



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:36 PM UTC

PDB ID : 7XSA / pdb_00007xsa
Title : Crystal structure of SARS-CoV-2 spike receptor binding domain bound with P2S-2E9 Fab
Authors : Wang, X.; Wang, Z.
Deposited on : 2022-05-13
Resolution : 2.20 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

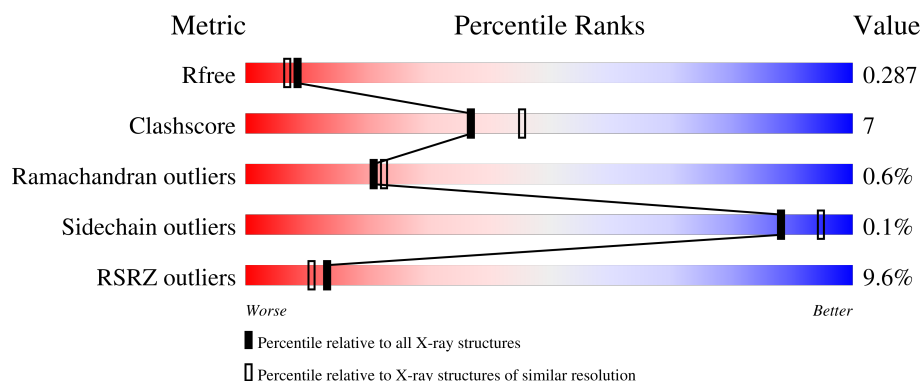
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	B	218	
1	H	218	
2	C	215	
2	I	215	
3	E	242	

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Mol	Chain	Length	Quality of chain
3	J	242	9% 64% 13% 22%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9284 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 P2S-2E9 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	215	Total	C	N	O	S	0	0	0
			1627	1035	267	319	6			
1	H	212	Total	C	N	O	S	0	0	0
			1610	1028	263	313	6			

