:212:LYS:HD3	1:D:213:VAL:N	2.19	0.56
1:D:40:LEU:HD21	1:D:107:PHE:HB3	1.86	0.55
1:D:42:ARG:HH12	1:D:54:SER:HG	1.53	0.55
1:D:17:PHE:CE2	1:D:40:LEU:HD22	2.42	0.55
1:E:42:ARG:HG3	1:E:52:ALA:HB3	1.87	0.55
1:E:13:LEU:HD11	1:E:86:ALA:HB2	1.88	0.54
1:A:163:HIS:HA	1:A:166:MET:HG3	1.89	0.54
1:D:147:ILE:HG22	1:D:151:LYS:HG3	1.89	0.54
1:F:42:ARG:HG3	1:F:52:ALA:HB3	1.89	0.54
1:D:16:PHE:O	1:D:115:PRO:HG3	2.08	0.54
1:E:21:THR:HG22	1:E:24:GLU:HG3	1.90	0.54
1:B:39:TYR:CE1	1:B:103:LEU:HB3	2.43	0.53
1:B:235:ASP:N	1:B:239:GLN:OE1	2.36	0.53
1:C:154:LEU:HG	1:C:155:GLU:HG3	1.91	0.53
1:E:17:PHE:O	1:E:115:PRO:HA	2.08	0.53
1:F:21:THR:HG21	1:F:246:TYR:CE2	2.43	0.53
1:B:17:PHE:O	1:B:115:PRO:HA	2.08	0.53
1:E:168:TRP:CZ3	1:E:194:ILE:HD11	2.43	0.53
1:D:14:PRO:O	1:D:109:ARG:HB2	2.07	0.53
1:C:179:GLU:HG3	1:C:213:VAL:HG11	1.90	0.52
1:D:122:ASP:HA	1:D:125:GLU:HB2	1.92	0.52
1:E:225:LYS:NZ	1:E:235:ASP:OD1	2.43	0.52
1:B:58:GLY:O	1:B:59:ARG:HG2	2.11	0.51
1:B:36:ASP:OD1	1:B:58:GLY:N	2.36	0.51
1:C:39:TYR:HB3	1:C:55:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:TYR:HD2	1:C:107:PHE:HE1	1.59	0.51
1:B:34:MET:HG3	1:B:56:ALA:HB1	1.91	0.51
1:E:217:ARG:CZ	1:E:219:ASP:HB3	2.40	0.51
1:E:17:PHE:HE1	1:E:109:ARG:HA	1.75	0.51
1:C:173:ILE:HG22	1:C:177:GLU:HB3	1.92	0.51
1:D:74:TYR:CD2	1:D:84:SER:HA	2.46	0.51
1:E:14:PRO:O	1:E:109:ARG:N	2.41	0.51
1:A:14:PRO:O	1:A:109:ARG:N	2.40	0.50
1:D:21:THR:HG23	1:D:24:GLU:H	1.77	0.50
1:C:21:THR:HA	1:C:45:ARG:HD2	1.92	0.50
1:E:256:THR:OG1	1:E:257:VAL:N	2.45	0.50
1:C:256:THR:OG1	1:C:257:VAL:N	2.45	0.50
1:F:256:THR:OG1	1:F:257:VAL:N	2.44	0.50
1:B:256:THR:OG1	1:B:257:VAL:N	2.45	0.49
1:F:38:LEU:HD21	1:F:107:PHE:HB2	1.93	0.49
1:B:120:PHE:CD2	1:B:238:TRP:HB2	2.48	0.49
1:D:39:TYR:CG	1:D:103:LEU:HD23	2.47	0.49
1:A:13:LEU:HD11	1:A:86:ALA:HB2	1.94	0.49
1:E:227:SER:HB3	1:E:233:LYS:HG2	1.93	0.49
1:B:42:ARG:HH12	1:B:54:SER:HG	1.53	0.49
1:D:102:LEU:HD23	1:D:104:LYS:HE3	1.94	0.49
1:E:117:THR:HG23	1:E:121:GLU:HB2	1.94	0.49
1:A:168:TRP:HB3	1:A:258:PRO:HB3	1.93	0.49
1:F:132:VAL:HG13	1:F:136:TRP:CE2	2.48	0.49
