



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:53 PM UTC

PDB ID : 5I8E / pdb_00005i8e
Title : Crystal Structure of Broadly Neutralizing HIV-1 Fusion Peptide-Targeting Antibody VRC34.01 Fab
Authors : Xu, K.; Zhou, T.; Liu, K.; Kwong, P.D.
Deposited on : 2016-02-18
Resolution : 2.65 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

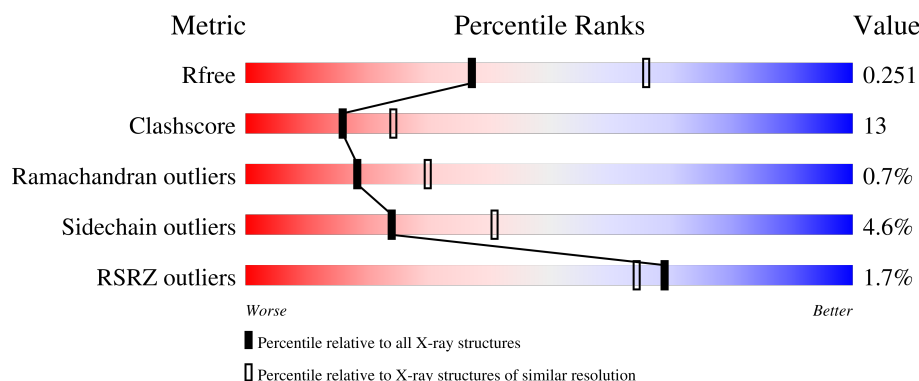
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	222	
1	C	222	
2	B	210	
2	D	210	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6546 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 VRC34.01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1633	1031	277	319	6			
1	C	216	Total	C	N	O	S	0	0	0
			1627	1027	276	318	6			

- Molecule 2 is a protein called VRC34.01 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	203	Total	C	N	O	S	0	0	0
			1541	976	258	302	5			
2	D	210	Total	C	N	O	S	0	0	0
			1610	1015	269	321	5			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Zn	0	0
			4	4		
3	B	1	Total	Zn	0	0
			1	1		
3	C	4	Total	Zn	0	0
			4	4		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	31	Total	O	0	0
			31	31		

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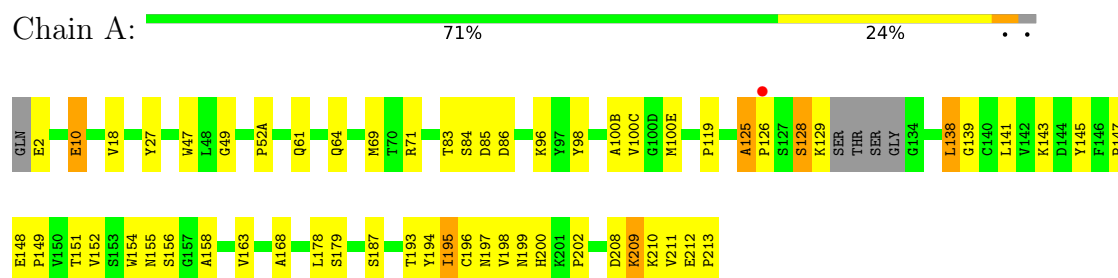
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	31	Total	O	0	0
			31	31		
4	D	30	Total	O	0	0
			30	30		

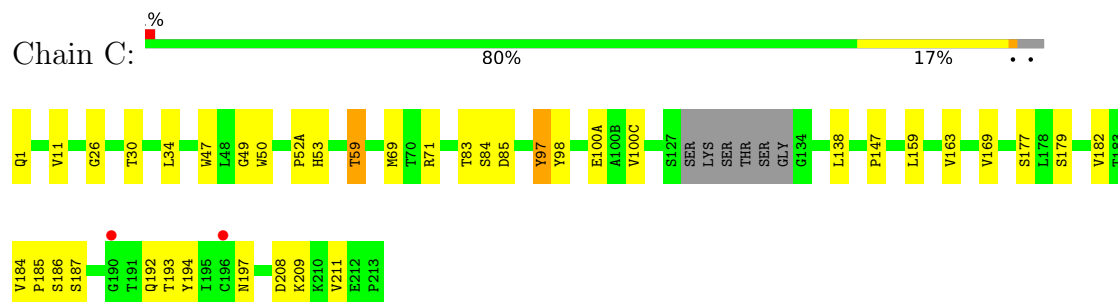
3 Residue-property plots

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.

