



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:45 AM UTC

PDB ID : 3TNN / pdb_00003tnn
Title : Crystal structure of N5-i5 Fab, an ADCC mediating and non-neutralizing CD4i anti-HIV- 1 antibody.
Authors : Wu, X.; Pazgier, M.
Deposited on : 2011-09-01
Resolution : 1.95 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
Mogul : 2022.3.0, CSD as543be (2022)
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

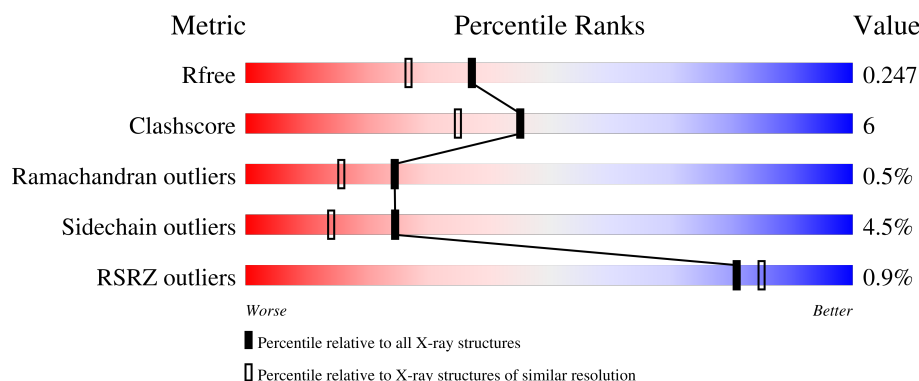
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	226	73% 19% 6%
1	C	226	2% 77% 15% 6%
1	E	226	76% 15% 7%
1	H	226	78% 12% 7%
2	B	217	% 87% 9% ..

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Mol	Chain	Length	Quality of chain
2	D	217	% 87% 9% ..
2	F	217	% 84% 12% ...
2	L	217	83% 13% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13429 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 Fab heavy chain of ADCC and non-neutralizing anti-HIV-1 antibody N5-i5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	211	Total	C	N	O	S	0	0	0
			1564	982	268	308	6			
1	A	212	Total	C	N	O	S	0	0	0
			1571	987	269	309	6			
1	C	212	Total	C	N	O	S	0	0	0
			1571	987	269	309	6			
1	E	210	Total	C	N	O	S	0	0	0
			1555	977	267	305	6			

- Molecule 2 is a protein called Fab light chain of ADCC and non-neutralizing anti-HIV-1 antibody N5-i5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1575	982	264	324	5			
2	B	212	Total	C	N	O	S	0	0	0
			1575	982	264	324	5			
2	D	212	Total	C	N	O	S	0	0	0
			1575	982	264	324	5			
2	F	212	Total	C	N	O	S	0	0	0
			1575	982	264	324	5			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Cl	0	0
			2	2		
5	L	2	Total	Cl	0	0
			2	2		
5	A	1	Total	Cl	0	0
			1	1		
5	B	2	Total	Cl	0	0
			2	2		
5	D	2	Total	Cl	0	0
			2	2		
5	E	3	Total	Cl	0	0
			3	3		
5	F	2	Total	Cl	0	0
			2	2		

- Molecule 6 is water.

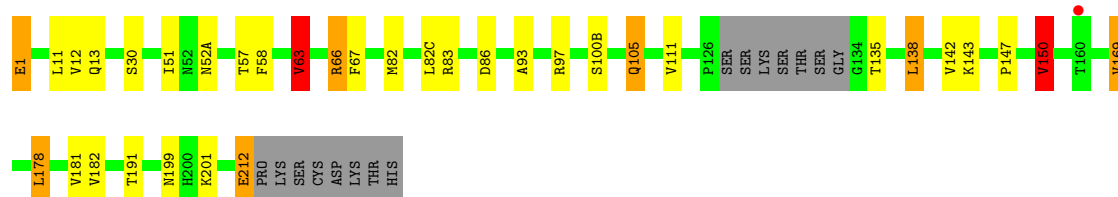
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	105	Total 105	O 105	0	0
6	L	116	Total 116	O 116	0	0
6	A	76	Total 76	O 76	0	0
6	B	91	Total 91	O 91	0	0
6	C	59	Total 59	O 59	0	0
6	D	97	Total 97	O 97	0	0
6	E	124	Total 124	O 124	0	0
6	F	134	Total 134	O 134	0	0

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.

