Full wwPDB X-ray Structure Validation Report ⓘ

Jul 2, 2024 – 08:16 PM JST

PDB ID	:	8XK2
Title	:	A neutralizing nanobody VHH60 against wt SARS-CoV-2
Authors	:	Lu, Y.; Guo, H.; Ji, X.; Yang, H.
Deposited on	:	2023-12-22
Resolution	:	3.40 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:

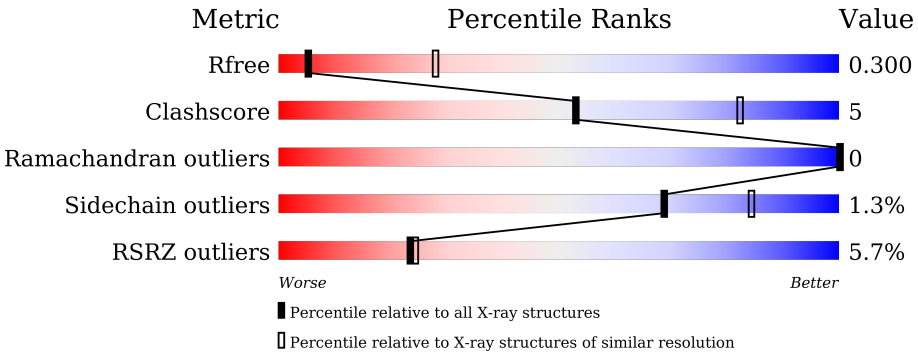
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	219	2% 83% 12%
1	C	219	4% 77% 8% 14%
1	E	219	9% 72% 6% 21%
1	G	219	5% 68% 8% 24%
2	B	121	3% 87% 13%
2	D	121	8% 81% 18%

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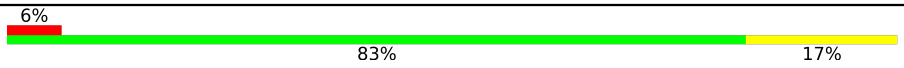
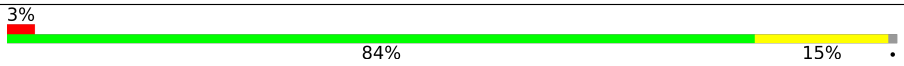
Mol	Chain	Length	Quality of chain
2	F	121	
2	H	121	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18253 atoms, of which 8847 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 protein S1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	193	Total	C	H	N	O	S	0	0	0
			2932	973	1419	249	284	7			
1	C	188	Total	C	H	N	O	S	0	0	0
			2862	947	1386	245	278	6			
1	E	172	Total	C	H	N	O	S	0	0	0
			2663	881	1291	229	256	6			
1	G	167	Total	C	H	N	O	S	0	0	0
			2579	851	1250	224	248	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	532	LEU	-	expression tag	UNP P0DTC2
A	533	GLU	-	expression tag	UNP P0DTC2
A	534	VAL	-	expression tag	UNP P0DTC2
A	535	LEU	-	expression tag	UNP P0DTC2
A	536	PHE	-	expression tag	UNP P0DTC2
A	537	GLN	-	expression tag	UNP P0DTC2
C	532	LEU	-	expression tag	UNP P0DTC2
C	533	GLU	-	expression tag	UNP P0DTC2
C	534	VAL	-	expression tag	UNP P0DTC2
C	535	LEU	-	expression tag	UNP P0DTC2
C	536	PHE	-	expression tag	UNP P0DTC2
C	537	GLN	-	expression tag	UNP P0DTC2
E	532	LEU	-	expression tag	UNP P0DTC2
E	533	GLU	-	expression tag	UNP P0DTC2
E	534	VAL	-	expression tag	UNP P0DTC2
E	535	LEU	-	expression tag	UNP P0DTC2
E	536	PHE	-	expression tag	UNP P0DTC2
E	537	GLN	-	expression tag	UNP P0DTC2
G	532	LEU	-	expression tag	UNP P0DTC2
G	533	GLU	-	expression tag	UNP P0DTC2
G	534	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	535	LEU	-	expression tag	UNP P0DTC2
G	536	PHE	-	expression tag	UNP P0DTC2
G	537	GLN	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called VHH60 nanobody.