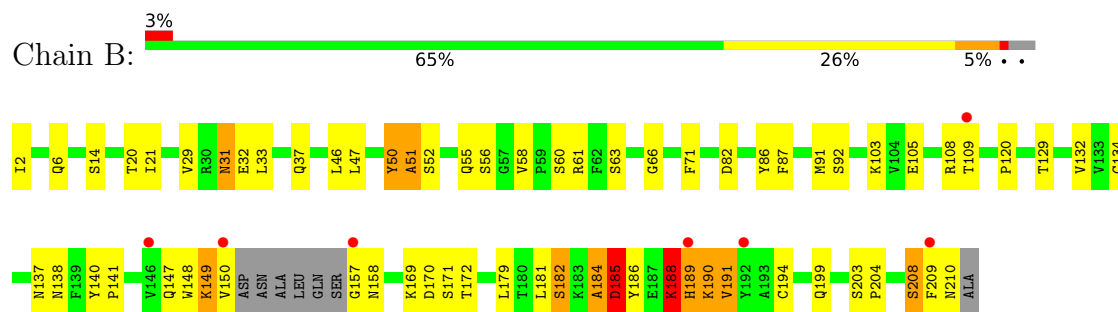
• Molecule 1: VRC34.01 Fab heavy chain



• Molecule 1: VRC34.01 Fab heavy chain

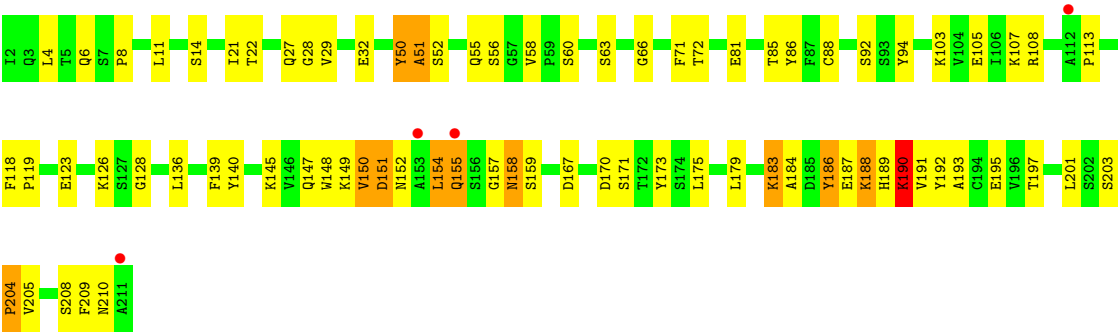


• Molecule 2: VRC34.01 Fab light chain



• Molecule 2: VRC34.01 Fab light chain





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	114.61Å 114.61Å 174.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.31 – 2.65 37.31 – 2.65	Depositor EDS
% Data completeness (in resolution range)	92.9 (37.31-2.65) 92.8 (37.31-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.186 , 0.248 0.190 , 0.251	Depositor DCC
R_{free} test set	1535 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.116 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6546	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 3.69% 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:
ZN

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	0.60	0/1673	1.05	11/2280 (0.5%)
1	C	0.62	0/1667	0.96	0/2273
2	B	0.67	0/1577	1.11	14/2145 (0.7%)
2	D	0.68	0/1647	1.10	13/2239 (0.6%)
All	All	0.64	0/6564	1.06	38/8937 (0.4%)