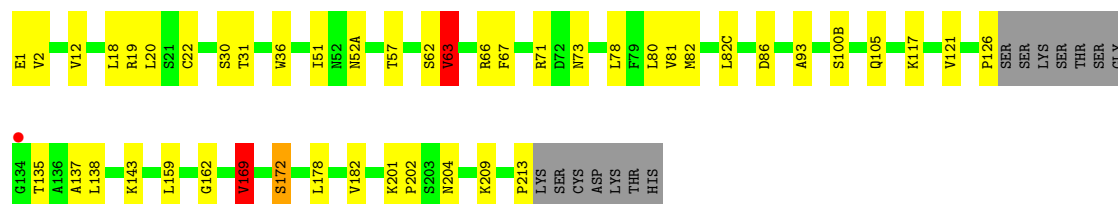
- Molecule 1: Fab heavy chain of ADCC and non-neutralizing anti-HIV-1 antibody N5-i5

Chain H: 



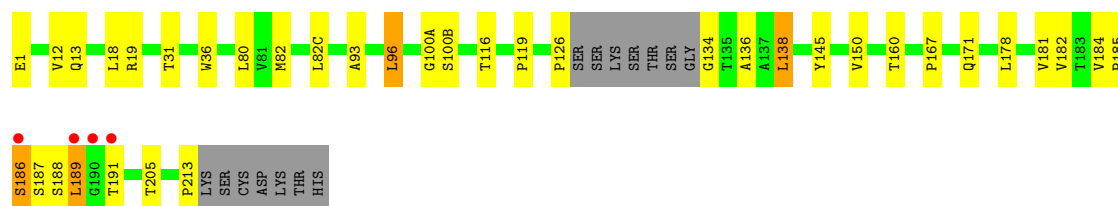
- Molecule 1: Fab heavy chain of ADCC and non-neutralizing anti-HIV-1 antibody N5-i5

Chain A: 



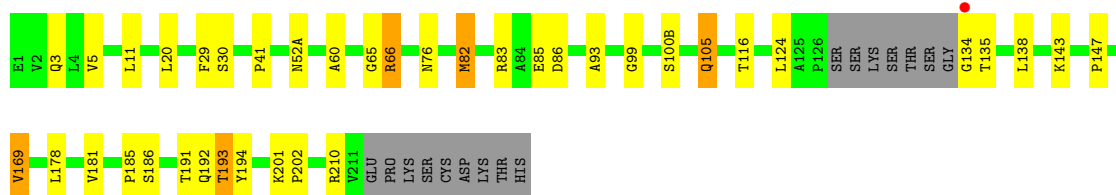
- Molecule 1: Fab heavy chain of ADCC and non-neutralizing anti-HIV-1 antibody N5-i5

Chain C: 



- Molecule 1: Fab heavy chain of ADCC and non-neutralizing anti-HIV-1 antibody N5-i5

Chain E: 



- Molecule 2: Fab light chain of ADCC and non-neutralizing anti-HIV-1 antibody N5-i5

Chain L: 83% 13% ..



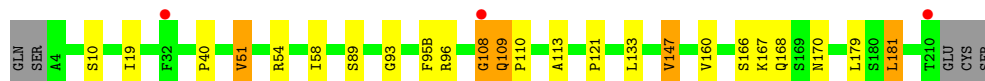
- Molecule 2: Fab light chain of ADCC and non-neutralizing anti-HIV-1 antibody N5-i5

Chain B: 87% 9% ..



- Molecule 2: Fab light chain of ADCC and non-neutralizing anti-HIV-1 antibody N5-i5

Chain D: 87% 9% ..



- Molecule 2: Fab light chain of ADCC and non-neutralizing anti-HIV-1 antibody N5-i5

Chain F: 84% 12% ...