- Molecule 2 is a protein called P2S-2E9 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	209	Total	C	N	O	S	0	0	0
			1532	954	252	320	6			
2	I	209	Total	C	N	O	S	0	0	0
			1529	950	252	321	6			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	187	Total	C	N	O	S	0	0	0
			1490	957	247	279	7			
3	J	188	Total	C	N	O	S	0	0	0
			1496	960	248	280	8			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	292	MET	-	initiating methionine	UNP P0DTC2
E	293	LEU	-	expression tag	UNP P0DTC2
E	294	LEU	-	expression tag	UNP P0DTC2
E	295	VAL	-	expression tag	UNP P0DTC2
E	296	ASN	-	expression tag	UNP P0DTC2
E	297	GLN	-	expression tag	UNP P0DTC2
E	298	SER	-	expression tag	UNP P0DTC2
E	299	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	300	GLN	-	expression tag	UNP P0DTC2
E	301	GLY	-	expression tag	UNP P0DTC2
E	302	PHE	-	expression tag	UNP P0DTC2
E	303	ASN	-	expression tag	UNP P0DTC2
E	304	LYS	-	expression tag	UNP P0DTC2
E	305	GLU	-	expression tag	UNP P0DTC2
E	306	HIS	-	expression tag	UNP P0DTC2
E	307	THR	-	expression tag	UNP P0DTC2
E	308	SER	-	expression tag	UNP P0DTC2
E	309	LYS	-	expression tag	UNP P0DTC2
E	310	MET	-	expression tag	UNP P0DTC2
E	311	VAL	-	expression tag	UNP P0DTC2
E	312	SER	-	expression tag	UNP P0DTC2
E	313	ALA	-	expression tag	UNP P0DTC2
E	314	ILE	-	expression tag	UNP P0DTC2
E	315	VAL	-	expression tag	UNP P0DTC2
E	316	LEU	-	expression tag	UNP P0DTC2
E	317	TYR	-	expression tag	UNP P0DTC2
E	318	VAL	-	expression tag	UNP P0DTC2
E	319	LEU	-	expression tag	UNP P0DTC2
E	320	LEU	-	expression tag	UNP P0DTC2
E	321	ALA	-	expression tag	UNP P0DTC2
E	322	ALA	-	expression tag	UNP P0DTC2
E	323	ALA	-	expression tag	UNP P0DTC2
E	324	ALA	-	expression tag	UNP P0DTC2
E	325	HIS	-	expression tag	UNP P0DTC2
E	326	SER	-	expression tag	UNP P0DTC2
E	327	ALA	-	expression tag	UNP P0DTC2
E	328	PHE	-	expression tag	UNP P0DTC2
E	329	ALA	-	expression tag	UNP P0DTC2
E	330	ALA	-	expression tag	UNP P0DTC2
E	331	ASP	-	expression tag	UNP P0DTC2
E	332	PRO	-	expression tag	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	484	LYS	GLU	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	528	HIS	-	expression tag	UNP P0DTC2
E	529	HIS	-	expression tag	UNP P0DTC2
E	530	HIS	-	expression tag	UNP P0DTC2
E	531	HIS	-	expression tag	UNP P0DTC2
E	532	HIS	-	expression tag	UNP P0DTC2
E	533	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	292	MET	-	initiating methionine	UNP P0DTC2
J	293	LEU	-	expression tag	UNP P0DTC2
J	294	LEU	-	expression tag	UNP P0DTC2
J	295	VAL	-	expression tag	UNP P0DTC2
J	296	ASN	-	expression tag	UNP P0DTC2
J	297	GLN	-	expression tag	UNP P0DTC2
J	298	SER	-	expression tag	UNP P0DTC2
J	299	HIS	-	expression tag	UNP P0DTC2
J	300	GLN	-	expression tag	UNP P0DTC2
J	301	GLY	-	expression tag	UNP P0DTC2
J	302	PHE	-	expression tag	UNP P0DTC2
J	303	ASN	-	expression tag	UNP P0DTC2
J	304	LYS	-	expression tag	UNP P0DTC2
J	305	GLU	-	expression tag	UNP P0DTC2
J	306	HIS	-	expression tag	UNP P0DTC2
J	307	THR	-	expression tag	UNP P0DTC2
J	308	SER	-	expression tag	UNP P0DTC2
J	309	LYS	-	expression tag	UNP P0DTC2
J	310	MET	-	expression tag	UNP P0DTC2
J	311	VAL	-	expression tag	UNP P0DTC2
J	312	SER	-	expression tag	UNP P0DTC2
J	313	ALA	-	expression tag	UNP P0DTC2
J	314	ILE	-	expression tag	UNP P0DTC2
J	315	VAL	-	expression tag	UNP P0DTC2
J	316	LEU	-	expression tag	UNP P0DTC2
J	317	TYR	-	expression tag	UNP P0DTC2
J	318	VAL	-	expression tag	UNP P0DTC2
J	319	LEU	-	expression tag	UNP P0DTC2
J	320	LEU	-	expression tag	UNP P0DTC2
J	321	ALA	-	expression tag	UNP P0DTC2
J	322	ALA	-	expression tag	UNP P0DTC2
J	323	ALA	-	expression tag	UNP P0DTC2
J	324	ALA	-	expression tag	UNP P0DTC2
J	325	HIS	-	expression tag	UNP P0DTC2
J	326	SER	-	expression tag	UNP P0DTC2
J	327	ALA	-	expression tag	UNP P0DTC2
J	328	PHE	-	expression tag	UNP P0DTC2
J	329	ALA	-	expression tag	UNP P0DTC2
J	330	ALA	-	expression tag	UNP P0DTC2
J	331	ASP	-	expression tag	UNP P0DTC2
J	332	PRO	-	expression tag	UNP P0DTC2
J	417	ASN	LYS	variant	UNP P0DTC2

