



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:31 PM UTC

PDB ID : 2GHW / pdb_00002ghw
Title : Crystal structure of SARS spike protein receptor binding domain in complex with a neutralizing antibody, 80R
Authors : Hwang, W.C.; Lin, Y.; Santelli, E.; Sui, J.; Jaroszewski, L.; Stec, B.; Farzan, M.; Marasco, W.A.; Liddington, R.C.
Deposited on : 2006-03-27
Resolution : 2.30 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

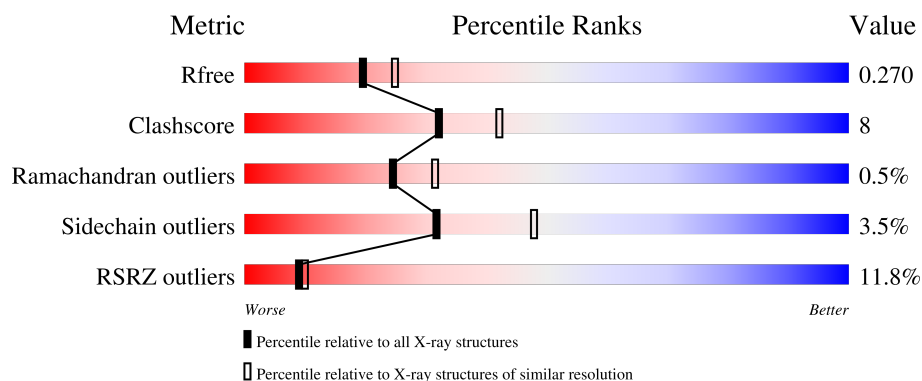
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	203	17% 80% 13% 6%
1	C	203	14% 79% 12% 7%
2	B	247	7% 75% 17% 6%
2	D	247	7% 76% 16% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	517	-	-	X	-
3	CL	A	88	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7089 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	191	Total	C	N	O	S	0	0	0
			1528	989	248	283	8			
1	C	188	Total	C	N	O	S	0	0	0
			1512	978	246	280	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	314	MET	-	cloning artifact	UNP P59594
C	315	ALA	-	cloning artifact	UNP P59594
C	316	ASP	-	cloning artifact	UNP P59594
C	511	SER	-	cloning artifact	UNP P59594
C	512	GLY	-	cloning artifact	UNP P59594
C	513	LEU	-	cloning artifact	UNP P59594
C	514	VAL	-	cloning artifact	UNP P59594
C	515	PRO	-	cloning artifact	UNP P59594
C	516	ARG	-	cloning artifact	UNP P59594
A	314	MET	-	cloning artifact	UNP P59594
A	315	ALA	-	cloning artifact	UNP P59594
A	316	ASP	-	cloning artifact	UNP P59594
A	511	SER	-	cloning artifact	UNP P59594
A	512	GLY	-	cloning artifact	UNP P59594
A	513	LEU	-	cloning artifact	UNP P59594
A	514	VAL	-	cloning artifact	UNP P59594
A	515	PRO	-	cloning artifact	UNP P59594
A	516	ARG	-	cloning artifact	UNP P59594

- Molecule 2 is a protein called anti-sars scFv antibody, 80R.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	232	Total	C	N	O	S	0	0	0
			1785	1118	312	349	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	231	Total	C	N	O	S	0	0	0
			1789	1120	314	349	6			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		
3	C	1	Total	Cl	0	0
			1	1		

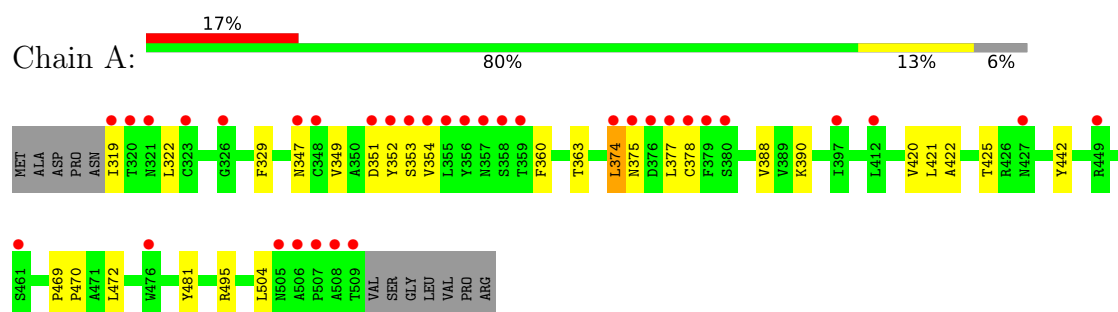
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	118	Total	O	0	0
			118	118		
4	C	115	Total	O	0	0
			115	115		
4	D	129	Total	O	0	0
			129	129		

