



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:34 PM UTC

PDB ID : 7X4I / pdb_00007x4i
Title : Crystal structure of nanobody aSA3 in complex with dimer SARS-CoV-1 RBD
Authors : Ma, H.; Zeng, W.H.; Jin, T.C.
Deposited on : 2022-03-02
Resolution : 3.38 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

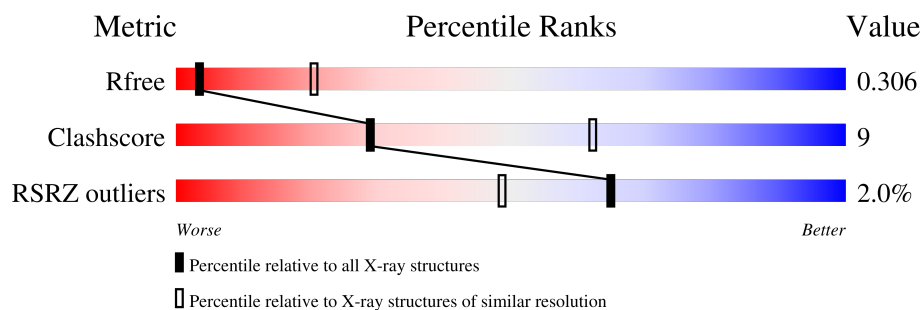
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	204	2% 72% 20% 9%
1	B	204	2% 81% 14% 5%
1	C	204	% 71% 22% 8%
1	D	204	3% 78% 14% 8%
2	E	123	% 79% 21%
2	F	123	% 71% 29%
2	G	123	2% 79% 21%

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Mol	Chain	Length	Quality of chain
2	H	123	2% 76% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9779 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1478	953	243	273	9			
1	B	194	Total	C	N	O	S	0	0	0
			1542	995	253	285	9			
1	C	188	Total	C	N	O	S	0	0	0
			1497	966	246	276	9			
1	D	187	Total	C	N	O	S	0	1	0
			1494	962	248	275	9			

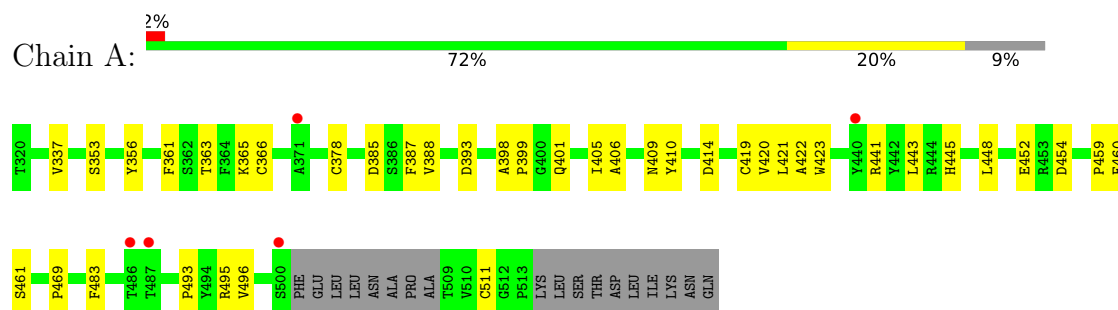
- Molecule 2 is a protein called nanobody aSA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	123	Total	C	N	O	S	0	0	0
			942	589	162	187	4			
2	F	123	Total	C	N	O	S	0	2	0
			948	593	162	189	4			
2	G	123	Total	C	N	O	S	0	2	0
			946	592	162	188	4			
2	H	121	Total	C	N	O	S	0	2	0
			932	583	161	184	4			