1:C:102:LEU:HD23	1:C:102:LEU:H	1.76	0.49
1:B:15:PHE:HE1	1:B:39:TYR:HE2	1.61	0.48
1:C:182:VAL:HG22	1:C:191:LYS:HE3	1.95	0.48
1:E:163:HIS:CD2	1:E:237:LEU:HD12	2.48	0.48
1:F:206:CYS:HA	1:F:214:LEU:O	2.13	0.48
1:B:70:LEU:H	1:B:70:LEU:HG	1.48	0.48
1:B:120:PHE:HZ	1:B:242:GLU:HB2	1.78	0.48
1:A:12:HIS:CD2	1:A:12:HIS:H	2.31	0.48
1:F:75:ALA:HB2	1:F:81:THR:HA	1.95	0.48
1:B:199:ASN:HB3	1:B:202:SER:HB3	1.96	0.47
1:C:227:SER:HB3	1:C:233:LYS:HG2	1.96	0.47
1:F:247:LYS:HD2	1:F:249:ASP:HB2	1.96	0.47
1:D:74:TYR:HD2	1:D:84:SER:HA	1.79	0.47
1:D:163:HIS:HA	1:D:166:MET:HG3	1.96	0.47
1:E:157:LEU:O	1:E:161:THR:HG22	2.13	0.47
1:D:197:ARG:CZ	1:D:197:ARG:HB3	2.45	0.47
1:D:256:THR:OG1	1:D:257:VAL:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:SER:O	1:E:182:VAL:HG23	2.13	0.47
1:B:125:GLU:OE2	1:B:129:ARG:NH2	2.42	0.47
1:D:16:PHE:CE2	1:D:41:LEU:HD22	2.44	0.47
1:D:181:ILE:HG22	1:D:259:CYS:SG	2.54	0.46
1:A:36:ASP:HA	1:A:56:ALA:O	2.15	0.46
1:C:74:TYR:CD2	1:C:85:PRO:HD3	2.50	0.46
1:E:163:HIS:HA	1:E:166:MET:HG3	1.97	0.46
1:E:169:PHE:HD1	1:E:194:ILE:HG13	1.79	0.46
1:A:70:LEU:HD13	1:F:73:THR:HG21	1.97	0.46
1:D:68:ARG:NH2	1:D:155:GLU:OE1	2.49	0.46
1:A:256:THR:OG1	1:A:257:VAL:N	2.46	0.46
1:B:212:LYS:HD3	1:B:213:VAL:N	2.30	0.46
1:C:247:LYS:HD2	1:C:249:ASP:HB2	1.98	0.46
1:E:129:ARG:HD2	1:E:143:LEU:HD21	1.98	0.46
1:D:157:LEU:O	1:D:161:THR:HG22	2.16	0.46
1:A:216:TYR:CE2	1:A:251:LEU:HD22	2.50	0.46
1:C:189:ASN:ND2	1:C:253:ARG:HG2	2.31	0.46
1:B:26:GLU:O	1:B:30:VAL:HG22	2.16	0.45
1:D:43:GLN:HA	1:D:51:PHE:HD2	1.81	0.45
1:D:216:TYR:CE2	1:D:251:LEU:HD22	2.52	0.45
1:F:172:LYS:HG2	1:F:196:ALA:HB3	1.98	0.45
1:A:92:HIS:HA	1:A:95:GLU:O	2.16	0.45
1:D:17:PHE:HE2	1:D:40:LEU:HD22	1.81	0.45
1:F:163:HIS:CD2	1:F:237:LEU:HD12	2.51	0.45
1:D:12:HIS:N	1:D:12:HIS:ND1	2.63	0.45
1:E:219:ASP:N	1:E:219:ASP:OD1	2.50	0.45
1:B:128:ILE:HG22	1:B:158:ILE:HG13	1.99	0.45
1:B:180:GLN:O	1:B:184:ILE:HG12	2.17	0.45
1:B:182:VAL:HG13	1:B:183:LEU:HD12	1.97	0.45
1:D:151:LYS:N	1:D:152:PRO:HD2	2.31	0.45
1:B:74:TYR:CD2	1:B:85:PRO:HD3	2.52	0.44