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	3
2	D	0	3
All	All	0	6

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	182	SER	N-CA-C	-10.20	99.67	112.72
2	D	204	PRO	N-CA-C	7.28	122.64	111.15
1	A	125	ALA	CA-C-N	7.15	126.91	119.76
1	A	125	ALA	C-N-CA	7.15	126.91	119.76
1	A	139	GLY	N-CA-C	6.75	120.31	110.80
2	D	190	LYS	CA-C-N	6.70	131.37	122.93
2	D	190	LYS	C-N-CA	6.70	131.37	122.93
2	D	58	VAL	CA-C-N	6.53	126.48	119.76
2	D	58	VAL	C-N-CA	6.53	126.48	119.76
2	B	208	SER	N-CA-C	6.25	117.72	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100(E)	MET	CA-C-N	6.17	130.29	121.71
1	A	100(E)	MET	C-N-CA	6.17	130.29	121.71
2	D	157	GLY	N-CA-C	6.07	127.56	113.18
2	B	185	ASP	N-CA-C	-6.04	101.23	110.30
2	D	188	LYS	N-CA-C	-6.01	105.90	113.72
1	A	194	TYR	CA-C-N	6.00	129.25	120.91
1	A	194	TYR	C-N-CA	6.00	129.25	120.91
2	D	186	TYR	CA-C-N	-5.97	113.54	123.33
2	D	186	TYR	C-N-CA	-5.97	113.54	123.33
2	D	189	HIS	N-CA-C	5.76	118.10	108.02
1	A	163	VAL	N-CA-C	5.59	116.28	109.30
2	B	58	VAL	CA-C-N	5.57	125.58	119.90
2	B	58	VAL	C-N-CA	5.57	125.58	119.90
2	D	151	ASP	N-CA-C	-5.53	101.79	110.36
2	D	154	LEU	N-CA-C	5.41	118.00	108.75
2	D	51	ALA	N-CA-C	5.39	122.28	110.80
1	A	195	ILE	CA-C-N	-5.30	114.54	122.39
1	A	195	ILE	C-N-CA	-5.30	114.54	122.39
2	B	157	GLY	CA-C-N	-5.30	114.72	122.19
2	B	157	GLY	C-N-CA	-5.30	114.72	122.19
2	B	191	VAL	N-CA-C	5.28	116.22	109.30
2	B	189	HIS	CA-C-N	-5.22	113.07	122.15
2	B	189	HIS	C-N-CA	-5.22	113.07	122.15
2	B	188	LYS	CA-C-N	-5.20	114.42	122.49
2	B	188	LYS	C-N-CA	-5.20	114.42	122.49
2	B	31	ASN	CA-C-N	-5.17	115.12	122.77
2	B	31	ASN	C-N-CA	-5.17	115.12	122.77
1	A	195	ILE	CA-C-O	-5.16	115.71	121.23

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	185	ASP	Peptide
2	B	190	LYS	Peptide
2	B	50	TYR	Peptide
2	D	150	VAL	Peptide
2	D	187	GLU	Peptide
2	D	50	TYR	Peptide

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	1633	0	1593	45	0
1	C	1627	0	1586	24	0
2	B	1541	0	1487	47	0
2	D	1610	0	1569	55	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
3	C	4	0	0	0	0
3	D	1	0	0	0	0
4	A	33	0	0	1	0
4	B	31	0	0	0	0
4	C	31	0	0	0	0
4	D	30	0	0	1	0
All	All	6546	0	6235	167	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 13.

