



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:33 AM UTC

PDB ID : 7SA7 / pdb_00007sa7
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 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

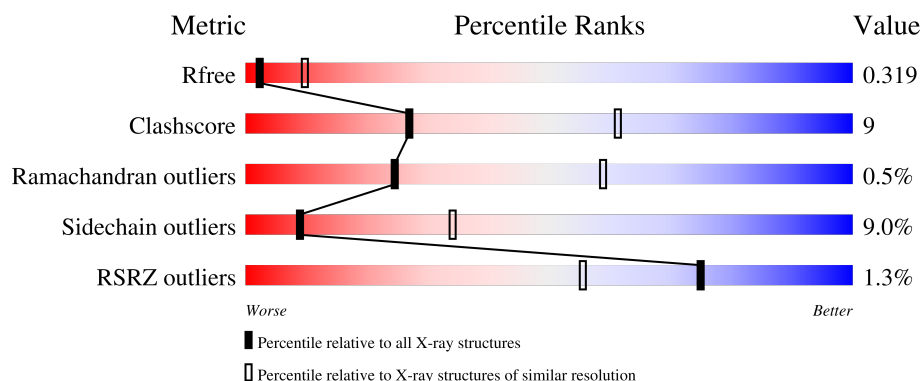
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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	61% 19% • 17%
1	B	267	64% 21% • 12%
1	C	267	3% 63% 16% • 18%
1	D	267	3% 57% 26% 8% 9%
1	E	267	72% 22% • 5%

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Mol	Chain	Length	Quality of chain
1	F	267	74% 18% • 5%

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

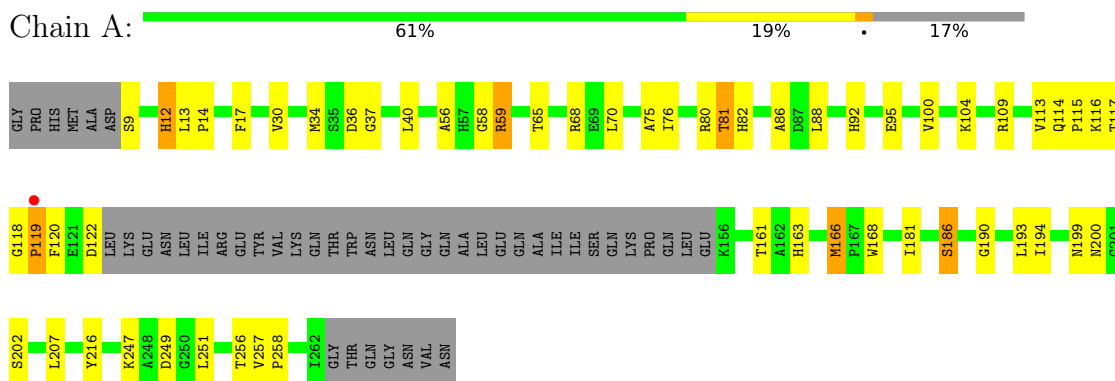
- Molecule 2 is water.

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

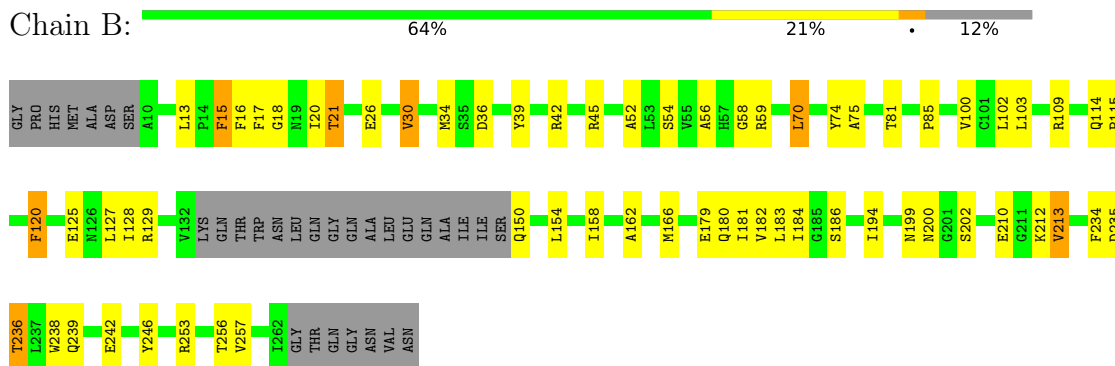
3 Residue-property plots

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.