1:E:21:THR:HG23	1:E:24:GLU:H	1.83	0.44
1:E:38:LEU:HA	1:E:105:LYS:O	2.17	0.44
1:B:15:PHE:HE1	1:B:39:TYR:CE2	2.35	0.44
1:D:27:ASP:O	1:D:30:VAL:HG22	2.17	0.44
1:A:109:ARG:HG2	1:A:113:VAL:HB	1.99	0.44
1:D:42:ARG:HG3	1:D:52:ALA:HB3	1.99	0.44
1:B:15:PHE:HD2	1:B:15:PHE:N	2.10	0.43
1:C:220:LYS:HE2	1:C:226:LEU:HG	2.00	0.43
1:F:181:ILE:HG22	1:F:259:CYS:SG	2.58	0.43
1:A:82:HIS:CD2	1:A:88:LEU:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LEU:HB2	1:C:16:PHE:HB2	1.99	0.43
1:E:132:VAL:HG13	1:E:136:TRP:CE3	2.54	0.43
1:E:109:ARG:HD2	1:E:113:VAL:O	2.18	0.43
1:F:151:LYS:N	1:F:152:PRO:HD2	2.34	0.43
1:D:39:TYR:CD2	1:D:103:LEU:HB3	2.54	0.43
1:D:219:ASP:OD1	1:D:219:ASP:N	2.50	0.43
1:D:111:GLN:H	1:D:111:GLN:HG2	1.63	0.43
1:E:64:TYR:OH	1:E:100:VAL:HG22	2.19	0.43
1:D:38:LEU:HD12	1:D:105:LYS:O	2.18	0.43
1:C:42:ARG:HG3	1:C:52:ALA:HB3	2.01	0.43
1:D:17:PHE:HE1	1:D:110:PRO:HD2	1.83	0.43
1:F:129:ARG:HG2	1:F:147:ILE:HD13	2.02	0.42
1:D:17:PHE:CE1	1:D:109:ARG:HG3	2.53	0.42
1:F:92:HIS:HE1	1:F:97:ASP:O	2.02	0.42
1:B:18:GLY:O	1:B:42:ARG:HB2	2.20	0.42
1:F:41:LEU:HD11	1:F:85:PRO:HB2	2.02	0.42
1:C:189:ASN:HD22	1:C:253:ARG:HG2	1.85	0.42
1:B:13:LEU:HD13	1:B:15:PHE:CE2	2.54	0.42
1:A:190:GLY:HA3	1:A:256:THR:HG23	2.01	0.42
1:B:236:THR:HG21	1:B:238:TRP:CZ3	2.55	0.42
1:D:123:LEU:HD21	1:D:238:TRP:CH2	2.55	0.42
1:B:199:ASN:OD1	1:B:200:ASN:N	2.53	0.42
1:E:207:LEU:HD13	1:E:255:LEU:HD23	2.02	0.41
1:A:247:LYS:HD2	1:A:249:ASP:HB2	2.02	0.41
1:D:64:TYR:OH	1:D:100:VAL:HG23	2.20	0.41
1:A:200:ASN:HB3	1:D:71:ASN:OD1	2.19	0.41
1:D:173:ILE:HG23	1:D:174:SER:O	2.21	0.41
1:F:198:ASP:OD1	1:F:198:ASP:N	2.53	0.41
1:F:207:LEU:HD13	1:F:255:LEU:HD23	2.03	0.41
1:A:9:SER:O	1:A:12:HIS:NE2	2.53	0.41
1:D:206:CYS:HA	1:D:214:LEU:O	2.21	0.41
1:E:134:GLN:HG2	1:E:135:THR:HG23	2.02	0.41
1:C:47:TYR:HE1	1:C:225:LYS:HZ1	1.67	0.41
1:D:38:LEU:HA	1:D:105:LYS:O	2.20	0.41
1:F:123:LEU:O	1:F:127:LEU:HB2	2.20	0.41
1:F:225:LYS:HB3	1:F:233:LYS:HB3	2.01	0.41
1:A:190:GLY:HA2	1:A:207:LEU:HD11	2.03	0.41
1:B:42:ARG:HG3	1:B:52:ALA:HB3	2.01	0.41
