



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2017 – 06:53 AM EDT

PDB ID : 5I8E
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 : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

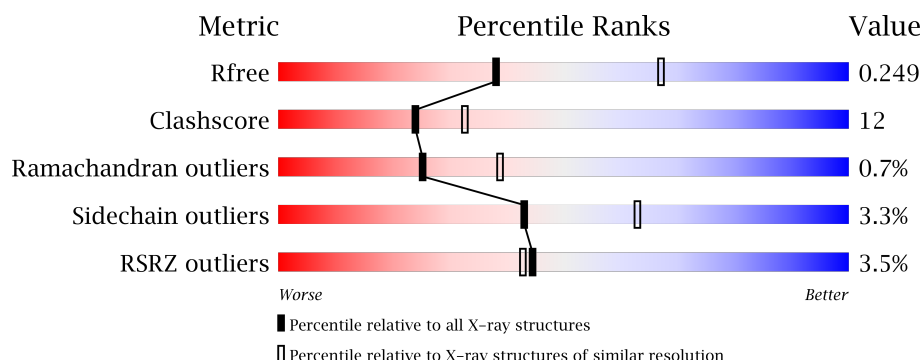
1 Overall quality at a glance

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}	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>8%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>
1	C	222	<div> <div>81%</div> <div>15%</div> <div>..</div> </div>
2	B	210	<div> <div>3%</div> <div>70%</div> <div>24%</div> <div>..</div> </div>
2	D	210	<div> <div>2%</div> <div>65%</div> <div>32%</div> <div>.</div> </div>

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 (three-letter code: ZN) (formula: Zn).

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

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

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 8% 74% 23%
- Legend:
- V I L M S A T P G Q N D E K R H Y C F W M L I V

- Chain C: 

- Chain B:
-
- 3% 70% 24%
- T2 Q6 S14 T20 I21 V29 R30 R31 E32 L33 Q37 L46 L47 Y50 A51 S52 Q55 S56 R61 P62 S63 G66 F71 D82 Y86 P87 R91 S92 K103 V104 E105 R108 T109 P120 T129 V132 V133 C134 Y140 P141 V146 Q147 W148 K149 V150 ASP ASN ALA LEU GLN SER G157 N158 S171 L181 S182 K183 A184 D185 Y186 E187 K188 H189 K190 V191 Y192 A193 C194 E195 S203 P204 S208 F209 N210 ALA

- Chain D:
-
- 2% 65% 32%
- I2 Q3 L4 T5 Q6 S7 P8 L11 S14 I21 T22 Q27 G28 V29 E32 Y0 A51 S52 Q55 S56 S63 G66 F71 T72 T85 Y86 F87 C88 M91 S92 S93 Y94 K103 V104 E105 I106 K107 R108 P113 F118 P119 E123 V126



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 – 2.66	Depositor EDS
% Data completeness (in resolution range)	92.9 (37.31-2.65) 92.9 (37.31-2.66)	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 0.187 , 0.249	Depositor DCC
R_{free} test set	1536 reflections (5.11%)	DCC
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 , 50.1	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	0.46	0/1673	0.71	0/2280
1	C	0.51	0/1667	0.66	0/2273
2	B	0.54	0/1577	0.77	0/2145
2	D	0.51	0/1647	0.76	1/2239 (0.0%)
All	All	0.51	0/6564	0.73	1/8937 (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	3
2	D	0	3
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	157	GLY	N-CA-C	5.78	127.56	113.10

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

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Mol	Chain	Res	Type	Group
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	41	0
1	C	1627	0	1586	22	0
2	B	1541	0	1487	44	0
2	D	1610	0	1569	54	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	0	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	158	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 12.