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.44Å 84.50Å 143.12Å 90.00° 101.08° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 20.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.00-1.95) 98.3 (20.00-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.245 0.200 , 0.247	Depositor DCC
R_{free} test set	6209 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtrriage
Anisotropy	0.555	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13429	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5582e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, GOL, 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	0.99	1/1605 (0.1%)	1.02	2/2184 (0.1%)
1	C	0.94	0/1605	0.98	1/2184 (0.0%)
1	E	1.24	3/1588 (0.2%)	1.15	4/2160 (0.2%)
1	H	1.18	1/1597 (0.1%)	1.16	4/2172 (0.2%)
2	B	1.04	2/1613 (0.1%)	1.03	2/2198 (0.1%)
2	D	1.01	1/1613 (0.1%)	1.07	6/2198 (0.3%)
2	F	1.18	1/1613 (0.1%)	1.10	1/2198 (0.0%)
2	L	1.21	2/1613 (0.1%)	1.12	0/2198
All	All	1.10	11/12847 (0.1%)	1.08	20/17492 (0.1%)

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
2	F	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	SER	C-N	11.60	1.49	1.33
2	L	10	SER	C-N	9.43	1.46	1.33
1	E	5	VAL	CA-CB	6.65	1.61	1.53
2	F	9	ALA	CA-CB	6.13	1.63	1.53
1	E	60	ALA	N-CA	6.12	1.53	1.45
1	A	137	ALA	CA-CB	6.01	1.62	1.53
1	H	58	PHE	N-CA	5.88	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	189	HIS	CA-C	-5.68	1.45	1.52
2	B	51	VAL	CA-CB	5.60	1.62	1.54
1	E	82	MET	SD-CE	-5.47	1.65	1.79
2	L	87	TYR	C-O	5.02	1.30	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	169	VAL	CB-CA-C	-9.45	98.26	111.21
2	F	169	SER	N-CA-C	-9.34	90.90	110.80
1	A	169	VAL	CB-CA-C	-7.72	100.17	111.68
1	E	66	ARG	NE-CZ-NH2	-7.21	112.71	119.20
2	D	113	ALA	CA-C-N	-6.62	113.17	119.85
2	D	113	ALA	C-N-CA	-6.62	113.17	119.85
1	H	63	VAL	N-CA-CB	-6.27	104.21	112.36
2	D	108	GLY	N-CA-C	6.24	121.58	113.27
2	D	109	GLN	N-CA-C	6.24	118.67	109.50
1	C	160	THR	N-CA-C	-5.98	106.96	114.56
1	H	169	VAL	CB-CA-C	-5.88	102.91	111.68
1	E	65	GLY	N-CA-C	-5.51	108.13	115.40
1	H	66	ARG	NE-CZ-NH2	-5.46	114.29	119.20
2	B	113	ALA	CA-C-N	-5.32	114.48	119.85
2	B	113	ALA	C-N-CA	-5.32	114.48	119.85
1	A	63	VAL	N-CA-CB	-5.19	106.15	112.33
2	D	147	VAL	CB-CA-C	5.11	118.58	110.81
2	D	160	VAL	CB-CA-C	-5.07	104.62	110.91
1	H	150	VAL	N-CA-C	-5.06	100.92	108.46
1	E	66	ARG	CG-CD-NE	-5.00	100.99	112.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	106	VAL	Peptide
2	D	108	GLY	Peptide
2	F	156	VAL	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	1571	0	1544	25	0
1	C	1571	0	1544	17	0
1	E	1555	0	1531	25	0
1	H	1564	0	1537	29	1
2	B	1575	0	1519	13	0
2	D	1575	0	1519	10	0
2	F	1575	0	1519	19	0
2	L	1575	0	1519	27	0
3	B	5	0	0	1	0
3	D	10	0	0	0	0
3	F	10	0	0	0	0
3	H	10	0	0	1	0
3	L	5	0	0	0	0
4	H	6	0	8	0	0
4	L	6	0	8	3	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	F	2	0	0	0	0
5	H	2	0	0	0	0
5	L	2	0	0	0	0
6	A	76	0	0	1	0
6	B	91	0	0	2	0
6	C	59	0	0	0	0
6	D	97	0	0	0	0
6	E	124	0	0	5	1
6	F	134	0	0	1	0
6	H	105	0	0	0	0
6	L	116	0	0	2	0
All	All	13429	0	12248	147	1

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 6.