1:C:182:VAL:HG13	1:C:183:LEU:HD23	2.01	0.41
1:F:191:LYS:HA	1:F:257:VAL:O	2.21	0.41
1:B:234:PHE:HB3	1:B:239:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LEU:HG	1:D:158:ILE:HD13	2.03	0.41
1:D:144:GLU:HB2	1:D:145:GLN:H	1.75	0.40
1:F:193:LEU:CD2	1:F:206:CYS:HB2	2.51	0.40
1:B:45:ARG:O	1:B:239:GLN:HB2	2.21	0.40
1:D:41:LEU:HD23	1:D:42:ARG:N	2.36	0.40
1:A:70:LEU:HD12	1:A:70:LEU:H	1.87	0.40
1:B:162:ALA:HB3	1:B:238:TRP:CZ3	2.57	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:SER:OG	1:D:27:ASP:OD2[4_445]	1.87	0.33
1:E:186:SER:OG	1:F:27:ASP:OD2[4_455]	2.06	0.14
1:A:186:SER:OG	1:C:27:ASP:OD2[4_456]	2.07	0.13
1:B:186:SER:OG	1:E:27:ASP:OD2[1_556]	2.18	0.02

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	217/267 (81%)	208 (96%)	8 (4%)	1 (0%)	29	67
1	B	232/267 (87%)	224 (97%)	8 (3%)	0	100	100
1	C	214/267 (80%)	205 (96%)	8 (4%)	1 (0%)	29	67
1	D	240/267 (90%)	228 (95%)	9 (4%)	3 (1%)	12	47
1	E	252/267 (94%)	241 (96%)	11 (4%)	0	100	100
1	F	252/267 (94%)	240 (95%)	10 (4%)	2 (1%)	19	58
All	All	1407/1602 (88%)	1346 (96%)	54 (4%)	7 (0%)	29	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	200	ASN
1	C	97	ASP
1	F	97	ASP
1	D	199	ASN
1	F	119	PRO
1	A	119	PRO
1	D	201	GLY

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	180/225 (80%)	165 (92%)	15 (8%)	11	40
1	B	196/225 (87%)	184 (94%)	12 (6%)	18	54
1	C	180/225 (80%)	167 (93%)	13 (7%)	14	47
1	D	205/225 (91%)	176 (86%)	29 (14%)	3	16
1	E	211/225 (94%)	198 (94%)	13 (6%)	18	53
1	F	212/225 (94%)	200 (94%)	12 (6%)	20	56
All	All	1184/1350 (88%)	1090 (92%)	94 (8%)	12	43

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	59	ARG
1	A	65	THR
1	A	68	ARG
1	A	80	ARG
1	A	81	THR
1	A	100	VAL
1	A	114	GLN
1	A	116	LYS
1	A	117	THR
1	A	161	THR
1	A	181	ILE

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Mol	Chain	Res	Type
1	A	186	SER
1	A	193	LEU
1	A	194	ILE
1	B	15	PHE
1	B	21	THR
1	B	30	VAL
1	B	70	LEU
1	B	100	VAL
1	B	102	LEU
1	B	114	GLN
1	B	120	PHE
1	B	127	LEU
1	B	181	ILE
1	B	194	ILE
1	B	236	THR
1	C	9	SER
1	C	11	ASN
1	C	12	HIS
1	C	21	THR
1	C	55	VAL