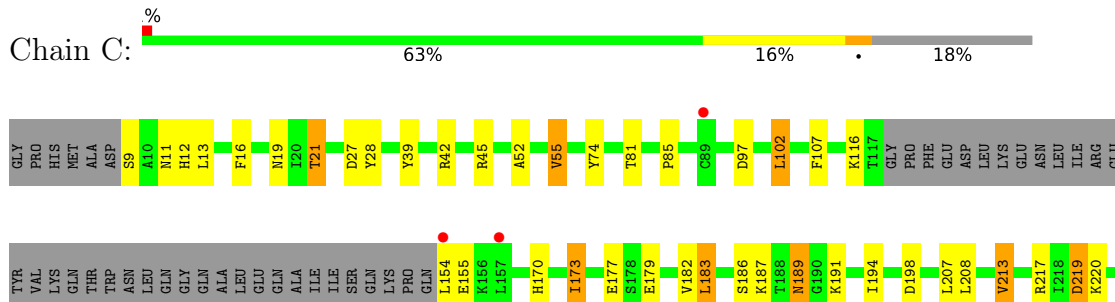
• Molecule 1: Tyrosine-protein kinase SYK



• Molecule 1: Tyrosine-protein kinase SYK

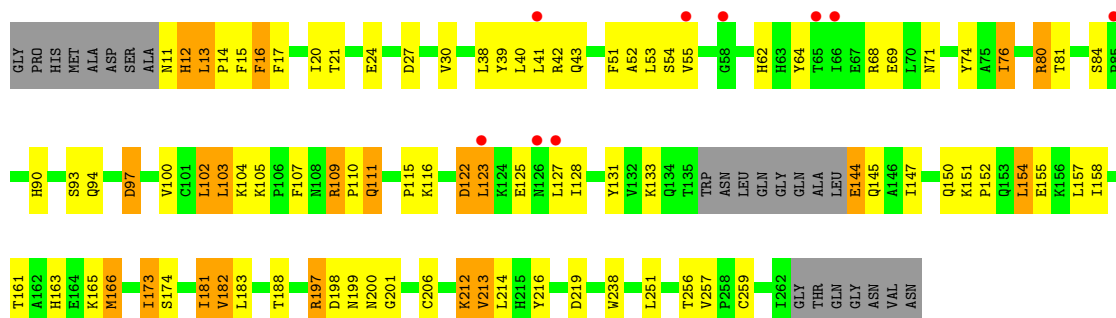


• Molecule 1: Tyrosine-protein kinase SYK

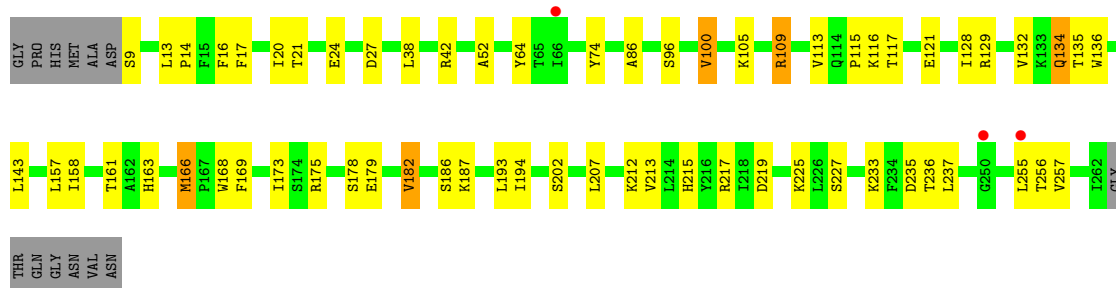




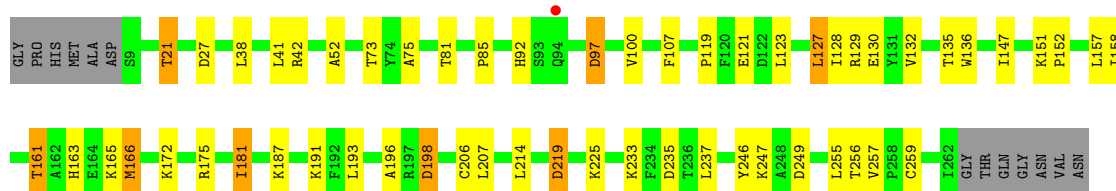
• Molecule 1: Tyrosine-protein kinase SYK



• 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 45.78 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.78-3.20) 99.7 (45.78-3.20)	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 0.284 , 0.319	Depositor DCC
R_{free} test set	1592 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)	0.31 , 33.8	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	0.16	0/1776	0.47	0/2399
1	B	0.13	0/1916	0.35	0/2586
1	C	0.12	0/1759	0.36	0/2374
1	D	0.13	0/1985	0.43	0/2678
1	E	0.11	0/2061	0.35	0/2784
1	F	0.12	0/2063	0.34	0/2788
All	All	0.13	0/11560	0.38	0/15609