All (147) 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:F:157:LYS:HD2	2:F:158:ALA:H	1.24	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:61:ARG:HE	4:L:215:GOL:H31	1.25	1.00
2:F:157:LYS:HD2	2:F:158:ALA:N	1.79	0.96
1:A:105:GLN:HG2	6:A:801:HOH:O	1.80	0.81
1:E:105:GLN:H	1:E:105:GLN:NE2	1.79	0.81
1:H:105:GLN:NE2	1:H:105:GLN:H	1.76	0.81
2:F:27:SER:HB3	6:F:658:HOH:O	1.82	0.78
2:B:133:LEU:HD12	2:B:179:LEU:HD23	1.68	0.75
2:L:170:ASN:O	2:L:171:ASN:HB2	1.88	0.74
1:E:66:ARG:HD3	6:E:794:HOH:O	1.86	0.73
2:F:168:GLN:C	2:F:169:SER:O	2.30	0.72
1:C:126:PRO:HD3	1:C:138:LEU:HB3	1.72	0.71
2:B:197:THR:HG23	6:B:395:HOH:O	1.91	0.70
2:L:61:ARG:HH21	4:L:215:GOL:H11	1.57	0.69
2:F:168:GLN:HA	2:F:168:GLN:OE1	1.85	0.68
1:A:51:ILE:HG13	1:A:57:THR:HG22	1.76	0.68
2:L:61:ARG:NE	4:L:215:GOL:H31	2.06	0.68
2:F:141:TYR:CD1	2:F:142:PRO:HA	2.30	0.67
2:D:40:PRO:HG3	2:D:167:LYS:HB3	1.78	0.66
1:A:12:VAL:HG11	1:A:82(C):LEU:HD13	1.78	0.65
1:C:82:MET:HE2	1:C:82(C):LEU:HD21	1.78	0.65
1:A:63:VAL:HG13	1:A:67:PHE:HB2	1.78	0.65
1:H:66:ARG:HD2	1:H:83:ARG:HH21	1.62	0.64
1:H:169:VAL:HG21	2:L:178:TYR:CD2	2.34	0.62
1:E:99:GLY:O	2:F:96:ARG:NH1	2.32	0.61
1:E:30:SER:O	1:E:52(A):ASN:HB2	2.00	0.61
1:E:134:GLY:HA2	1:E:186:SER:H	1.65	0.61
2:F:111:LYS:HD2	2:F:142:PRO:HD3	1.83	0.60
1:H:82:MET:HE2	1:H:82(C):LEU:HD21	1.83	0.59
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.84	0.59
2:B:59:SER:HB2	3:B:214:SO4:O4	2.02	0.59
2:L:121:PRO:HD3	2:L:133:LEU:HD21	1.84	0.58
1:C:126:PRO:HD3	1:C:138:LEU:CB	2.32	0.58
1:H:11:LEU:HB2	1:H:147:PRO:HG3	1.85	0.58
1:A:30:SER:O	1:A:52(A):ASN:HB2	2.03	0.57
1:H:97:ARG:NH2	2:L:32:PHE:HE1	2.03	0.57
2:B:103:LYS:HE3	6:B:613:HOH:O	2.03	0.57
1:A:20:LEU:HG	1:A:82:MET:HE2	1.85	0.57
1:A:126:PRO:HG2	1:A:213:PRO:HA	1.87	0.57
1:H:105:GLN:H	1:H:105:GLN:HE21	1.51	0.56
2:L:141:TYR:CD1	2:L:142:PRO:HA	2.41	0.55
1:C:119:PRO:HD2	1:C:205:THR:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:ARG:NH1	6:E:251:HOH:O	2.26	0.55
1:H:178:LEU:C	1:H:178:LEU:HD12	2.32	0.54
1:H:169:VAL:HG21	2:L:178:TYR:CE2	2.43	0.54