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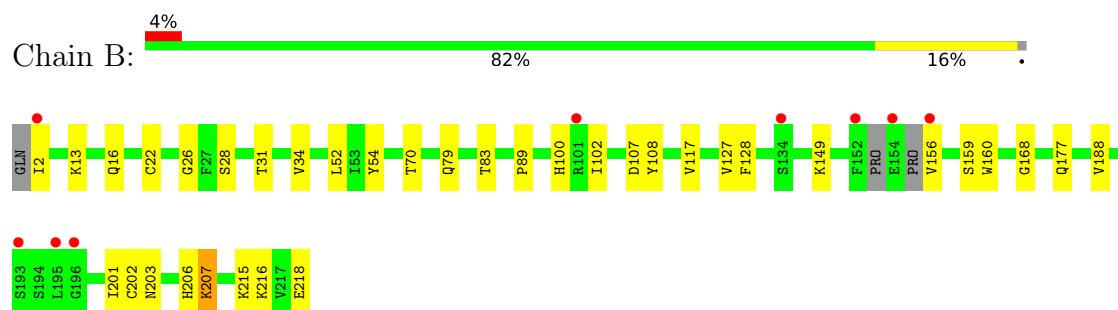
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Chain	Residue	Modelled	Actual	Comment	Reference
J	484	LYS	GLU	variant	UNP P0DTC2
J	501	TYR	ASN	variant	UNP P0DTC2
J	528	HIS	-	expression tag	UNP P0DTC2
J	529	HIS	-	expression tag	UNP P0DTC2
J	530	HIS	-	expression tag	UNP P0DTC2
J	531	HIS	-	expression tag	UNP P0DTC2
J	532	HIS	-	expression tag	UNP P0DTC2
J	533	HIS	-	expression tag	UNP P0DTC2

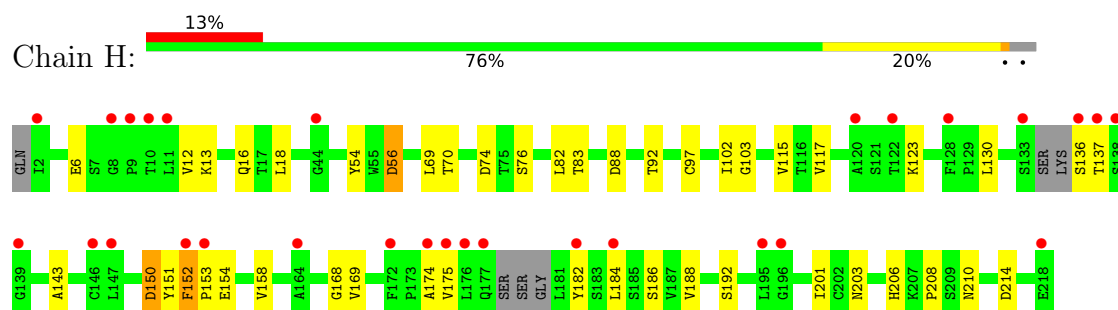
3 Residue-property plots [i](#)

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.