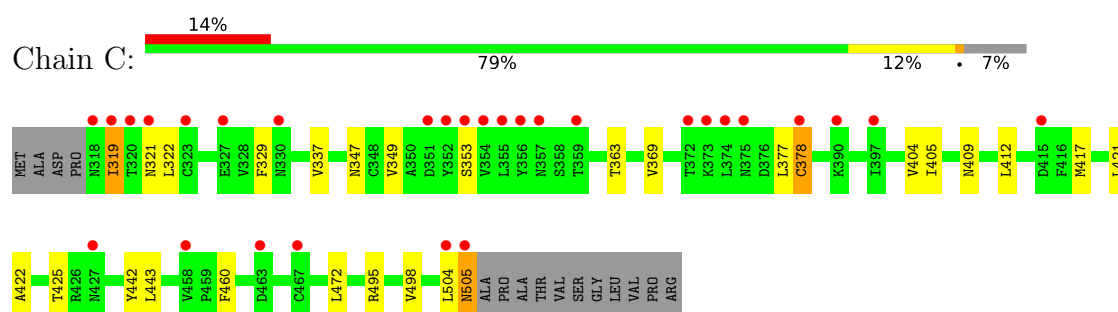
3 Residue-property plots [i](#)

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.

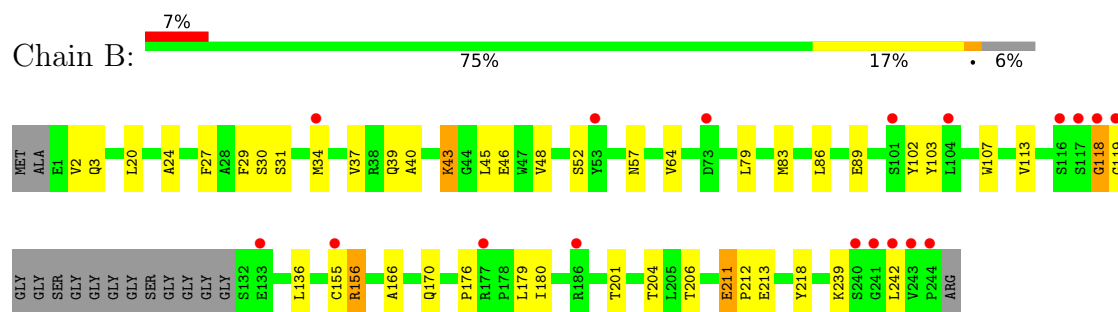
- Molecule 1: Spike glycoprotein



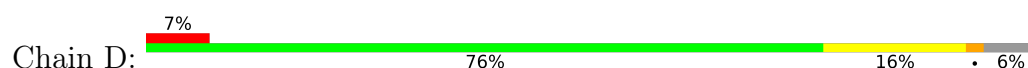
- Molecule 1: Spike glycoprotein

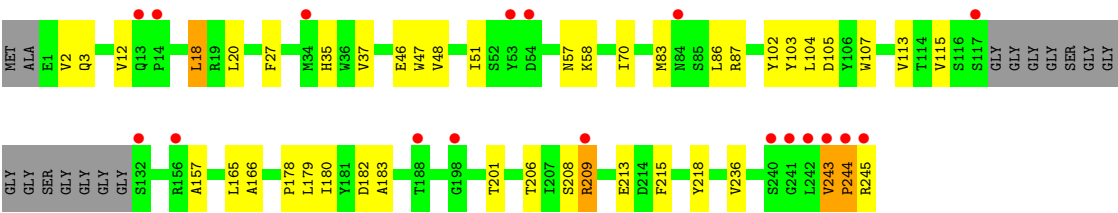


- Molecule 2: anti-sars scFv antibody, 80R



- Molecule 2: anti-sars scFv antibody, 80R





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.45Å 175.90Å 67.56Å 90.00° 96.55° 90.00°	Depositor
Resolution (Å)	45.55 – 2.30 45.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.8 (45.55-2.30) 93.8 (45.55-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.248 , 0.295 0.263 , 0.270	Depositor DCC
R_{free} test set	2617 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	1.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.8	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	0.88	EDS
Total number of atoms	7089	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.61% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.64	1/1576 (0.1%)	0.79	1/2152 (0.0%)
1	C	0.60	0/1559	0.77	0/2127
2	B	0.56	0/1827	0.71	0/2481
2	D	0.57	0/1831	0.71	1/2485 (0.0%)
All	All	0.59	1/6793 (0.0%)	0.74	2/9245 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	PRO	CA-C	6.76	1.55	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	PHE	N-CA-C	5.53	118.82	111.75
2	D	48	VAL	CB-CA-C	-5.18	107.31	111.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	102	TYR	Peptide
2	D	102	TYR	Peptide

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	1528	0	1455	27	0
1	C	1512	0	1439	20	0
2	B	1785	0	1722	28	0
2	D	1789	0	1729	28	0
3	A	4	0	0	5	0
3	C	1	0	0	1	0
4	A	108	0	0	4	0
4	B	118	0	0	2	0
4	C	115	0	0	0	0
4	D	129	0	0	1	0
All	All	7089	0	6345	103	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 8.