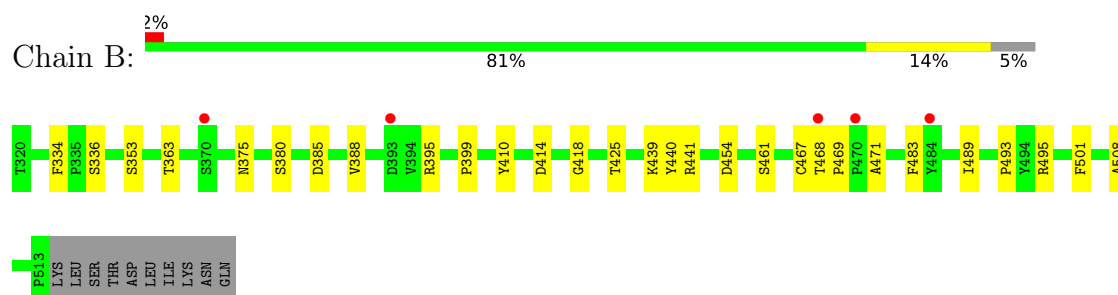
3 Residue-property plots [i](#)

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.

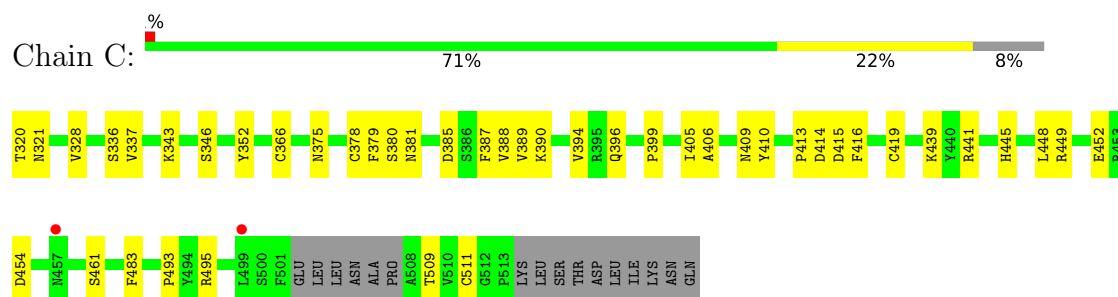
• Molecule 1: Spike glycoprotein



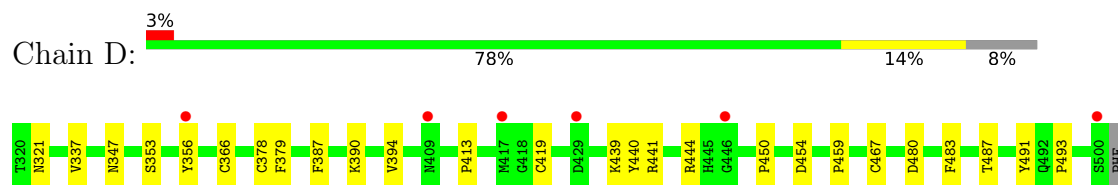
• Molecule 1: Spike glycoprotein

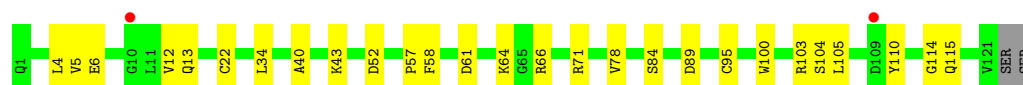


• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.70Å 112.01Å 151.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.52 – 3.38 75.52 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.0 (75.52-3.38) 99.0 (75.52-3.38)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.41Å)	Xtriage
Refinement program	PHENIX dev_2481	Depositor
R, R_{free}	0.267 , 0.321 (Not available) , 0.306	Depositor DCC
R_{free} test set	1217 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.948	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9779	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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	A	0.21	0/1524	0.39	0/2079
1	B	0.22	0/1591	0.40	0/2173
1	C	0.21	0/1544	0.39	0/2106
1	D	0.22	0/1543	0.39	0/2104
2	E	0.25	0/964	0.53	0/1306
2	F	0.25	0/975	0.52	0/1319
2	G	0.25	0/974	0.47	0/1319
2	H	0.23	0/959	0.51	0/1299
All	All	0.23	0/10074	0.44	0/13705

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 [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	1478	0	1399	24	0
1	B	1542	0	1464	21	0
1	C	1497	0	1417	27	0
1	D	1494	0	1421	17	0
2	E	942	0	880	18	0
2	F	948	0	890	30	0
2	G	946	0	886	18	0
2	H	932	0	876	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9779	0	9233	165	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 9.