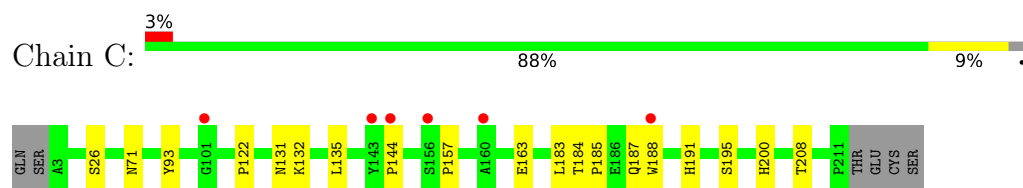
- Molecule 1: P2S-2E9 Heavy chain



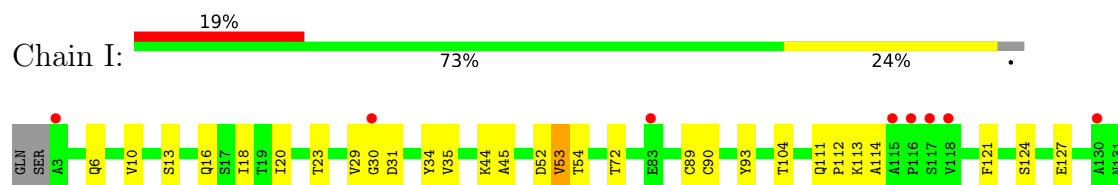
- Molecule 1: P2S-2E9 Heavy chain

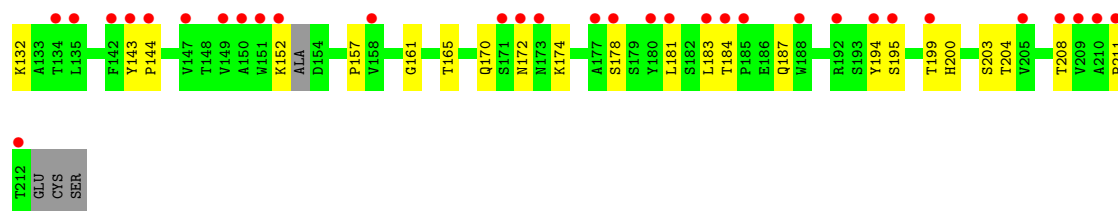


- Molecule 2: P2S-2E9 Light chain

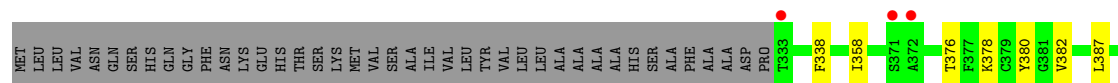


- Molecule 2: P2S-2E9 Light chain

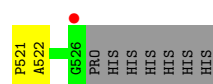
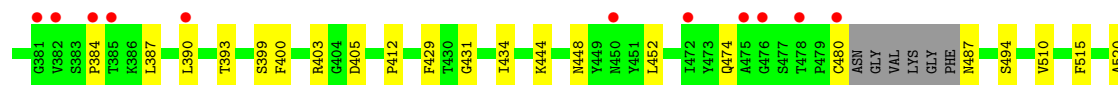
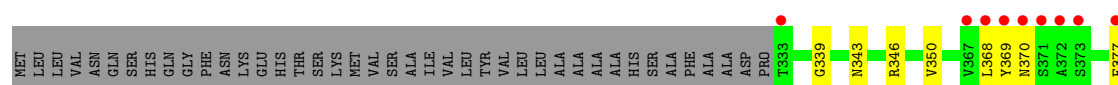




• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.95Å 70.80Å 127.80Å 90.00° 95.98° 90.00°	Depositor
Resolution (Å)	32.41 – 2.20 32.41 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.41-2.20) 99.0 (32.41-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.231 , 0.283 0.237 , 0.287	Depositor DCC
R_{free} test set	3585 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9284	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 [i](#)

5.1 Standard geometry [i](#)

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	B	0.39	0/1664	0.66	0/2268
1	H	0.36	0/1649	0.69	2/2252 (0.1%)
2	C	0.44	0/1568	0.79	0/2141
2	I	0.44	0/1562	0.70	0/2129
3	E	0.44	0/1532	0.62	1/2086 (0.0%)
3	J	0.49	0/1538	0.72	1/2094 (0.0%)
All	All	0.43	0/9513	0.70	4/12970 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	475	ALA	N-CA-C	-5.75	106.27	113.28
1	H	56	ASP	CA-C-N	-5.73	113.31	122.66
1	H	56	ASP	C-N-CA	-5.73	113.31	122.66
3	J	370	ASN	N-CA-C	-5.03	105.26	111.90

There are no chirality outliers.

There are no planarity outliers.

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	B	1627	0	1624	25	0
1	H	1610	0	1607	31	0
2	C	1532	0	1470	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1529	0	1474	35	0
3	E	1490	0	1409	14	0
3	J	1496	0	1412	18	0
All	All	9284	0	8996	129	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 7.