All (103) 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:C:369:VAL:HG22	1:C:417:MET:HE3	1.61	0.81
2:B:39:GLN:HE22	2:B:170:GLN:HE22	1.31	0.77
1:A:472:LEU:HD13	2:B:206:THR:HG21	1.67	0.75
3:A:88:CL:CL	4:B:411:HOH:O	2.42	0.75
2:B:40:ALA:HB3	2:B:43:LYS:HG2	1.71	0.72
1:A:322:LEU:HD12	1:A:349:VAL:CG2	2.20	0.72
2:D:35:HIS:HD2	2:D:47:TRP:HE1	1.35	0.72
3:A:246:CL:CL	4:A:596:HOH:O	2.48	0.69
2:D:83:MET:HE1	2:D:113:VAL:HG21	1.73	0.69
3:A:517:CL:CL	4:A:567:HOH:O	2.48	0.69
2:D:243:VAL:HB	2:D:244:PRO:HD3	1.75	0.68
3:C:20:CL:CL	4:D:291:HOH:O	2.48	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:LEU:HG	2:B:83:MET:HE2	1.75	0.68
1:A:347:ASN:HD22	1:A:504:LEU:HD11	1.61	0.63
1:A:329:PHE:CZ	1:A:421:LEU:HD22	2.36	0.61
2:B:39:GLN:NE2	2:B:170:GLN:HE22	1.99	0.60
2:B:2:VAL:HG13	2:B:27:PHE:CD2	2.39	0.57
2:D:20:LEU:CD1	2:D:83:MET:HE2	2.34	0.57
1:C:319:ILE:CD1	1:C:377:LEU:HD13	2.34	0.56
1:A:319:ILE:HA	1:A:322:LEU:HD13	1.87	0.56
2:B:39:GLN:HE22	2:B:170:GLN:NE2	2.03	0.56
2:D:12:VAL:HG21	2:D:86:LEU:HD23	1.88	0.55
1:C:472:LEU:HD13	2:D:206:THR:HG21	1.88	0.55
1:A:363:THR:HB	1:A:422:ALA:HB3	1.89	0.55
3:A:88:CL:CL	2:B:31:SER:O	2.63	0.54
2:D:83:MET:HB2	2:D:86:LEU:HD11	1.90	0.54
1:C:369:VAL:H	1:C:417:MET:HE3	1.72	0.54
2:D:12:VAL:HG11	2:D:18:LEU:HD23	1.89	0.54
1:C:425:THR:HG21	1:C:495:ARG:HD2	1.90	0.54
2:B:136:LEU:HD22	2:B:155:CYS:SG	2.48	0.53
3:A:517:CL:CL	4:A:595:HOH:O	2.56	0.53
2:D:103:TYR:CD2	2:D:166:ALA:HB2	2.43	0.52
2:B:83:MET:HE1	2:B:113:VAL:HG21	1.91	0.52
2:B:156:ARG:HH11	2:B:156:ARG:HG2	1.75	0.51
1:A:374:LEU:O	1:A:374:LEU:HD12	2.10	0.51
2:D:182:ASP:O	2:D:183:ALA:HB3	2.11	0.51
1:A:351:ASP:OD2	1:A:354:VAL:HG23	2.10	0.51
2:B:37:VAL:HG13	2:B:46:GLU:O	2.11	0.50
1:A:349:VAL:HB	1:A:377:LEU:HD23	1.94	0.50
2:D:83:MET:CB	2:D:86:LEU:HD11	2.41	0.50
1:A:349:VAL:HG21	1:A:377:LEU:HD21	1.93	0.49
1:C:425:THR:HG21	1:C:495:ARG:HG3	1.95	0.49
2:D:179:LEU:HD11	2:D:218:TYR:CE2	2.47	0.49
1:A:319:ILE:O	1:A:319:ILE:HG22	2.12	0.49
1:A:425:THR:HG21	1:A:495:ARG:HG3	1.95	0.49
2:B:40:ALA:HB3	2:B:43:LYS:CG	2.42	0.48
1:C:329:PHE:CZ	1:C:421:LEU:HD22	2.48	0.48
1:C:322:LEU:HD23	1:C:349:VAL:HB	1.94	0.48
1:A:442:TYR:HD2	4:A:526:HOH:O	1.96	0.47
1:C:404:VAL:HG23	1:C:405:ILE:HD13	1.96	0.47
1:A:425:THR:HG21	1:A:495:ARG:CG	2.45	0.47
2:B:34:MET:HB3	2:B:79:LEU:HD22	1.97	0.47
2:D:208:SER:O	2:D:209:ARG:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:LEU:HD11	2:D:83:MET:CE	2.45	0.47
2:D:104:LEU:HD12	2:D:107:TRP:CZ2	2.49	0.47