1:C:93:ALA:HB1	1:C:100(B):SER:HB3	1.89	0.54
1:H:97:ARG:CZ	2:L:32:PHE:HE1	2.20	0.54
1:H:169:VAL:CG2	2:L:178:TYR:CE2	2.91	0.53
1:A:159:LEU:HD21	1:A:182:VAL:HG21	1.90	0.53
1:A:66:ARG:NH2	1:A:86:ASP:OD1	2.41	0.53
1:A:172:SER:HB3	1:E:193:THR:OG1	2.09	0.53
2:L:209:PRO:O	2:L:210:THR:C	2.53	0.52
2:L:111:LYS:NZ	2:L:199:GLU:OE2	2.42	0.52
1:A:93:ALA:HB1	1:A:100(B):SER:HB3	1.92	0.52
1:H:12:VAL:HG11	1:H:82(C):LEU:HD13	1.92	0.51
1:E:83:ARG:HG3	1:E:85:GLU:HG2	1.92	0.51
1:E:3:GLN:NE2	6:E:740:HOH:O	2.26	0.51
2:F:168:GLN:O	2:F:169:SER:O	2.29	0.51
2:D:133:LEU:HD12	2:D:179:LEU:HD23	1.92	0.51
1:E:178:LEU:C	1:E:178:LEU:HD12	2.36	0.50
1:E:11:LEU:HB2	1:E:147:PRO:HG3	1.92	0.50
2:L:19:ILE:HD11	2:L:75:ILE:HD12	1.94	0.50
1:E:66:ARG:CD	6:E:794:HOH:O	2.52	0.50
1:C:12:VAL:HG11	1:C:82(C):LEU:HD13	1.93	0.50
1:H:181:VAL:HG11	2:L:136:LEU:HD12	1.94	0.49
2:F:141:TYR:CG	2:F:142:PRO:HA	2.47	0.49
1:A:20:LEU:HG	1:A:82:MET:CE	2.42	0.49
1:C:182:VAL:HG12	1:C:184:VAL:HG13	1.94	0.49
2:D:89:SER:OG	2:D:96:ARG:NH1	2.45	0.48
1:E:20:LEU:HG	1:E:82:MET:HE2	1.95	0.48
1:E:105:GLN:H	1:E:105:GLN:CD	2.21	0.48
2:L:121:PRO:HD3	2:L:133:LEU:CD2	2.42	0.48
2:B:170:ASN:O	2:B:171:ASN:HB2	2.14	0.48
1:C:13:GLN:HG2	2:F:129:ASN:OD1	2.13	0.47
1:H:97:ARG:NH2	2:L:32:PHE:CE1	2.82	0.47
1:A:1:GLU:CG	1:A:2:VAL:H	2.27	0.47
2:D:121:PRO:HD3	2:D:133:LEU:CD2	2.44	0.47
1:E:93:ALA:HB1	1:E:100(B):SER:HB3	1.96	0.47
1:H:169:VAL:HG22	2:L:163:THR:CG2	2.44	0.47
2:F:157:LYS:O	2:F:158:ALA:HB3	2.15	0.47
2:F:168:GLN:N	2:F:172:LYS:O	2.43	0.46
2:L:32:PHE:O	2:L:90:SER:HA	2.15	0.46
1:E:29:PHE:CD2	1:E:76:ASN:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:GLN:H	1:H:105:GLN:CD	2.22	0.46
1:H:143:LYS:HE2	3:H:222:SO4:O1	2.15	0.46
1:E:192:GLN:HG2	1:E:194:TYR:CZ	2.51	0.46
1:C:167:PRO:HG2	2:D:166:SER:OG	2.16	0.45
1:E:116:THR:HG21	1:E:202:PRO:C	2.42	0.45
1:H:138:LEU:CD1	1:H:182:VAL:HG13	2.46	0.45
1:C:134:GLY:O	1:C:185:PRO:HA	2.17	0.45
1:E:143:LYS:CE	6:E:734:HOH:O	2.64	0.45
2:L:105:THR:HG23	6:L:331:HOH:O	2.17	0.45
1:E:116:THR:HG21	1:E:202:PRO:O	2.17	0.45