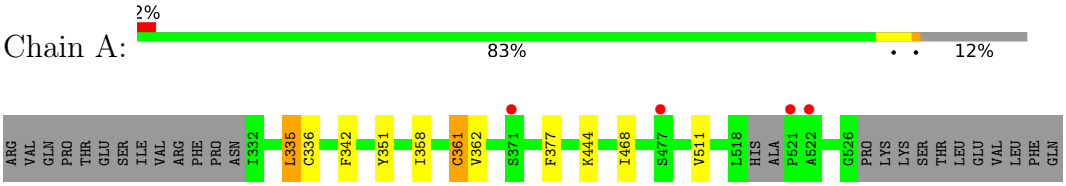
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	121	Total	C	H	N	O	S	0	0	0
			1822	585	886	163	183	5			
2	D	120	Total	C	H	N	O	S	0	0	0
			1788	577	866	159	181	5			
2	F	121	Total	C	H	N	O	S	0	0	0
			1806	582	875	160	184	5			
2	H	120	Total	C	H	N	O	S	0	0	0
			1801	580	874	162	180	5			

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.

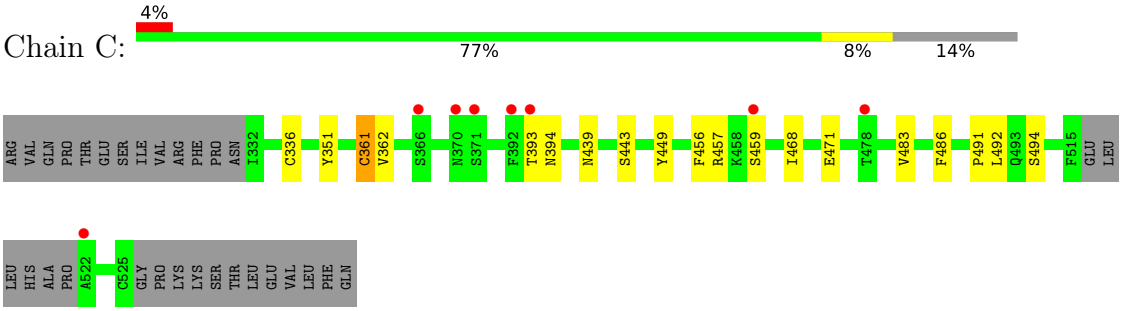
• Molecule 1: Spike protein S1

Chain A:



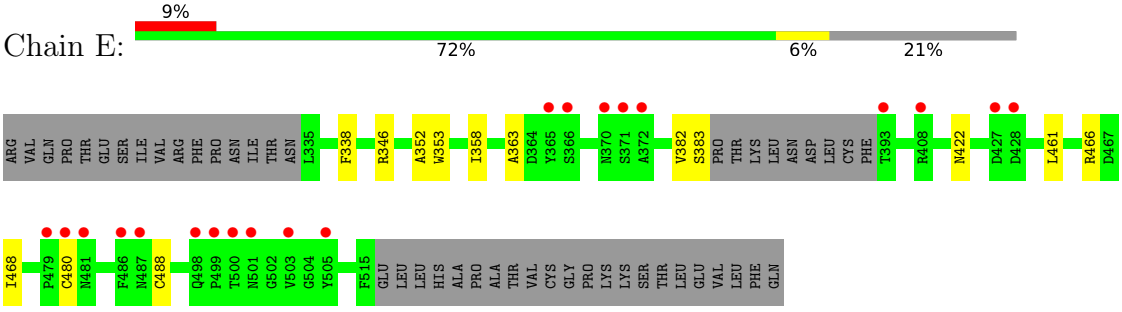
• Molecule 1: Spike protein S1

Chain C:



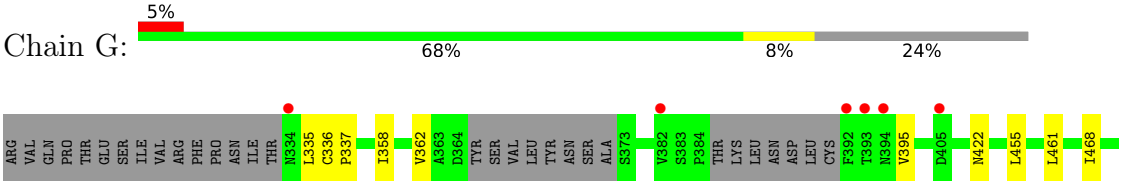
• Molecule 1: Spike protein S1

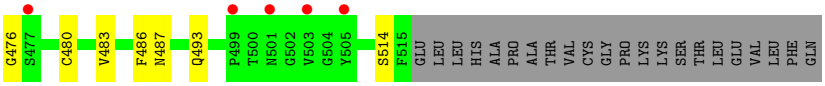
Chain E:



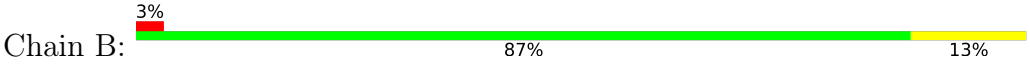
• Molecule 1: Spike protein S1

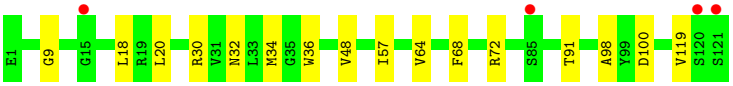
Chain G:



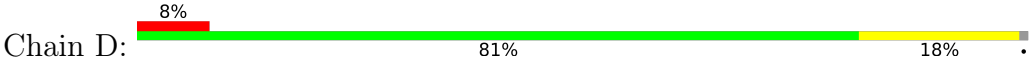


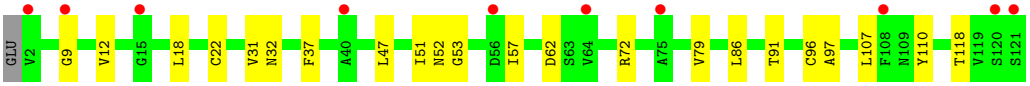
• Molecule 2: VHH60 nanobody



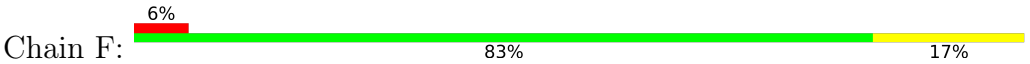


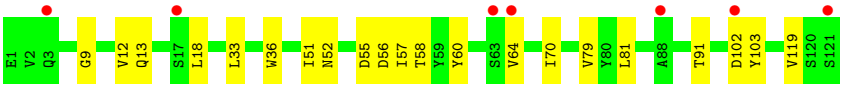
• Molecule 2: VHH60 nanobody



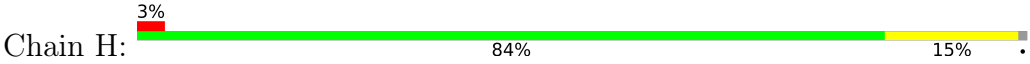


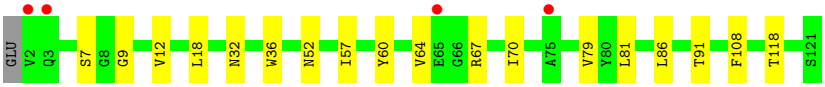
• Molecule 2: VHH60 nanobody





• Molecule 2: VHH60 nanobody





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	80.85Å 100.61Å 227.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.21 – 3.40 31.21 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.21-3.40) 99.8 (31.21-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.256 , 0.300 0.259 , 0.300	Depositor DCC
R_{free} test set	1998 reflections (7.62%)	wwPDB-VP
Wilson B-factor (Å^2)	60.3	Xtriage
Anisotropy	0.900	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	18253	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0/1554	0.51	0/2114
1	C	0.29	0/1515	0.52	0/2061
1	E	0.26	0/1410	0.49	0/1915
1	G	0.29	0/1365	0.53	0/1852
2	B	0.29	0/955	0.56	0/1292
2	D	0.30	0/941	0.55	0/1273
2	F	0.29	0/950	0.55	0/1285
2	H	0.33	0/946	0.59	0/1279
All	All	0.29	0/9636	0.53	0/13071

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	1513	1419	1419	9	0
1	C	1476	1386	1386	14	0
1	E	1372	1291	1291	10	0
1	G	1329	1250	1249	12	0
2	B	936	886	886	10	0
2	D	922	866	866	16	0
2	F	931	875	875	23	0
2	H	927	874	874	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9406	8847	8846	98	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 5.