2:D:208:SER:C	2:D:209:ARG:HG2	2.40	0.47
2:B:2:VAL:HG13	2:B:27:PHE:CE2	2.50	0.46
2:B:211:GLU:HG3	2:B:212:PRO:HD2	1.95	0.46
2:B:179:LEU:HD11	2:B:218:TYR:CE2	2.50	0.46
2:D:105:ASP:HA	2:D:178:PRO:HG3	1.98	0.46
2:D:179:LEU:HD11	2:D:218:TYR:HE2	1.80	0.46
1:C:363:THR:HB	1:C:422:ALA:HB3	1.97	0.46
2:D:215:PHE:HD2	2:D:236:VAL:HG12	1.81	0.45
1:A:329:PHE:CE1	1:A:421:LEU:HD22	2.51	0.45
1:A:470:PRO:HB2	2:B:204:THR:HG23	1.99	0.45
1:C:443:LEU:HD13	1:C:460:PHE:CD2	2.52	0.45
2:D:51:ILE:HB	2:D:70:ILE:HD13	1.98	0.45
1:C:442:TYR:CE1	1:C:443:LEU:HG	2.51	0.45
1:A:349:VAL:HG23	1:A:349:VAL:O	2.17	0.45
1:C:442:TYR:CD1	1:C:443:LEU:HG	2.52	0.45
1:A:319:ILE:HA	1:A:322:LEU:CD1	2.47	0.45
2:B:118:GLY:HA3	2:B:119:GLY:HA3	1.75	0.45
1:A:420:VAL:C	1:A:421:LEU:HD12	2.41	0.45
1:C:337:VAL:HG22	1:C:409:ASN:HB3	1.98	0.44
2:B:107:TRP:CE3	2:B:176:PRO:HD2	2.52	0.44
1:C:425:THR:HG21	1:C:495:ARG:CD	2.47	0.44
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.99	0.44
2:D:20:LEU:HG	2:D:83:MET:CE	2.47	0.44
2:D:12:VAL:HG21	2:D:86:LEU:CD2	2.47	0.44
1:C:347:ASN:ND2	1:C:504:LEU:HD13	2.33	0.43
1:A:322:LEU:HD12	1:A:349:VAL:HG22	1.98	0.43
2:B:156:ARG:HH11	2:B:156:ARG:CG	2.31	0.43
2:B:48:VAL:HG13	2:B:64:VAL:HG21	1.99	0.43
1:C:425:THR:HG21	1:C:495:ARG:CG	2.49	0.43
2:B:83:MET:HB3	2:B:86:LEU:HD21	2.01	0.43
2:B:103:TYR:CD2	2:B:166:ALA:HB2	2.54	0.43
2:D:20:LEU:HG	2:D:83:MET:HE2	1.99	0.43
2:D:157:ALA:HB3	2:D:201:THR:HA	2.00	0.43
2:D:37:VAL:HG13	2:D:46:GLU:C	2.45	0.42
2:B:201:THR:HG21	4:B:426:HOH:O	2.19	0.41
1:A:390:LYS:HB2	1:A:481:TYR:CE2	2.55	0.41
1:A:375:ASN:O	1:C:505:ASN:HB3	2.21	0.41
1:A:425:THR:HG21	1:A:495:ARG:HD2	2.03	0.41
2:D:2:VAL:HG13	2:D:27:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:TYR:CE2	1:A:374:LEU:HD13	2.56	0.41
2:B:39:GLN:HB2	2:B:45:LEU:HD23	2.03	0.41
1:A:378:CYS:SG	1:C:378:CYS:SG	3.19	0.40
2:D:87:ARG:O	2:D:115:VAL:HG21	2.21	0.40
2:B:52:SER:HB3	2:B:57:ASN:HB2	2.02	0.40
1:C:412:LEU:HD21	1:C:498:VAL:HG11	2.02	0.40
1:A:351:ASP:OD2	1:A:354:VAL:CG2	2.70	0.40
2:B:24:ALA:CB	2:B:29:PHE:CD1	3.05	0.40
2:D:20:LEU:CD1	2:D:83:MET:CE	2.99	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	189/203 (93%)	178 (94%)	11 (6%)	0	100	100
1	C	186/203 (92%)	171 (92%)	15 (8%)	0	100	100
2	B	228/247 (92%)	211 (92%)	16 (7%)	1 (0%)	30	38
2	D	227/247 (92%)	214 (94%)	10 (4%)	3 (1%)	9	10
All	All	830/900 (92%)	774 (93%)	52 (6%)	4 (0%)	24	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	209	ARG
2	D	243	VAL
2	B	118	GLY
2	D	244	PRO