All (129) 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)
2:I:184:THR:HB	2:I:187:GLN:HB2	1.57	0.86
2:I:53:VAL:HG23	2:I:54:THR:HG23	1.58	0.86
3:J:444:LYS:HG2	3:J:448:ASN:HB2	1.65	0.78
1:H:92:THR:HG22	1:H:117:VAL:H	1.48	0.76
2:C:183:LEU:HD11	2:C:188:TRP:HB2	1.71	0.71
3:J:387:LEU:HA	3:J:390:LEU:HD12	1.71	0.71
1:B:127:VAL:O	1:B:215:LYS:NZ	2.24	0.70
3:J:403:ARG:NH2	3:J:405:ASP:OD2	2.27	0.68
1:B:31:THR:HG23	1:B:34:VAL:HG21	1.75	0.68
1:B:216:LYS:NZ	1:B:218:GLU:OE1	2.26	0.68
2:C:184:THR:OG1	2:C:187:GLN:HG3	1.93	0.68
1:B:54:TYR:CZ	3:E:444:LYS:HB2	2.29	0.67
1:H:158:VAL:HG11	1:H:186:SER:HB2	1.76	0.67
2:I:195:SER:OG	2:I:208:THR:HG22	1.97	0.64
1:B:177:GLN:HG2	2:C:163:GLU:OE1	1.98	0.64
1:H:136:SER:HB2	1:H:143:ALA:HB3	1.81	0.63
1:H:175:VAL:HG22	2:I:165:THR:HG22	1.81	0.62
2:C:184:THR:HG23	2:C:187:GLN:HE21	1.65	0.61
1:B:28:SER:O	1:B:31:THR:HG22	2.01	0.60
3:E:393:THR:HG23	3:E:516:GLU:HG3	1.83	0.60
1:H:103:GLY:HA2	2:I:34:TYR:CD1	2.38	0.59
2:I:113:LYS:HE2	2:I:200:HIS:CE1	2.37	0.59
2:I:114:ALA:HB3	2:I:143:TYR:H	1.68	0.59
2:I:170:GLN:HG2	2:I:174:LYS:O	2.03	0.58
2:I:52:ASP:O	2:I:53:VAL:HG22	2.02	0.58
2:C:184:THR:H	2:C:187:GLN:HE21	1.49	0.58
1:H:18:LEU:HD13	1:H:115:VAL:HG11	1.87	0.57
1:H:13:LYS:HB2	1:H:16:GLN:NE2	2.20	0.57
3:E:444:LYS:HG2	3:E:448:ASN:HB2	1.86	0.56
2:I:44:LYS:HG3	2:I:45:ALA:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:PHE:HE1	1:B:149:LYS:HE2	1.71	0.55
1:H:54:TYR:CZ	3:J:444:LYS:HB2	2.41	0.55
1:H:153:PRO:HB2	1:H:208:PRO:HG2	1.88	0.55
1:B:2:ILE:HG22	1:B:26:GLY:HA3	1.88	0.54
1:B:206:HIS:O	1:B:207:LYS:HB2	2.07	0.54
2:I:30:GLY:O	2:I:31:ASP:HB2	2.06	0.54
1:H:203:ASN:ND2	1:H:214:ASP:OD2	2.41	0.53
1:H:130:LEU:HB3	2:I:121:PHE:CD1	2.44	0.53
1:H:152:PHE:HB3	1:H:153:PRO:HD3	1.90	0.53
2:I:199:THR:OG1	2:I:204:THR:HG22	2.08	0.52
1:B:100:HIS:CE1	1:B:102:ILE:H	2.28	0.52
1:B:102:ILE:HD11	3:E:444:LYS:HA	1.91	0.52
3:J:412:PRO:HG3	3:J:429:PHE:HB3	1.92	0.52
2:C:195:SER:OG	2:C:208:THR:HG22	2.09	0.51
2:I:6:GLN:HE22	2:I:89:CYS:HA	1.75	0.51
2:I:124:SER:HB3	2:I:127:GLU:HB2	1.92	0.51