All (98) 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:336:CYS:N	1:A:361:CYS:SG	2.54	0.81
1:C:336:CYS:N	1:C:361:CYS:SG	2.54	0.80
1:C:361:CYS:SG	1:C:362:VAL:N	2.54	0.80
2:B:91:THR:HG22	2:B:119:VAL:H	1.47	0.79
1:A:361:CYS:SG	1:A:362:VAL:N	2.57	0.78
2:F:51:ILE:HG22	2:F:58:THR:HG22	1.67	0.76
1:G:468:ILE:HD13	2:H:57:ILE:HG21	1.68	0.75
1:E:468:ILE:HD11	2:F:57:ILE:HG23	1.72	0.71
2:B:32:ASN:OD1	2:B:72:ARG:NH1	2.24	0.70
1:E:468:ILE:HD11	2:F:57:ILE:CG2	2.23	0.68
2:H:64:VAL:HG12	2:H:64:VAL:O	1.95	0.66
1:G:468:ILE:CD1	2:H:57:ILE:HG21	2.28	0.64
1:E:353:TRP:O	1:E:466:ARG:NH1	2.31	0.62
2:B:9:GLY:HA2	2:B:18:LEU:HD21	1.81	0.62
2:F:102:ASP:OD1	2:F:103:TYR:N	2.33	0.61
2:F:55:ASP:HB3	2:F:57:ILE:HD12	1.83	0.59
1:G:455:LEU:HD11	1:G:493:GLN:HG3	1.85	0.59
1:C:439:ASN:O	1:C:443:SER:OG	2.22	0.58
2:D:52:ASN:OD1	2:D:53:GLY:N	2.38	0.56
2:B:34:MET:SD	2:B:72:ARG:NH1	2.79	0.56
1:C:393:THR:HG23	1:C:394:ASN:H	1.70	0.56
2:D:9:GLY:HA2	2:D:18:LEU:HD21	1.87	0.56
1:G:455:LEU:HD11	1:G:493:GLN:CG	2.36	0.56
1:G:358:ILE:O	1:G:395:VAL:CG1	2.54	0.55
2:F:51:ILE:HD11	2:F:79:VAL:HG23	1.89	0.55
1:C:393:THR:HG23	1:C:394:ASN:N	2.22	0.55
2:F:64:VAL:HG23	2:F:64:VAL:O	2.07	0.54
2:F:51:ILE:CG2	2:F:58:THR:HG22	2.36	0.54
2:H:60:TYR:CE1	2:H:70:ILE:HG22	2.44	0.53
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.90	0.53
2:H:36:TRP:CG	2:H:81:LEU:HD22	2.43	0.53
2:H:36:TRP:CZ3	2:H:79:VAL:HG22	2.44	0.53
1:C:471:GLU:CD	2:D:47:LEU:HD12	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:VAL:HG21	2:D:86:LEU:HD13	1.92	0.50
2:H:91:THR:HG23	2:H:118:THR:HA	1.94	0.50
1:A:362:VAL:O	1:A:362:VAL:HG23	2.13	0.49
2:H:36:TRP:HZ3	2:H:79:VAL:HG22	1.77	0.49
2:B:64:VAL:HG11	2:B:68:PHE:CG	2.48	0.48
1:A:335:LEU:O	1:A:335:LEU:HD12	2.13	0.48
1:C:492:LEU:O	2:D:107:LEU:HD12	2.13	0.48
1:A:342:PHE:CZ	1:A:511:VAL:HG11	2.50	0.47
1:E:422:ASN:N	1:E:461:LEU:HD12	2.30	0.47
2:F:91:THR:HG22	2:F:119:VAL:H	1.80	0.47
1:A:444:LYS:HA	2:F:102:ASP:OD2	2.14	0.47
2:H:64:VAL:O	2:H:64:VAL:CG1	2.62	0.46
2:F:51:ILE:HG23	2:F:70:ILE:HG23	1.97	0.46
1:G:395:VAL:HA	1:G:514:SER:O	2.16	0.46
1:C:468:ILE:HD11	2:D:57:ILE:HG21	1.98	0.46
1:G:337:PRO:HD2	1:G:358:ILE:HG23	1.97	0.46
2:F:33:LEU:HD12	2:F:51:ILE:O	2.16	0.46
2:D:22:CYS:SG	2:D:79:VAL:CG1	3.04	0.45
2:B:36:TRP:O	2:B:48:VAL:HG12	2.17	0.45
1:E:358:ILE:HG22	1:E:358:ILE:O	2.16	0.45
1:E:468:ILE:HD11	2:F:57:ILE:HG21	1.99	0.45
1:G:362:VAL:HG23	1:G:362:VAL:O	2.16	0.45
1:A:468:ILE:HG21	2:B:57:ILE:HD11	2.00	0.44
1:C:457:ARG:NH1	1:C:459:SER:O	2.50	0.44
2:F:91:THR:HG22	2:F:119:VAL:N	2.32	0.44
2:H:36:TRP:HH2	2:H:79:VAL:C	2.21	0.43