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1734	0	1682	28	1
1	B	1872	0	1841	40	1
1	C	1719	0	1688	22	2
1	D	1941	0	1909	56	1
1	E	2014	0	1985	32	2
1	F	2016	0	1980	29	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	205	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 (205) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.54	0.55
1:D:17:PHE:CE2	1:D:40:LEU:HD22	2.42	0.55
1:F:225:LYS:NZ	1:F:235:ASP:OD1	2.29	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
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:B:42:ARG:HH12	1:B:54:SER:HG	1.56	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:30:VAL:HG13	1:B:34:MET:HE3	1.97	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:A:256:THR:OG1	1:A:257:VAL:N	2.46	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:OD1	1:E:219:ASP:N	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:A:118:GLY:C	1:A:120:PHE:H	2.25	0.43
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
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:A:58:GLY:C	1:A:59:ARG:HG3	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ASP:OD1	1:D:219:ASP:N	2.50	0.43
1:F:256:THR:OG1	1:F:257:VAL:N	2.44	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:B:120:PHE:HB3	1:B:166:MET:HE1	2.03	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: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
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:E:166:MET:HE2	1:E:166:MET:HB3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24	59
1	B	232/267 (87%)	224 (97%)	8 (3%)	0	100	100
1	C	214/267 (80%)	205 (96%)	8 (4%)	1 (0%)	24	59
1	D	240/267 (90%)	228 (95%)	9 (4%)	3 (1%)	9	40
1	E	252/267 (94%)	241 (96%)	11 (4%)	0	100	100
1	F	252/267 (94%)	240 (95%)	10 (4%)	2 (1%)	16	50
All	All	1407/1602 (88%)	1346 (96%)	54 (4%)	7 (0%)	24	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	200	ASN

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Mol	Chain	Res	Type
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%)	164 (91%)	16 (9%)	9	34
1	B	196/225 (87%)	182 (93%)	14 (7%)	13	44
1	C	180/225 (80%)	164 (91%)	16 (9%)	9	34
1	D	205/225 (91%)	171 (83%)	34 (17%)	2	11
1	E	211/225 (94%)	196 (93%)	15 (7%)	13	44
1	F	212/225 (94%)	200 (94%)	12 (6%)	18	51
All	All	1184/1350 (88%)	1077 (91%)	107 (9%)	9	34

All (107) 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	166	MET

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Mol	Chain	Res	Type
1	A	181	ILE
1	A	186	SER
1	A	193	LEU
1	A	194	ILE
1	B	15	PHE
1	B	20	ILE
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	213	VAL
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	81	THR
1	C	102	LEU
1	C	173	ILE
1	C	183	LEU
1	C	189	ASN
1	C	194	ILE
1	C	198	ASP
1	C	207	LEU
1	C	213	VAL
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

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Mol	Chain	Res	Type
1	D	81	THR
1	D	90	HIS
1	D	97	ASP
1	D	102	LEU
1	D	103	LEU
1	D	109	ARG
1	D	111	GLN
1	D	116	LYS
1	D	122	ASP
1	D	123	LEU
1	D	128	ILE
1	D	131	TYR
1	D	133	LYS
1	D	144	GLU
1	D	150	GLN
1	D	154	LEU
1	D	165	LYS
1	D	166	MET
1	D	173	ILE
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	213	VAL
1	E	20	ILE
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	173	ILE
1	E	182	VAL
1	E	187	LYS
1	E	193	LEU
1	E	212	LYS
1	E	213	VAL
1	E	215	HIS
1	E	236	THR
1	F	21	THR

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Mol	Chain	Res	Type
1	F	100	VAL
1	F	121	GLU
1	F	127	LEU
1	F	135	THR
1	F	161	THR
1	F	166	MET
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	200	ASN
1	B	19	ASN
1	C	12	HIS
1	C	57	HIS
1	C	189	ASN
1	C	209	HIS
1	E	126	ASN
1	E	137	ASN
1	E	150	GLN
1	F	62	HIS
1	F	92	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	221/267 (82%)	0.16	1 (0%) 87 76	34, 60, 100, 157	0
1	B	236/267 (88%)	0.25	0 100 100	40, 65, 101, 111	0
1	C	218/267 (81%)	0.52	4 (1%) 67 48	60, 87, 110, 137	0
1	D	244/267 (91%)	0.55	9 (3%) 45 28	50, 102, 136, 173	0
1	E	254/267 (95%)	0.38	3 (1%) 76 58	52, 80, 112, 147	0
1	F	254/267 (95%)	0.25	1 (0%) 88 79	39, 65, 86, 118	0
All	All	1427/1602 (89%)	0.35	18 (1%) 75 55	34, 75, 118, 173	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	154	LEU	4.1
1	D	66	ILE	3.7
1	D	85	PRO	3.5
1	D	55	VAL	2.7
1	C	89	CYS	2.7
1	D	58	GLY	2.6
1	E	66	ILE	2.5
1	C	157	LEU	2.5
1	D	123	LEU	2.5
1	F	94	GLN	2.4
1	D	41	LEU	2.3
1	E	250	GLY	2.3
1	D	126	ASN	2.3
1	D	127	LEU	2.3
1	E	255	LEU	2.2
1	C	237	LEU	2.2
1	D	65	THR	2.2
1	A	119	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.