All (165) 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:A:409:ASN:HD21	1:A:441:ARG:H	1.17	0.89
1:C:389:VAL:HG11	1:C:405:ILE:HD12	1.54	0.88
1:D:440:TYR:OH	2:F:115:GLN:NE2	2.13	0.81
2:G:24:ALA:HB3	2:G:76:ASN:HB3	1.63	0.78
2:H:100:TRP:HH2	2:H:110:TYR:HA	1.56	0.70
2:F:24:ALA:HB3	2:F:76:ASN:HB3	1.74	0.70
2:H:71:ARG:HB3	2:H:78:VAL:HG12	1.73	0.69
2:H:103:ARG:NH2	2:H:104:SER:O	2.28	0.67
2:E:71:ARG:HG2	2:E:78:VAL:HG12	1.76	0.67
2:G:2:VAL:HG13	2:G:26:GLY:HA3	1.77	0.66
2:G:52:ASP:OD1	2:G:56:ASN:N	2.29	0.65
1:B:440:TYR:OH	2:E:115:GLN:NE2	2.29	0.64
1:C:346:SER:OG	1:C:381:ASN:ND2	2.31	0.64
1:B:467:CYS:HB2	1:B:469:PRO:HD2	1.81	0.62
2:E:52:ASP:O	2:E:71:ARG:NH1	2.32	0.62
2:F:34:LEU:HD13	2:F:78:VAL:HG22	1.82	0.61
2:E:98:GLY:HA3	2:E:100:TRP:CZ3	2.37	0.59
1:B:363:THR:OG1	2:F:106:ASN:ND2	2.36	0.58
1:B:489:ILE:N	2:F:44:GLU:OE2	2.37	0.57
1:A:441:ARG:NH2	1:A:454:ASP:O	2.37	0.57
1:B:399:PRO:HB3	1:B:414:ASP:HA	1.87	0.57
1:B:418:GLY:HA2	1:B:501:PHE:HE2	1.71	0.56
2:E:66:ARG:NH1	2:E:84:SER:O	2.37	0.56
1:A:361:PHE:HA	1:A:423:TRP:HB3	1.87	0.56
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.87	0.56
2:F:52:ASP:OD1	2:F:56:ASN:N	2.38	0.56
1:A:363:THR:HB	1:A:422:ALA:HB3	1.88	0.55
1:B:441:ARG:NH2	1:B:454:ASP:O	2.39	0.54
1:D:441:ARG:NH2	1:D:454:ASP:O	2.41	0.54
2:F:100:TRP:HD1	2:F:102:GLY:H	1.54	0.54
2:F:100:TRP:HD1	2:F:102:GLY:N	2.06	0.54
1:B:388:VAL:HG22	1:B:495:ARG:HG2	1.90	0.53
1:D:379:PHE:O	1:D:509:THR:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:66:ARG:NH1	2:G:84:SER:O	2.42	0.53
2:E:33:ALA:HA	2:E:71:ARG:HH12	1.74	0.52
2:E:39:GLN:HB2	2:E:45:ARG:HB3	1.90	0.52
2:F:33:ALA:HA	2:F:71:ARG:HH12	1.73	0.52
1:C:385:ASP:OD2	1:C:410:TYR:OH	2.22	0.52
1:D:444:ARG:HH21	1:D:454:ASP:HB2	1.75	0.52
1:A:353:SER:HA	1:A:356:TYR:CE2	2.45	0.52
2:F:96:ALA:HB2	2:F:113:TRP:CE3	2.44	0.52
1:C:388:VAL:HG22	1:C:495:ARG:HG2	1.91	0.51
2:G:34:LEU:HD12	2:G:71:ARG:CZ	2.40	0.51
1:B:395:ARG:NE	2:F:108:PHE:O	2.43	0.51
2:E:5:VAL:O	2:E:22:CYS:HA	2.10	0.51
2:G:3:GLN:HB3	2:G:25[B]:SER:HB2	1.92	0.51