2:D:12:VAL:HG21	2:D:86:LEU:CD1	2.47	0.43
2:F:60:TYR:CE1	2:F:70:ILE:HG22	2.54	0.43
2:B:30:ARG:N	2:B:100:ASP:OD1	2.49	0.43
2:H:9:GLY:HA2	2:H:18:LEU:HD21	2.00	0.43
1:C:483:VAL:O	1:C:483:VAL:HG23	2.19	0.43
2:H:36:TRP:CH2	2:H:79:VAL:HG13	2.54	0.43
1:E:382:VAL:HG12	1:E:383:SER:N	2.33	0.42
2:B:20:LEU:N	2:B:20:LEU:HD12	2.34	0.42
1:E:338:PHE:HE2	1:E:363:ALA:HB1	1.83	0.42
2:H:64:VAL:HG13	2:H:67:ARG:HH11	1.84	0.42
1:A:336:CYS:SG	1:A:358:ILE:HG23	2.60	0.42
2:D:97:ALA:HA	2:D:110:TYR:O	2.20	0.42
1:C:456:PHE:CE1	1:C:491:PRO:HA	2.55	0.42
2:F:12:VAL:HG12	2:F:13:GLN:H	1.83	0.42
1:G:476:GLY:HA3	1:G:487:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:480:CYS:O	1:G:483:VAL:HG12	2.19	0.42
2:F:36:TRP:CD1	2:F:81:LEU:HB2	2.55	0.42
2:F:52:ASN:O	2:F:56:ASP:N	2.53	0.42
2:D:91:THR:HG23	2:D:118:THR:HA	2.02	0.42
2:F:55:ASP:CB	2:F:57:ILE:HD12	2.50	0.42
1:A:358:ILE:O	1:A:358:ILE:HG22	2.19	0.41
2:H:32:ASN:O	2:H:32:ASN:OD1	2.38	0.41
2:H:52:ASN:O	2:H:52:ASN:OD1	2.39	0.41
1:G:335:LEU:HD23	1:G:336:CYS:N	2.35	0.41
2:D:51:ILE:HG23	2:D:72:ARG:HH21	1.85	0.41
2:H:64:VAL:HG13	2:H:67:ARG:NH1	2.35	0.41
1:C:449:TYR:O	1:C:494:SER:OG	2.30	0.41
2:D:37:PHE:CE2	2:D:47:LEU:HD22	2.55	0.41
2:B:34:MET:HG2	2:B:98:ALA:HA	2.02	0.41
2:F:51:ILE:HG23	2:F:70:ILE:CG2	2.51	0.41
1:E:352:ALA:HB1	2:F:57:ILE:HD13	2.02	0.41
2:F:12:VAL:HG12	2:F:13:GLN:N	2.36	0.41
2:D:12:VAL:CG1	2:D:18:LEU:HD22	2.51	0.40
2:F:9:GLY:HA2	2:F:18:LEU:HD21	2.03	0.40
1:C:468:ILE:CD1	2:D:57:ILE:HG21	2.51	0.40
2:D:31:VAL:HG12	2:D:32:ASN:N	2.36	0.40
1:E:480:CYS:HG	1:E:488:CYS:CB	2.35	0.40
1:C:471:GLU:HA	2:D:47:LEU:CD1	2.51	0.40
1:G:422:ASN:N	1:G:461:LEU:HD12	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	189/219 (86%)	179 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	184/219 (84%)	172 (94%)	12 (6%)	0	100	100
1	E	168/219 (77%)	159 (95%)	9 (5%)	0	100	100
1	G	161/219 (74%)	150 (93%)	11 (7%)	0	100	100
2	B	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
2	D	118/121 (98%)	115 (98%)	3 (2%)	0	100	100
2	F	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
2	H	118/121 (98%)	112 (95%)	6 (5%)	0	100	100
All	All	1176/1360 (86%)	1116 (95%)	60 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	A	161/192 (84%)	157 (98%)	4 (2%)	47	72
1	C	158/192 (82%)	155 (98%)	3 (2%)	57	78
1	E	147/192 (77%)	146 (99%)	1 (1%)	84	92
1	G	143/192 (74%)	142 (99%)	1 (1%)	84	92
2	B	97/98 (99%)	97 (100%)	0	100	100
2	D	95/98 (97%)	93 (98%)	2 (2%)	53	76
2	F	96/98 (98%)	96 (100%)	0	100	100
2	H	95/98 (97%)	93 (98%)	2 (2%)	53	76
All	All	992/1160 (86%)	979 (99%)	13 (1%)	69	84