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	167/177 (94%)	165 (99%)	2 (1%)	63	79
1	C	166/177 (94%)	161 (97%)	5 (3%)	36	53
2	B	192/196 (98%)	182 (95%)	10 (5%)	21	31
2	D	193/196 (98%)	185 (96%)	8 (4%)	27	41
All	All	718/746 (96%)	693 (96%)	25 (4%)	32	48

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	353	SER
1	A	374	LEU
2	B	3	GLN
2	B	30	SER
2	B	43	LYS
2	B	89	GLU
2	B	156	ARG
2	B	180	ILE
2	B	211	GLU
2	B	213	GLU
2	B	239	LYS
2	B	242	LEU
1	C	319	ILE
1	C	321	ASN
1	C	353	SER
1	C	378	CYS
1	C	505	ASN
2	D	3	GLN
2	D	18	LEU
2	D	57	ASN
2	D	58	LYS
2	D	165	LEU
2	D	180	ILE
2	D	213	GLU
2	D	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	ASN
1	A	375	ASN
1	A	505	ASN
2	B	3	GLN
2	B	35	HIS
2	B	39	GLN
2	B	82	GLN
2	B	169	GLN
2	B	174	GLN
1	C	321	ASN
1	C	347	ASN
1	C	505	ASN
2	D	3	GLN
2	D	35	HIS
2	D	39	GLN
2	D	170	GLN
2	D	174	GLN