All (167) 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:D:29:VAL:HG13	2:D:92:SER:HB3	1.50	0.92
2:B:186:TYR:HD1	2:B:188:LYS:HD2	1.36	0.88
2:B:129:THR:HG23	2:B:182:SER:HB2	1.57	0.86
1:C:138:LEU:HD13	1:C:211:VAL:HG21	1.57	0.85
2:B:186:TYR:CD1	2:B:188:LYS:HD2	2.11	0.85
1:A:52(A):PRO:HA	1:A:71:ARG:HD2	1.61	0.82
2:B:181:LEU:HD13	2:B:186:TYR:HB2	1.64	0.80
2:D:190:LYS:HG3	2:D:191:VAL:N	1.97	0.80
1:C:83:THR:HG22	1:C:85:ASP:H	1.46	0.79
1:C:197:ASN:ND2	1:C:208:ASP:OD1	2.16	0.79
2:D:148:TRP:O	2:D:154:LEU:HD12	1.82	0.79
2:D:190:LYS:HG3	2:D:191:VAL:H	1.49	0.78
1:C:49:GLY:HA3	1:C:69:MET:HE1	1.66	0.77
2:D:154:LEU:HD23	2:D:155:GLN:N	1.99	0.77
2:B:29:VAL:HG13	2:B:92:SER:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:VAL:HG22	2:D:210:ASN:HA	1.70	0.72
2:B:32:GLU:HB3	2:B:91:MET:HB2	1.73	0.71
2:B:186:TYR:CD1	2:B:188:LYS:HB3	2.27	0.70
2:B:33:LEU:HB3	2:B:51:ALA:HB2	1.74	0.70
1:A:49:GLY:HA3	1:A:69:MET:HE1	1.73	0.69
1:C:184:VAL:HG21	1:C:194:TYR:OH	1.93	0.69
2:B:150:VAL:HG13	2:B:188:LYS:HE2	1.77	0.67
2:D:150:VAL:HG23	2:D:151:ASP:H	1.59	0.67
2:D:151:ASP:HA	2:D:190:LYS:HD3	1.78	0.66
2:D:184:ALA:O	2:D:188:LYS:HG3	1.95	0.66
2:D:123:GLU:HA	2:D:126:LYS:HD2	1.77	0.66
1:C:52(A):PRO:HA	1:C:71:ARG:HD2	1.77	0.65
1:A:187:SER:OG	4:A:401:HOH:O	2.14	0.65
1:A:155:ASN:HA	1:A:195:ILE:HG13	1.79	0.64
2:D:191:VAL:HG13	2:D:209:PHE:O	1.97	0.64
2:D:128:GLY:HA2	2:D:183:LYS:HD3	1.79	0.63
1:A:152:VAL:HG22	1:A:198:VAL:HG22	1.81	0.62
1:C:11:VAL:HG21	1:C:147:PRO:HG3	1.79	0.62
2:B:186:TYR:CE1	2:B:188:LYS:HB3	2.34	0.62
2:D:150:VAL:O	2:D:190:LYS:HG2	2.00	0.61
2:D:105:GLU:OE1	2:D:173:TYR:OH	2.15	0.61
1:A:155:ASN:HA	1:A:195:ILE:CG1	2.30	0.61
2:B:6:GLN:HE22	2:B:87:PHE:HA	1.66	0.61
2:D:190:LYS:HE3	2:D:191:VAL:O	2.01	0.61
2:D:148:TRP:C	2:D:154:LEU:HD12	2.25	0.61
2:D:148:TRP:HB2	2:D:154:LEU:HD11	1.81	0.60
2:D:186:TYR:O	2:D:192:TYR:OH	2.09	0.60
1:C:159:LEU:HD21	1:C:182:VAL:HG11	1.84	0.60
2:B:103:LYS:HE2	2:B:105:GLU:HG2	1.84	0.59
2:B:189:HIS:O	2:B:189:HIS:ND1	2.36	0.59
1:A:2:GLU:HG2	1:A:27:TYR:HB3	1.85	0.58
1:C:59:THR:HG22	1:C:69:MET:HE3	1.85	0.58
1:A:209:LYS:HZ1	1:A:211:VAL:HG13	1.67	0.58
2:D:149:LYS:NZ	2:D:152:ASN:O	2.25	0.58
1:A:155:ASN:HA	1:A:195:ILE:HB	1.86	0.58
1:C:71:ARG:HH21	1:C:71:ARG:HG2	1.69	0.57
2:D:123:GLU:OE1	2:D:123:GLU:N	2.35	0.56
2:B:108:ARG:NH1	2:B:109:THR:O	2.38	0.56
1:A:195:ILE:HD13	1:A:210:LYS:NZ	2.21	0.56
2:B:66:GLY:HA3	2:B:71:PHE:CD2	2.41	0.56
1:A:197:ASN:ND2	1:A:208:ASP:OD1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:HB3	1:A:158:ALA:HB3	1.88	0.55