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	LEU
1	A	351	TYR

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Mol	Chain	Res	Type
1	A	361	CYS
1	A	377	PHE
1	C	351	TYR
1	C	361	CYS
1	C	486	PHE
2	D	62	ASP
2	D	96	CYS
1	E	346	ARG
1	G	486	PHE
2	H	7	SER
2	H	108	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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, 95^{th} 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	193/219 (88%)	0.36	4 (2%)	63	62	47, 60, 101, 252	0
1	C	188/219 (85%)	0.58	8 (4%)	35	35	51, 65, 106, 212	0
1	E	172/219 (78%)	0.68	20 (11%)	4	5	61, 81, 132, 175	0
1	G	167/219 (76%)	0.54	11 (6%)	18	20	53, 74, 96, 148	0
2	B	121/121 (100%)	0.43	4 (3%)	46	45	50, 66, 102, 119	0
2	D	120/121 (99%)	0.68	10 (8%)	11	13	61, 80, 107, 136	0
2	F	121/121 (100%)	0.42	7 (5%)	23	24	57, 73, 101, 132	0
2	H	120/121 (99%)	0.41	4 (3%)	46	45	54, 68, 100, 123	0
All	All	1202/1360 (88%)	0.51	68 (5%)	23	24	47, 72, 107, 252	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	522	ALA	4.6
1	C	522	ALA	4.6
1	C	371	SER	4.4
1	E	481	ASN	4.3
1	E	371	SER	4.1
1	C	370	ASN	4.1
1	E	366	SER	4.0
2	B	15	GLY	3.9
1	E	370	ASN	3.8
1	C	393	THR	3.6
1	G	382	VAL	3.6
1	A	371	SER	3.6
2	D	120	SER	3.5
1	G	499	PRO	3.3
1	G	393	THR	3.3
2	F	3	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	121	SER	3.2
1	C	478	THR	3.1
2	D	121	SER	3.1
1	E	499	PRO	3.0
2	D	9	GLY	3.0
2	H	65	GLU	2.9
1	E	486	PHE	2.9
1	G	477	SER	2.9
1	E	365	TYR	2.7
1	E	427	ASP	2.7
1	C	366	SER	2.7
1	G	334	ASN	2.7
1	G	503	VAL	2.7
1	E	480	CYS	2.6
1	E	503	VAL	2.6
2	F	64	VAL	2.6
2	B	120	SER	2.6
1	A	521	PRO	2.5
2	F	63	SER	2.5
2	H	2	VAL	2.4
1	G	501	ASN	2.4
2	F	88	ALA	2.4
1	G	394	ASN	2.3
1	G	392	PHE	2.3
2	B	85	SER	2.3
1	E	500	THR	2.3
1	E	372	ALA	2.3
1	E	479	PRO	2.2
2	D	75	ALA	2.2
2	D	40	ALA	2.2
1	E	501	ASN	2.2
2	F	17	SER	2.2
2	D	15	GLY	2.2
2	D	64	VAL	2.2
1	C	392	PHE	2.1
1	C	459	SER	2.1
1	E	487	ASN	2.1
1	E	428	ASP	2.1
2	H	3	GLN	2.1
1	A	477	SER	2.1
2	D	108	PHE	2.1
1	E	393	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	505	TYR	2.0
2	F	102	ASP	2.0
2	F	121	SER	2.0
1	E	498	GLN	2.0
1	G	405	ASP	2.0
2	D	2	VAL	2.0
1	E	408	ARG	2.0
1	G	505	TYR	2.0
2	D	56	ASP	2.0
2	H	75	ALA	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.