3:J:346:ARG:HD3	3:J:346:ARG:H	1.73	0.51
3:J:384:PRO:HA	3:J:387:LEU:HD12	1.93	0.51
2:I:29:VAL:HG23	2:I:93:TYR:O	2.11	0.51
2:C:184:THR:H	2:C:187:GLN:NE2	2.09	0.50
3:J:474:GLN:HG2	3:J:480:CYS:SG	2.51	0.50
3:E:403:ARG:HG2	3:E:406:GLU:CD	2.36	0.50
2:I:20:ILE:HD13	2:I:104:THR:HB	1.93	0.50
2:I:35:VAL:HG22	2:I:53:VAL:HG12	1.93	0.50
3:E:376:THR:HB	3:E:435:ALA:HB3	1.94	0.50
2:I:23:THR:HG22	2:I:72:THR:OG1	2.12	0.50
2:C:157:PRO:HD2	1:H:201:ILE:HD12	1.94	0.50
2:I:200:HIS:N	2:I:203:SER:O	2.39	0.49
1:B:156:VAL:HG12	1:B:206:HIS:CD2	2.47	0.49
3:J:487:ASN:N	3:J:487:ASN:OD1	2.45	0.49
1:B:13:LYS:HB2	1:B:16:GLN:OE1	2.12	0.49
2:I:144:PRO:HB2	2:I:200:HIS:NE2	2.28	0.49
1:B:31:THR:HG23	1:B:34:VAL:CG2	2.43	0.49
3:J:452:LEU:HD23	3:J:494:SER:HA	1.95	0.48
1:H:102:ILE:HD11	3:J:444:LYS:HA	1.94	0.48
3:E:393:THR:CG2	3:E:516:GLU:HG3	2.43	0.48
2:I:152:LYS:HD3	2:I:157:PRO:HA	1.94	0.47
2:I:183:LEU:HD21	2:I:194:TYR:CZ	2.50	0.47
1:B:89:PRO:HA	1:B:117:VAL:HB	1.97	0.47
2:C:144:PRO:HD2	2:C:200:HIS:CE1	2.50	0.47
1:H:158:VAL:HG11	1:H:186:SER:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:338:PHE:CE1	3:E:358:ILE:HD13	2.49	0.47
3:E:378:LYS:HD2	3:E:380:TYR:OH	2.15	0.47
3:E:441:LEU:HD23	3:E:509:ARG:NH2	2.30	0.46
2:I:35:VAL:HG22	2:I:53:VAL:HA	1.98	0.46
1:H:12:VAL:O	1:H:117:VAL:HA	2.15	0.46
3:J:520:ALA:HB1	3:J:521:PRO:HD2	1.96	0.46
1:H:123:LYS:NZ	1:H:150:ASP:O	2.36	0.46
2:I:13:SER:O	2:I:16:GLN:HG2	2.16	0.46
1:H:88:ASP:C	1:H:117:VAL:HG11	2.42	0.45
1:H:74:ASP:OD2	1:H:76:SER:OG	2.28	0.45
1:H:69:LEU:HD22	1:H:82:LEU:HD11	1.99	0.45
2:C:131:ASN:HA	2:C:185:PRO:HG2	1.99	0.45
3:E:382:VAL:HG21	3:E:387:LEU:HD13	1.98	0.45
3:J:377:PHE:CD1	3:J:434:ILE:HG12	2.52	0.44
1:B:168:GLY:O	1:B:188:VAL:HA	2.17	0.44
2:I:44:LYS:HG3	2:I:45:ALA:H	1.82	0.44
2:C:131:ASN:O	2:C:132:LYS:HD3	2.16	0.44
1:H:6:GLU:HG3	1:H:97:CYS:SG	2.58	0.44
1:H:210:ASN:O	1:H:210:ASN:ND2	2.51	0.43
2:I:6:GLN:NE2	2:I:90:CYS:H	2.17	0.43
1:B:159:SER:OG	1:B:203:ASN:HB2	2.19	0.43
2:I:132:LYS:HA	2:I:132:LYS:HD3	1.87	0.43
2:I:183:LEU:HD21	2:I:194:TYR:CE1	2.53	0.43