1:C:1:GLN:O	1:C:26:GLY:HA3	2.07	0.54
2:D:11:LEU:HD22	2:D:21:ILE:HD11	1.89	0.54
2:B:150:VAL:HG12	2:B:191:VAL:O	2.06	0.54
2:B:50:TYR:O	2:B:52:SER:N	2.39	0.54
2:D:145:LYS:HB3	2:D:197:THR:OG1	2.08	0.54
2:D:190:LYS:CG	2:D:191:VAL:N	2.71	0.53
1:A:96:LYS:HE3	2:B:55:GLN:HE21	1.74	0.53
2:D:29:VAL:HG12	2:D:32:GLU:H	1.74	0.52
2:B:55:GLN:HG2	2:B:56:SER:N	2.25	0.52
1:A:151:THR:O	1:A:198:VAL:HA	2.10	0.52
1:A:147:PRO:O	1:A:200:HIS:NE2	2.31	0.52
1:C:1:GLN:O	1:C:1:GLN:HG3	2.07	0.52
2:B:134:CYS:HB2	2:B:148:TRP:CZ2	2.44	0.52
2:D:22:THR:HG22	2:D:72:THR:HG22	1.92	0.52
1:C:71:ARG:HG2	1:C:71:ARG:NH2	2.25	0.52
2:B:29:VAL:HG12	2:B:32:GLU:H	1.75	0.51
2:D:154:LEU:HD23	2:D:155:GLN:H	1.75	0.51
1:A:71:ARG:HG2	1:A:71:ARG:HH21	1.76	0.51
1:A:155:ASN:HA	1:A:195:ILE:CB	2.40	0.51
1:C:163:VAL:HG22	1:C:182:VAL:HG22	1.92	0.51
2:D:8:PRO:HD2	2:D:21:ILE:HD12	1.93	0.51
1:A:141:LEU:HD21	1:A:143:LYS:HD2	1.93	0.50
2:B:46:LEU:HD23	2:B:47:LEU:N	2.26	0.50
2:B:108:ARG:HD2	2:B:171:SER:O	2.12	0.50
2:D:136:LEU:HB2	2:D:175:LEU:HB3	1.93	0.50
2:B:6:GLN:HE22	2:B:87:PHE:CA	2.24	0.50
1:A:126:PRO:HG3	1:A:138:LEU:HG	1.94	0.50
2:D:50:TYR:O	2:D:52:SER:N	2.43	0.49
2:D:63:SER:HB3	4:D:404:HOH:O	2.13	0.49
2:B:150:VAL:CG2	2:B:188:LYS:HG3	2.42	0.49
1:C:47:TRP:CH2	1:C:49:GLY:HA2	2.47	0.49
2:B:189:HIS:O	2:B:189:HIS:CG	2.65	0.49
2:D:85:THR:OG1	2:D:103:LYS:HD3	2.13	0.49
2:D:108:ARG:HD2	2:D:171:SER:HB2	1.94	0.49
1:A:128:SER:O	1:A:128:SER:OG	2.21	0.49
2:D:203:SER:OG	2:D:204:PRO:HD2	2.13	0.48
1:A:100(B):ALA:O	2:B:91:MET:HG3	2.13	0.48
1:A:156:SER:N	1:A:195:ILE:HG21	2.29	0.48
1:C:50:TRP:HZ2	2:D:94:TYR:HH	1.61	0.48
1:C:169:VAL:HG22	1:C:177:SER:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:LEU:HD13	2:D:175:LEU:HD22	1.96	0.48
2:D:197:THR:HG22	2:D:204:PRO:HG3	1.96	0.48
2:D:193:ALA:HB2	2:D:208:SER:HB2	1.97	0.47
2:B:186:TYR:C	2:B:188:LYS:N	2.70	0.47
1:A:148:GLU:HG2	1:A:149:PRO:HA	1.97	0.47
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.96	0.47
2:D:150:VAL:HG21	2:D:155:GLN:OE1	2.15	0.47
2:D:167:ASP:HB3	2:D:170:ASP:OD1	2.15	0.47
1:A:168:ALA:HA	1:A:178:LEU:HB3	1.97	0.47
2:D:4:LEU:HD13	2:D:88:CYS:SG	2.55	0.46
2:B:6:GLN:NE2	2:B:86:TYR:O	2.49	0.46
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.95	0.46
2:D:148:TRP:HB2	2:D:154:LEU:CD1	2.46	0.46
1:A:47:TRP:CH2	1:A:49:GLY:HA2	2.50	0.46
1:A:83:THR:HG22	1:A:86:ASP:OD2	2.15	0.46
2:B:184:ALA:O	2:B:185:ASP:C	2.55	0.46
1:A:83:THR:HG23	1:A:85:ASP:HB2	1.98	0.46
1:A:10:GLU:HG2	1:A:18:VAL:HG23	1.97	0.46
1:A:200:HIS:CE1	1:A:202:PRO:HB2	2.51	0.46
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.98	0.46