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](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	191/203 (94%)	1.26	34 (17%) 4 4	11, 20, 32, 42	1 (0%)
1	C	188/203 (92%)	1.11	29 (15%) 5 6	15, 21, 30, 41	0
2	B	232/247 (93%)	0.78	18 (7%) 19 21	10, 20, 26, 38	2 (0%)
2	D	231/247 (93%)	0.79	18 (7%) 19 21	10, 20, 25, 44	2 (0%)
All	All	842/900 (93%)	0.97	99 (11%) 9 10	10, 20, 29, 44	5 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	PRO	8.2
1	A	508	ALA	6.5
2	D	244	PRO	6.4
2	B	244	PRO	5.9
1	C	505	ASN	5.8
1	A	506	ALA	5.7
1	A	352	TYR	5.7
1	A	355	LEU	5.2
2	D	243	VAL	4.9
2	B	116	SER	4.7
1	A	353	SER	4.7
1	A	354	VAL	4.6
2	B	242	LEU	4.6
2	B	117	SER	4.5
1	C	320	THR	4.4
2	D	242	LEU	4.3
1	A	357	ASN	4.2
1	C	319	ILE	4.2
2	B	243	VAL	4.2
1	A	377	LEU	4.2
1	C	321	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	319	ILE	4.1
2	B	186	ARG	4.0
2	B	34	MET	3.9
1	A	323	CYS	3.8
2	D	117	SER	3.8
1	A	509	THR	3.8
1	C	323	CYS	3.8
2	D	245	ARG	3.7
2	D	132	SER	3.6
2	B	118	GLY	3.5
1	A	505	ASN	3.5
1	C	352	TYR	3.4
2	D	34	MET	3.4
2	B	240	SER	3.4
1	C	354	VAL	3.3
1	A	321	ASN	3.3
1	C	355	LEU	3.2
1	A	359	THR	3.2
1	A	351	ASP	3.2
1	A	320	THR	3.2
1	A	374	LEU	3.1
1	A	449	ARG	3.0
1	C	318	ASN	3.0
1	A	375	ASN	3.0
2	B	133	GLU	3.0
1	A	358	SER	2.9
2	D	241	GLY	2.9
1	C	353	SER	2.8
2	D	209	ARG	2.8
1	C	463	ASP	2.8
1	C	356	TYR	2.8
1	C	357	ASN	2.7
1	C	378	CYS	2.7
2	B	101	SER	2.7
2	B	241	GLY	2.6
1	A	347	ASN	2.6
1	A	397	ILE	2.6
1	C	359	THR	2.5
1	A	356	TYR	2.5
1	A	378	CYS	2.5
1	C	330	ASN	2.5
2	D	13	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	119	GLY	2.5
1	A	427	ASN	2.4
1	C	351	ASP	2.4
1	A	326	GLY	2.4
1	A	461	SER	2.4
1	C	373	LYS	2.4
1	C	375	ASN	2.4
1	C	458	VAL	2.4
1	C	467	CYS	2.4
2	B	73	ASP	2.3
2	D	240	SER	2.3
2	B	155	CYS	2.3
1	A	412	LEU	2.3
2	D	188	THR	2.3
2	D	156	ARG	2.3
2	D	198	GLY	2.3
1	C	374	LEU	2.3
1	C	372	THR	2.3
1	A	379	PHE	2.2
1	C	427	ASN	2.2
1	C	397	ILE	2.2
1	C	504	LEU	2.2
2	D	14	PRO	2.2
2	B	104	LEU	2.2
2	D	54	ASP	2.2
1	C	327	GLU	2.1
1	A	348	CYS	2.1
2	B	177	ARG	2.1
2	B	53	TYR	2.1
2	D	53	TYR	2.1
1	A	476	TRP	2.1
1	C	390	LYS	2.1
2	D	84	ASN	2.0
1	A	380	SER	2.0
1	A	376	ASP	2.0
1	C	415	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	142	1/1	0.81	0.22	8,8,8,8	0
3	CL	A	517	1/1	0.87	0.26	17,17,17,17	0
3	CL	A	246	1/1	0.89	0.32	14,14,14,14	0
3	CL	A	88	1/1	0.92	0.30	3,3,3,3	0
3	CL	C	20	1/1	0.98	0.20	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.