1	C	102	LEU
1	C	173	ILE
1	C	183	LEU
1	C	194	ILE
1	C	198	ASP
1	C	207	LEU
1	C	219	ASP
1	C	236	THR
1	D	11	ASN
1	D	12	HIS
1	D	13	LEU
1	D	15	PHE
1	D	16	PHE
1	D	69	GLU
1	D	76	ILE
1	D	80	ARG
1	D	81	THR
1	D	90	HIS
1	D	94	GLN
1	D	97	ASP
1	D	102	LEU
1	D	109	ARG

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Mol	Chain	Res	Type
1	D	111	GLN
1	D	116	LYS
1	D	122	ASP
1	D	123	LEU
1	D	131	TYR
1	D	133	LYS
1	D	144	GLU
1	D	166	MET
1	D	181	ILE
1	D	182	VAL
1	D	188	THR
1	D	197	ARG
1	D	198	ASP
1	D	212	LYS
1	D	233	LYS
1	E	96	SER
1	E	100	VAL
1	E	109	ARG
1	E	116	LYS
1	E	134	GLN
1	E	166	MET
1	E	187	LYS
1	E	193	LEU
1	E	212	LYS
1	E	213	VAL
1	E	215	HIS
1	E	217	ARG
1	E	236	THR
1	F	21	THR
1	F	100	VAL
1	F	121	GLU
1	F	122	ASP
1	F	127	LEU
1	F	135	THR
1	F	161	THR
1	F	175	ARG
1	F	181	ILE
1	F	187	LYS
1	F	198	ASP
1	F	219	ASP

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

Mol	Chain	Res	Type
1	A	114	GLN
1	A	200	ASN
1	F	92	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	221/267 (82%)	0.04	1 (0%) 91 86	34, 60, 100, 157	0
1	B	236/267 (88%)	0.08	3 (1%) 77 65	40, 65, 101, 111	0
1	C	218/267 (81%)	0.23	10 (4%) 32 20	60, 87, 110, 137	0
1	D	244/267 (91%)	0.32	11 (4%) 33 21	50, 102, 136, 173	0
1	E	254/267 (95%)	0.05	3 (1%) 79 67	52, 80, 112, 147	0
1	F	254/267 (95%)	0.13	5 (1%) 65 51	39, 65, 86, 118	0
All	All	1427/1602 (89%)	0.14	33 (2%) 60 47	34, 75, 118, 173	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	85	PRO	4.7
1	F	12	HIS	3.6
1	D	69	GLU	3.0
1	F	94	GLN	3.0
1	E	255	LEU	2.9
1	D	59	ARG	2.7
1	F	142	ALA	2.6
1	C	107	PHE	2.6
1	C	89	CYS	2.6
1	D	66	ILE	2.6
1	B	198	ASP	2.5
1	D	58	GLY	2.5
1	D	126	ASN	2.4
1	F	143	LEU	2.3
1	E	66	ILE	2.3
1	B	131	TYR	2.3
1	D	151	LYS	2.3
1	D	98	GLY	2.2
1	C	161	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	216	TYR	2.2
1	C	51	PHE	2.2
1	D	55	VAL	2.2
1	C	244	TYR	2.2
1	D	51	PHE	2.2
1	C	237	LEU	2.2
1	C	157	LEU	2.1
1	C	53	LEU	2.1
1	F	78	GLY	2.1
1	A	198	ASP	2.1
1	B	111	GLN	2.1
1	C	236	THR	2.1
1	C	84	SER	2.0
1	D	150	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.