2:B:147:GLN:O	2:B:194:CYS:HA	2.16	0.46
1:A:98:TYR:HB2	1:A:100(C):VAL:HG21	1.98	0.45
2:D:66:GLY:HA3	2:D:71:PHE:CD1	2.52	0.45
1:C:47:TRP:CZ2	1:C:49:GLY:HA2	2.51	0.45
2:B:185:ASP:O	2:B:186:TYR:C	2.60	0.45
2:B:190:LYS:NZ	2:B:210:ASN:O	2.32	0.45
2:B:209:PHE:CD2	2:B:210:ASN:N	2.85	0.45
2:B:208:SER:OG	2:B:209:PHE:N	2.51	0.44
2:D:6:GLN:NE2	2:D:86:TYR:O	2.51	0.44
2:B:170:ASP:OD2	2:B:172:THR:OG1	2.29	0.44
2:B:150:VAL:HG21	2:B:188:LYS:HG3	2.00	0.44
2:D:81:GLU:H	2:D:81:GLU:CD	2.25	0.44
1:A:196:CYS:O	1:A:208:ASP:HA	2.17	0.43
2:B:190:LYS:HD2	2:B:190:LYS:HA	1.57	0.43
1:C:98:TYR:HB2	1:C:100(C):VAL:HG21	1.99	0.43
2:D:108:ARG:NE	2:D:170:ASP:O	2.51	0.43
1:A:195:ILE:HD13	1:A:210:LYS:CE	2.49	0.43
2:D:55:GLN:HG2	2:D:56:SER:N	2.31	0.43
1:A:100(C):VAL:C	2:B:91:MET:HE2	2.44	0.43
2:D:201:LEU:HD22	2:D:205:VAL:HG23	2.00	0.43
1:A:155:ASN:CB	1:A:158:ALA:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:HA	1:A:64:GLN:CD	2.44	0.43
1:A:141:LEU:HD23	1:A:143:LYS:HB2	2.00	0.43
1:A:125:ALA:HA	1:A:126:PRO:HD3	1.74	0.43
2:D:113:PRO:HB3	2:D:139:PHE:HB3	2.00	0.43
2:D:118:PHE:HA	2:D:119:PRO:HD3	1.86	0.43
2:D:147:GLN:HB2	2:D:195:GLU:HG2	2.01	0.42
1:A:156:SER:H	1:A:195:ILE:HG21	1.83	0.42
2:B:140:TYR:CG	2:B:141:PRO:HA	2.54	0.42
1:C:184:VAL:HG22	1:C:185:PRO:HD2	2.00	0.42
1:A:154:TRP:CE3	1:A:195:ILE:O	2.73	0.42
2:D:158:ASN:OD1	2:D:158:ASN:N	2.45	0.42
1:C:97:TYR:HA	1:C:100(A):GLU:O	2.20	0.42
1:A:128:SER:HA	1:A:129:LYS:HA	1.89	0.42
2:B:20:THR:O	2:B:21:ILE:HD13	2.19	0.41
2:B:61:ARG:NE	2:B:82:ASP:OD2	2.47	0.41
2:B:137:ASN:CG	2:B:138:ASN:HD22	2.27	0.41
2:B:203:SER:HB3	2:B:204:PRO:HD2	2.03	0.41
2:D:108:ARG:HD2	2:D:171:SER:O	2.20	0.41
1:A:212:GLU:HG2	1:A:213:PRO:HD3	2.03	0.41
1:C:30:THR:HB	1:C:53:HIS:HB2	2.03	0.41
2:D:27:GLN:HG2	2:D:28:GLY:N	2.36	0.41
2:D:107:LYS:HA	2:D:140:TYR:OH	2.21	0.41
1:A:155:ASN:H	1:A:195:ILE:HB	1.86	0.41
1:C:34:LEU:HD23	1:C:34:LEU:HA	1.91	0.41
1:A:141:LEU:CD2	1:A:143:LYS:HB2	2.51	0.40
2:D:150:VAL:HG23	2:D:151:ASP:N	2.30	0.40
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.57	0.40
1:C:192:GLN:OE1	1:C:193:THR:N	2.54	0.40
1:A:147:PRO:HD2	1:A:202:PRO:CB	2.51	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	A	213/222 (96%)	204 (96%)	9 (4%)	0	100	100
1	C	212/222 (96%)	203 (96%)	9 (4%)	0	100	100
2	B	199/210 (95%)	188 (94%)	7 (4%)	4 (2%)	6	10
2	D	208/210 (99%)	197 (95%)	9 (4%)	2 (1%)	12	20
All	All	832/864 (96%)	792 (95%)	34 (4%)	6 (1%)	18	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	ALA
2	D	51	ALA
2	B	31	ASN
2	D	190	LYS
2	B	149	LYS
2	B	184	ALA