3:E:462:LYS:HA	3:E:462:LYS:HE2	2.01	0.43
1:B:52:LEU:HD21	1:B:100:HIS:CD2	2.54	0.42
2:C:26:SER:HA	2:C:71:ASN:ND2	2.34	0.42
2:C:122:PRO:HA	2:C:135:LEU:HD22	2.00	0.42
1:H:154:GLU:HG3	1:H:182:TYR:CD1	2.54	0.42
1:B:107:ASP:OD1	1:B:108:TYR:N	2.43	0.42
2:C:184:THR:HG1	2:C:187:GLN:HG3	1.81	0.42
1:H:151:TYR:O	1:H:182:TYR:N	2.48	0.42
2:I:165:THR:HG23	2:I:178:SER:O	2.18	0.42
3:J:393:THR:HA	3:J:522:ALA:HA	2.01	0.42
1:B:22:CYS:O	1:B:79:GLN:HA	2.20	0.42
2:I:10:VAL:HG22	2:I:18:ILE:HD12	2.02	0.42
1:H:70:THR:HB	1:H:83:THR:OG1	2.20	0.42
2:I:161:GLY:O	2:I:181:LEU:HA	2.20	0.42
1:H:153:PRO:HD2	1:H:206:HIS:CE1	2.55	0.42
1:H:54:TYR:O	1:H:56:ASP:O	2.38	0.42
1:H:168:GLY:O	1:H:188:VAL:HA	2.20	0.41
1:H:169:VAL:HG22	1:H:188:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:399:SER:HA	3:J:510:VAL:O	2.20	0.41
1:B:160:TRP:CH2	1:B:202:CYS:HB3	2.56	0.41
3:J:350:VAL:HG23	3:J:400:PHE:CD1	2.56	0.41
1:B:102:ILE:HA	2:C:93:TYR:OH	2.21	0.41
1:B:201:ILE:HG12	1:B:216:LYS:HA	2.01	0.41
2:I:111:GLN:HB2	2:I:143:TYR:CZ	2.56	0.41
1:B:70:THR:HB	1:B:83:THR:OG1	2.20	0.41
3:E:393:THR:HA	3:E:522:ALA:HA	2.02	0.41
1:H:137:THR:HG23	1:H:192:SER:OG	2.20	0.41
3:J:339:GLY:O	3:J:343:ASN:HB2	2.21	0.41
1:B:128:PHE:CE1	1:B:149:LYS:HE2	2.53	0.41
2:C:183:LEU:HD12	2:C:183:LEU:C	2.46	0.41
1:H:174:ALA:HB2	1:H:184:LEU:HB3	2.03	0.41
2:I:111:GLN:HA	2:I:112:PRO:HD3	1.90	0.40
2:I:170:GLN:HG3	2:I:172:ASN:OD1	2.21	0.40
3:J:431:GLY:HA2	3:J:515:PHE:CE2	2.56	0.40
3:E:393:THR:HG22	3:E:516:GLU:O	2.21	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	B	210/218 (96%)	200 (95%)	9 (4%)	1 (0%)	24	27
1	H	206/218 (94%)	192 (93%)	12 (6%)	2 (1%)	12	11
2	C	207/215 (96%)	195 (94%)	11 (5%)	1 (0%)	24	27
2	I	205/215 (95%)	191 (93%)	12 (6%)	2 (1%)	12	11
3	E	183/242 (76%)	176 (96%)	7 (4%)	0	100	100
3	J	184/242 (76%)	173 (94%)	10 (5%)	1 (0%)	24	27
All	All	1195/1350 (88%)	1127 (94%)	61 (5%)	7 (1%)	21	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	LYS
2	I	211	PRO
3	J	369	TYR
1	H	152	PHE
2	C	191	HIS
1	H	150	ASP
2	I	53	VAL