All (158) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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: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: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
1:A:209:LYS:HZ1	1:A:211:VAL:HG13	1.67	0.59
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: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:N	2:D:123:GLU:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:LYS:NZ	2:D:152:ASN:O	2.25	0.56
2:D:148:TRP:C	2:D:154:LEU:HD12	2.25	0.56
1:A:197:ASN:ND2	1:A:208:ASP:OD1	2.38	0.55
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:HG3	1:C:1:GLN:O	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:155:ASN:HA	1:A:195:ILE:CB	2.40	0.51
1:A:71:ARG:HG2	1:A:71:ARG:HH21	1.76	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:108:ARG:HD2	2:B:171:SER:O	2.12	0.50
2:B:46:LEU:HD23	2:B:47:LEU:N	2.26	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:C:50:TRP:HZ2	2:D:94:TYR:HH	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:VAL:HG22	1:C:177:SER:O	2.14	0.48
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
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
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:147:GLN:O	2:B:194:CYS:HA	2.16	0.46
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.98	0.46
1:A:98:TYR:HB2	1:A:100(C):VAL:HG21	1.98	0.45
2:B:186:TYR:C	2:B:188:LYS:N	2.70	0.45
2:D:55:GLN:HG2	2:D:56:SER:N	2.31	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: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:150:VAL:HG21	2:B:188:LYS:HG3	2.00	0.44
1:A:196:CYS:O	1:A:208:ASP:HA	2.17	0.43
2:B:190:LYS:HA	2:B:190:LYS:HD2	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:184:ALA:O	2:B:185:ASP:C	2.55	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: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
2:D:27:GLN:HG2	2:D:28:GLY:N	2.36	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: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:HA	1:C:34:LEU:HD23	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
2:B:185:ASP:O	2:B:186:TYR:C	2.60	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	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%)	9	13
2	D	208/210 (99%)	197 (95%)	9 (4%)	2 (1%)	18	28
All	All	832/864 (96%)	792 (95%)	34 (4%)	6 (1%)	25	39

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%)	175 (96%)	7 (4%)	38	57
1	C	181/186 (97%)	175 (97%)	6 (3%)	43	63
2	B	171/183 (93%)	166 (97%)	5 (3%)	48	68
2	D	183/183 (100%)	177 (97%)	6 (3%)	43	63
All	All	717/738 (97%)	693 (97%)	24 (3%)	43	63

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	TRP
1	A	97	TYR
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
2	B	2	ILE
2	B	14	SER
2	B	63	SER
2	B	158	ASN
2	B	188	LYS
1	C	50	TRP
1	C	59	THR
1	C	84	SER
1	C	97	TYR
1	C	186	SER
1	C	187	SER
2	D	14	SER
2	D	63	SER
2	D	91	MET
2	D	155	GLN
2	D	158	ASN
2	D	159	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	155	ASN
2	B	6	GLN
2	B	38	GLN
2	B	55	GLN
2	B	138	ASN
1	C	199	ASN
2	D	147	GLN

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 [i](#)

There are no carbohydrates 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 ⓘ

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	217/222 (97%)	0.08	18 (8%) 12 10	40, 73, 167, 214	0
1	C	216/222 (97%)	-0.23	1 (0%) 90 91	39, 69, 109, 134	0
2	B	203/210 (96%)	-0.01	7 (3%) 46 44	40, 71, 166, 229	0
2	D	210/210 (100%)	-0.11	4 (1%) 67 66	41, 79, 152, 210	0
All	All	846/864 (97%)	-0.07	30 (3%) 44 43	39, 74, 156, 229	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	157	GLY	7.8
1	A	129	LYS	4.6
1	A	137	ALA	4.5
1	A	138	LEU	4.3
1	A	158	ALA	4.1
1	A	182	VAL	4.1
1	A	139	GLY	3.9
1	A	211	VAL	3.5
1	A	189	LEU	3.5
1	A	154	TRP	3.5
2	B	195	GLU	3.4
2	D	192	TYR	3.4
2	B	192	TYR	3.4
1	A	121	VAL	3.4
1	A	193	THR	3.3
1	A	122	PHE	3.1
2	D	153	ALA	3.0
1	A	160	THR	3.0
2	B	146	VAL	2.9
2	B	209	PHE	2.9
1	A	126	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	183	LYS	2.7
2	B	188	LYS	2.6
1	A	210	LYS	2.5
1	A	207	VAL	2.4
2	D	155	GLN	2.3
1	C	1	GLN	2.2
1	A	159	LEU	2.1
2	D	209	PHE	2.1
1	A	123	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	ZN	A	303	1/1	0.98	0.18	1.23	51,51,51,51	0
3	ZN	C	303	1/1	0.99	0.14	0.23	49,49,49,49	0
3	ZN	C	304	1/1	0.97	0.16	-0.03	103,103,103,103	0
3	ZN	A	304	1/1	0.97	0.14	-0.13	109,109,109,109	0
3	ZN	A	301	1/1	0.92	0.12	-0.81	118,118,118,118	0
3	ZN	C	301	1/1	0.87	0.09	-2.64	113,113,113,113	0
3	ZN	B	301	1/1	1.00	0.22	-	94,94,94,94	0
3	ZN	C	302	1/1	0.99	0.16	-	72,72,72,72	0
3	ZN	A	302	1/1	0.99	0.24	-	81,81,81,81	0
3	ZN	D	301	1/1	0.99	0.23	-	58,58,58,58	0

6.5 Other polymers

There are no such residues in this entry.