2:G:3:GLN:HB3	2:G:25[A]:SER:HB2	1.92	0.51
2:F:68:THR:O	2:F:81:GLN:N	2.34	0.51
2:F:5:VAL:O	2:F:22:CYS:HA	2.11	0.50
2:H:6:GLU:CD	2:H:115:GLN:H	2.18	0.50
1:A:448:LEU:HD22	1:A:452:GLU:HB3	1.93	0.50
1:D:366:CYS:HA	1:D:419:CYS:HA	1.94	0.50
1:B:380:SER:HA	1:B:508:ALA:HA	1.93	0.50
2:F:24:ALA:HB1	2:F:27:PHE:CE1	2.46	0.50
2:G:71:ARG:HA	2:G:78:VAL:HA	1.94	0.50
1:C:328:VAL:HG22	1:C:343:LYS:HD3	1.92	0.50
2:H:71:ARG:CB	2:H:78:VAL:HG12	2.42	0.50
2:G:1:GLN:HA	2:G:27:PHE:HE2	1.77	0.49
1:C:379:PHE:O	1:C:509:THR:N	2.45	0.49
1:D:353:SER:HA	1:D:356:TYR:CE2	2.47	0.49
1:A:366:CYS:HA	1:A:419:CYS:HA	1.95	0.49
1:A:399:PRO:HB3	1:A:414:ASP:HA	1.94	0.49
2:E:66:ARG:HH22	2:E:89:ASP:CG	2.21	0.49
2:F:100:TRP:HZ3	2:F:109:ASP:O	1.95	0.49
2:H:52:ASP:OD1	2:H:103:ARG:HA	2.13	0.48
1:C:409:ASN:ND2	1:C:441:ARG:O	2.36	0.48
1:C:378:CYS:HA	1:C:511:CYS:HA	1.95	0.48
2:F:34:LEU:HD13	2:F:78:VAL:CG2	2.42	0.48
2:H:95:CYS:O	2:H:114:GLY:N	2.46	0.48
1:D:413:PRO:HD3	1:D:450:PRO:HB3	1.95	0.48
2:G:51:ILE:HD12	2:G:56:ASN:O	2.14	0.48
1:A:459:PRO:HG3	1:A:469:PRO:HG3	1.96	0.48
2:G:51:ILE:HD12	2:G:56:ASN:C	2.38	0.48
2:E:12:VAL:HG11	2:E:18:LEU:HG	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:GLN:HB3	1:C:406:ALA:HB2	1.96	0.48
2:E:52:ASP:OD1	2:E:53:SER:N	2.45	0.48
2:H:12:VAL:HG12	2:H:13:GLN:H	1.80	0.47
1:A:337:VAL:HA	1:A:387:PHE:HB2	1.97	0.47
1:C:413:PRO:HB2	1:C:415:ASP:OD1	2.15	0.47
2:E:39:GLN:NE2	2:E:43:LYS:O	2.48	0.47
1:B:385:ASP:OD2	1:B:410:TYR:OH	2.27	0.47
1:C:337:VAL:HG22	1:C:409:ASN:HB3	1.97	0.47
1:C:396:GLN:OE1	1:C:405:ILE:HG23	2.15	0.47
2:E:6:GLU:HG3	2:E:22:CYS:HB2	1.95	0.47
2:F:104:SER:O	2:F:110:TYR:OH	2.30	0.47
2:H:66:ARG:HH22	2:H:89:ASP:CG	2.23	0.46
1:A:443:LEU:HD13	1:A:460:PHE:CD2	2.51	0.46
2:H:5:VAL:O	2:H:22:CYS:HA	2.14	0.46
2:F:75:LYS:HA	2:F:75:LYS:HD2	1.65	0.46
2:H:100:TRP:HE3	2:H:104:SER:HG	1.63	0.46
2:E:51:ILE:HG21	2:E:71:ARG:HG3	1.98	0.46
1:B:483:PHE:CE2	1:B:493:PRO:HB3	2.50	0.46
1:C:399:PRO:HB3	1:C:414:ASP:HA	1.98	0.46
2:E:96:ALA:HB2	2:E:113:TRP:CE3	2.51	0.46
1:A:483:PHE:CE2	1:A:493:PRO:HB3	2.51	0.45