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	B	188/191 (98%)	188 (100%)	0	100	100
1	H	186/191 (97%)	186 (100%)	0	100	100
2	C	174/182 (96%)	174 (100%)	0	100	100
2	I	175/182 (96%)	175 (100%)	0	100	100
3	E	162/206 (79%)	162 (100%)	0	100	100
3	J	163/206 (79%)	162 (99%)	1 (1%)	78	89
All	All	1048/1158 (90%)	1047 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	368	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	GLN
1	B	170	HIS
2	C	40	GLN
2	C	81	GLN

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Mol	Chain	Res	Type
2	C	111	GLN
2	C	187	GLN
2	C	200	HIS
3	E	354	ASN
3	E	474	GLN
1	H	16	GLN
1	H	78	ASN
1	H	170	HIS
1	H	198	GLN
1	H	210	ASN
2	I	6	GLN
2	I	41	HIS
2	I	111	GLN
2	I	173	ASN
2	I	197	GLN
3	J	487	ASN

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 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 ⓘ

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	B	215/218 (98%)	0.57	9 (4%) 40 37	36, 53, 83, 92	0
1	H	212/218 (97%)	0.94	29 (13%) 6 5	42, 68, 84, 109	0
2	C	209/215 (97%)	0.54	6 (2%) 53 50	37, 56, 76, 86	0
2	I	209/215 (97%)	1.13	40 (19%) 3 2	40, 67, 103, 111	0
3	E	187/242 (77%)	0.44	12 (6%) 25 22	35, 49, 79, 99	0
3	J	188/242 (77%)	0.50	21 (11%) 10 8	30, 48, 84, 101	0
All	All	1220/1350 (90%)	0.69	117 (9%) 13 11	30, 56, 92, 111	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	370	ASN	6.2
3	J	526	GLY	5.0
3	J	369	TYR	4.8
3	E	526	GLY	4.4
2	I	158	VAL	4.4
2	I	188	TRP	4.2
1	H	152	PHE	4.2
2	I	180	TYR	4.2
2	I	115	ALA	4.1
1	B	195	LEU	3.7
1	H	176	LEU	3.7
3	J	371	SER	3.6
3	J	368	LEU	3.5
1	H	9	PRO	3.5
2	I	143	TYR	3.5
1	B	2	ILE	3.4
2	I	210	ALA	3.4
1	B	152	PHE	3.4
1	H	8	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	101	GLY	3.1
2	I	142	PHE	3.1
2	I	212	THR	3.0
1	B	156	VAL	3.0
1	H	175	VAL	3.0
2	I	178	SER	3.0
3	E	479	PRO	3.0
2	I	183	LEU	2.9
1	H	136	SER	2.8
2	C	143	TYR	2.8
2	I	192	ARG	2.8
2	I	144	PRO	2.8
1	H	174	ALA	2.8
2	I	117	SER	2.7
3	E	372	ALA	2.7
2	I	151	TRP	2.7
3	J	475	ALA	2.7
2	I	181	LEU	2.7
2	I	194	TYR	2.6
3	E	333	THR	2.6
3	J	367	VAL	2.6
3	J	373	SER	2.6
2	I	208	THR	2.6
1	B	134	SER	2.5
1	H	138	SER	2.5
3	J	372	ALA	2.5
2	I	177	ALA	2.5
3	E	478	THR	2.5
2	I	205	VAL	2.5
3	E	487	ASN	2.4
2	C	144	PRO	2.4
2	I	185	PRO	2.4
2	I	134	THR	2.4
3	J	333	THR	2.4
2	C	156	SER	2.4
3	J	382	VAL	2.4
2	C	188	TRP	2.4
1	H	184	LEU	2.4
1	H	139	GLY	2.4
2	C	160	ALA	2.4
1	H	10	THR	2.4
2	I	149	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	218	GLU	2.4
1	B	196	GLY	2.3
2	I	3	ALA	2.3
3	J	377	PHE	2.3
2	I	211	PRO	2.3
1	H	164	ALA	2.3
2	I	173	ASN	2.3
2	I	150	ALA	2.3
2	I	171	SER	2.3
1	H	177	GLN	2.3
2	I	209	VAL	2.3
1	H	11	LEU	2.3
1	H	195	LEU	2.3
2	I	135	LEU	2.3
3	J	450	ASN	2.3
1	H	122	THR	2.3
2	I	199	THR	2.3
3	E	371	SER	2.3
2	I	116	PRO	2.2
1	H	44	GLY	2.2
1	H	196	GLY	2.2
1	B	154	GLU	2.2
1	H	120	ALA	2.2
1	H	182	TYR	2.2
2	I	172	ASN	2.2
2	I	130	ALA	2.2
1	H	133	SER	2.2
3	E	473	TYR	2.2
2	I	118	VAL	2.2
1	H	128	PHE	2.2
3	E	489	TYR	2.2
3	E	450	ASN	2.2
3	E	476	GLY	2.2
3	J	480	CYS	2.2
2	I	83	GLU	2.1
3	J	385	THR	2.1
1	H	147	LEU	2.1
2	I	184	THR	2.1
3	J	478	THR	2.1
2	I	152	LYS	2.1
1	H	2	ILE	2.1
3	J	390	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	153	PRO	2.1
3	J	384	PRO	2.1
3	J	381	GLY	2.1
3	J	476	GLY	2.1
1	B	193	SER	2.1
1	H	146	CYS	2.1
3	E	488	CYS	2.1
3	J	472	ILE	2.1
2	I	147	VAL	2.1
1	B	101	ARG	2.1
1	H	137	THR	2.0
2	I	30	GLY	2.0
1	H	172	PHE	2.0
2	I	195	SER	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 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.