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	182/186 (98%)	174 (96%)	8 (4%)	25	43
1	C	181/186 (97%)	174 (96%)	7 (4%)	28	48
2	B	171/183 (93%)	161 (94%)	10 (6%)	18	31
2	D	183/183 (100%)	175 (96%)	8 (4%)	25	43
All	All	717/738 (97%)	684 (95%)	33 (5%)	24	41

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	84	SER
1	A	128	SER
1	A	138	LEU
1	A	179	SER

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Mol	Chain	Res	Type
1	A	193	THR
1	A	199	ASN
1	A	209	LYS
2	B	2	ILE
2	B	14	SER
2	B	60	SER
2	B	63	SER
2	B	149	LYS
2	B	158	ASN
2	B	169	LYS
2	B	179	LEU
2	B	188	LYS
2	B	199	GLN
1	C	59	THR
1	C	84	SER
1	C	97	TYR
1	C	179	SER
1	C	186	SER
1	C	187	SER
1	C	209	LYS
2	D	14	SER
2	D	60	SER
2	D	155	GLN
2	D	158	ASN
2	D	159	SER
2	D	179	LEU
2	D	183	LYS
2	D	190	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	76	ASN
1	A	155	ASN
2	B	6	GLN
2	B	38	GLN
2	B	55	GLN
2	B	138	ASN
1	C	64	GLN
2	D	55	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 10 ligands modelled in this entry, 10 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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	217/222 (97%)	-0.10	1 (0%) 87 85	40, 73, 167, 214	0
1	C	216/222 (97%)	-0.23	2 (0%) 81 78	39, 69, 109, 134	0
2	B	203/210 (96%)	-0.02	7 (3%) 48 40	40, 71, 166, 229	0
2	D	210/210 (100%)	-0.06	4 (1%) 66 61	41, 79, 152, 210	0
All	All	846/864 (97%)	-0.10	14 (1%) 69 64	39, 74, 156, 229	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	157	GLY	4.0
2	B	150	VAL	3.6
2	B	189	HIS	3.5
1	C	196	CYS	3.2
2	B	192	TYR	2.9
1	C	190	GLY	2.5
2	D	211	ALA	2.5
2	D	155	GLN	2.4
2	B	209	PHE	2.3
2	D	153	ALA	2.2
2	D	112	ALA	2.1
2	B	146	VAL	2.1
2	B	109	THR	2.1
1	A	126	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](#)

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	ZN	A	301	1/1	0.95	0.10	118,118,118,118	0
3	ZN	C	301	1/1	0.95	0.08	113,113,113,113	0
3	ZN	A	304	1/1	0.97	0.04	109,109,109,109	0
3	ZN	B	301	1/1	0.98	0.10	94,94,94,94	0
3	ZN	C	304	1/1	0.98	0.06	103,103,103,103	0
3	ZN	A	302	1/1	0.99	0.05	81,81,81,81	0
3	ZN	C	302	1/1	0.99	0.02	72,72,72,72	0
3	ZN	C	303	1/1	0.99	0.05	49,49,49,49	0
3	ZN	A	303	1/1	0.99	0.02	51,51,51,51	0
3	ZN	D	301	1/1	0.99	0.07	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.