1:C:320:THR:OG1	1:C:321:ASN:N	2.48	0.45
1:A:398:ALA:HB3	1:A:401:GLN:HG3	1.99	0.45
1:A:459:PRO:CG	1:A:469:PRO:HG3	2.46	0.45
1:C:413:PRO:HA	2:F:28:THR:O	2.17	0.45
1:D:337:VAL:HA	1:D:387:PHE:HB2	1.99	0.45
2:E:51:ILE:HA	2:E:57:PRO:HA	1.99	0.45
1:D:459:PRO:HB2	1:D:467:CYS:O	2.17	0.44
1:A:337:VAL:HG22	1:A:409:ASN:HB3	2.00	0.44
1:D:321:ASN:ND2	1:D:347:ASN:O	2.40	0.44
1:A:406:ALA:HA	1:A:410:TYR:O	2.18	0.44
1:B:425:THR:HG21	1:B:495:ARG:HD2	2.00	0.44
1:C:337:VAL:HA	1:C:387:PHE:HB2	1.99	0.44
2:G:58:PHE:CE2	2:G:103:ARG:HG2	2.53	0.44
1:D:356:TYR:O	2:E:103:ARG:NH2	2.50	0.44
2:F:3:GLN:HB3	2:F:25[B]:SER:HB2	2.00	0.44
2:H:4:LEU:HB2	2:H:114:GLY:HA2	1.99	0.44
1:A:393:ASP:HB3	1:A:405:ILE:HG13	2.00	0.44
1:A:363:THR:HG23	2:H:105:LEU:HG	1.99	0.43
2:H:22:CYS:HB3	2:H:78:VAL:CG2	2.48	0.43
2:H:66:ARG:NH1	2:H:84:SER:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:12:VAL:HG12	2:F:13:GLN:H	1.83	0.43
1:A:365:LYS:HG3	1:A:420:VAL:HB	2.01	0.43
2:F:11:LEU:HD11	2:F:122:SER:HB3	2.01	0.43
2:H:57:PRO:C	2:H:58:PHE:HD1	2.27	0.43
2:F:3:GLN:HB3	2:F:25[A]:SER:HB2	2.00	0.43
2:F:34:LEU:HD12	2:F:71:ARG:CZ	2.49	0.43
2:G:111:ASP:OD1	2:G:111:ASP:N	2.48	0.43
2:F:100:TRP:CZ3	2:F:109:ASP:O	2.71	0.43
2:G:100:TRP:HD1	2:G:102:GLY:N	2.15	0.43
2:F:1:GLN:HB3	2:F:2:VAL:H	1.70	0.43
1:B:336:SER:HB3	1:B:439:LYS:O	2.18	0.42
1:B:469:PRO:C	1:B:471:ALA:H	2.27	0.42
1:C:390:LYS:O	1:C:394:VAL:HG23	2.18	0.42
2:H:34:LEU:HB3	2:H:78:VAL:HG11	2.00	0.42
1:B:468:THR:N	1:B:469:PRO:CD	2.82	0.42
1:C:445:HIS:NE2	1:C:461:SER:O	2.50	0.42
1:C:399:PRO:HG3	1:C:416:PHE:HB3	2.01	0.42
1:A:445:HIS:NE2	1:A:461:SER:O	2.52	0.42
1:C:449:ARG:HG3	1:C:452:GLU:OE1	2.20	0.42
1:D:378:CYS:HA	1:D:511:CYS:HA	2.02	0.42
1:C:380:SER:O	1:C:509:THR:OG1	2.32	0.42
1:D:439:LYS:HD3	1:D:480:ASP:HB3	2.02	0.42
1:B:395:ARG:HH21	2:F:110:TYR:H	1.67	0.42
2:G:4:LEU:HD23	2:G:24:ALA:HA	2.02	0.42
2:H:61:ASP:HA	2:H:64:LYS:HG3	2.02	0.42
1:C:441:ARG:NH2	1:C:454:ASP:O	2.52	0.41
1:C:448:LEU:HD22	1:C:452:GLU:HB3	2.02	0.41
1:D:487:THR:HB	1:D:491:TYR:HB2	2.01	0.41
1:C:336:SER:HB3	1:C:439:LYS:O	2.21	0.41
1:C:366:CYS:HA	1:C:419:CYS:HA	2.02	0.41
1:C:483:PHE:CE2	1:C:493:PRO:HB3	2.54	0.41
2:G:96:ALA:HB2	2:G:113:TRP:CZ3	2.56	0.41
2:H:40:ALA:HB3	2:H:43:LYS:HD3	2.01	0.41
1:B:353:SER:HB3	1:B:375:ASN:ND2	2.35	0.41
1:A:385:ASP:OD2	1:A:410:TYR:OH	2.23	0.41
1:D:483:PHE:CE2	1:D:493:PRO:HB3	2.55	0.41
1:D:390:LYS:O	1:D:394:VAL:HG23	2.20	0.41
1:B:353:SER:N	1:B:375:ASN:OD1	2.54	0.41
2:E:104:SER:O	2:E:110:TYR:OH	2.25	0.41
1:B:334:PHE:HB3	1:B:388:VAL:HG23	2.03	0.41
2:G:68:THR:O	2:G:81:GLN:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:SER:HA	2:F:82:MET:O	2.20	0.41
1:B:461:SER:HB3	1:B:467:CYS:SG	2.61	0.40
1:C:352:TYR:N	1:C:375:ASN:OD1	2.54	0.40
1:D:353:SER:HA	1:D:356:TYR:CZ	2.56	0.40
2:G:51:ILE:HG12	2:G:71:ARG:HG3	2.03	0.40
1:A:378:CYS:HA	1:A:511:CYS:HA	2.02	0.40
1:A:421:LEU:O	1:A:496:VAL:HA	2.21	0.40
2:F:52:ASP:O	2:F:71:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 [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	186/204 (91%)	0.41	5 (2%)	56 41	73, 95, 145, 155	0
1	B	194/204 (95%)	0.39	5 (2%)	57 42	72, 95, 141, 147	0
1	C	188/204 (92%)	0.45	2 (1%)	78 64	84, 101, 137, 153	0
1	D	187/204 (91%)	0.35	6 (3%)	50 36	54, 96, 137, 148	1 (0%)
2	E	123/123 (100%)	0.35	1 (0%)	82 70	76, 90, 105, 117	0
2	F	123/123 (100%)	0.34	1 (0%)	82 70	64, 94, 105, 118	2 (1%)
2	G	123/123 (100%)	0.32	3 (2%)	59 44	54, 100, 114, 122	2 (1%)
2	H	121/123 (98%)	0.35	2 (1%)	69 53	59, 104, 114, 120	2 (1%)
All	All	1245/1308 (95%)	0.37	25 (2%)	65 49	54, 97, 137, 155	7 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	54	ASP	3.6
1	B	393	ASP	3.3
2	G	50	CYS	3.2
1	D	356	TYR	3.1
2	H	10	GLY	3.1
1	A	486	THR	3.1
1	D	429	ASP	2.9
2	H	109	ASP	2.8
1	D	417	MET	2.7
1	A	440	TYR	2.5
1	D	446	GLY	2.5
2	G	28	THR	2.3
1	A	487	THR	2.3
1	A	500	SER	2.3
1	B	370	SER	2.2
1	B	468	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	10	GLY	2.2
1	B	484	TYR	2.1
1	C	499	LEU	2.1
2	F	99	LEU	2.1
1	C	457	ASN	2.1
1	D	500	SER	2.1
1	A	371	ALA	2.1
1	D	409	ASN	2.0
1	B	470	PRO	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.