1:H:63:VAL:HG13	1:H:67:PHE:HB2	1.99	0.44
1:E:134:GLY:HA2	1:E:135:THR:HA	1.68	0.44
1:A:22:CYS:HB3	1:A:78:LEU:HB3	2.00	0.44
1:E:66:ARG:NH2	1:E:86:ASP:OD1	2.33	0.44
2:L:11:VAL:HG23	2:L:104:LEU:HD13	1.99	0.44
1:H:142:VAL:HG11	1:H:150:VAL:HG11	1.99	0.44
2:L:50:GLU:O	2:L:51:VAL:HG13	2.17	0.44
2:B:133:LEU:HG	2:B:181:LEU:HD11	1.99	0.44
2:B:51:VAL:HG21	2:B:66:LYS:HG2	2.00	0.44
2:D:54:ARG:HG2	2:D:58:ILE:HB	1.99	0.44
1:C:96:LEU:HG	1:C:100(A):GLY:O	2.18	0.44
2:F:32:PHE:O	2:F:90:SER:HA	2.18	0.44
1:A:169:VAL:HG21	2:B:178:TYR:CD2	2.53	0.43
1:C:136:ALA:CB	1:C:189:LEU:HD21	2.48	0.43
1:E:134:GLY:HA2	1:E:185:PRO:HA	2.00	0.43
2:F:167:LYS:NZ	2:F:171:ASN:OD1	2.50	0.43
1:H:212:GLU:OE2	1:H:212:GLU:HA	2.18	0.43
1:A:143:LYS:HE3	2:B:132:THR:OG1	2.18	0.43
1:A:162:GLY:O	1:A:182:VAL:HA	2.18	0.43
2:D:168:GLN:HE21	2:D:170:ASN:HB2	1.82	0.43
2:B:121:PRO:HD3	2:B:133:LEU:CD2	2.48	0.43
2:L:96:ARG:NH1	6:L:617:HOH:O	2.50	0.43
1:A:36:TRP:NE1	1:A:80:LEU:HB2	2.34	0.43
1:A:51:ILE:HD13	1:A:71:ARG:HG2	2.01	0.43
1:H:30:SER:O	1:H:52(A):ASN:HB2	2.18	0.43
1:H:169:VAL:CG2	2:L:178:TYR:HE2	2.31	0.43
2:D:109:GLN:HA	2:D:110:PRO:HD2	1.90	0.43
2:D:93:GLY:O	2:D:95(B):PHE:HA	2.19	0.43
1:H:66:ARG:NH2	1:H:86:ASP:OD1	2.41	0.43
1:A:169:VAL:HG22	2:B:178:TYR:CE2	2.54	0.43
2:B:181:LEU:HD23	2:B:192:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:GLU:O	2:B:51:VAL:HG13	2.19	0.42
1:A:67:PHE:HA	1:A:81:VAL:O	2.19	0.42
1:E:124:LEU:HB3	2:F:119:PHE:CG	2.55	0.42
2:D:181:LEU:H	2:D:181:LEU:HD23	1.85	0.42
1:A:201:LYS:N	1:A:202:PRO:CD	2.82	0.41
1:H:199:ASN:OD1	1:H:201:LYS:HG3	2.19	0.41
1:H:181:VAL:CG1	2:L:136:LEU:CD1	2.99	0.41
1:C:145:TYR:CE1	1:C:150:VAL:HG23	2.54	0.41
1:E:138:LEU:O	1:E:181:VAL:HG23	2.21	0.41
2:F:60:ASN:OD1	2:F:60:ASN:C	2.63	0.41
2:L:143:GLY:O	2:L:165:PRO:HG2	2.20	0.41
1:A:126:PRO:HD3	1:A:138:LEU:HB3	2.03	0.41
2:F:150:LYS:HE2	2:F:195:GLN:NE2	2.36	0.41
1:C:36:TRP:CE2	1:C:80:LEU:HB2	2.56	0.41
1:C:126:PRO:HG2	1:C:213:PRO:HA	2.02	0.41
1:C:186:SER:O	1:C:188:SER:N	2.54	0.41
2:F:5:LEU:HD22	2:F:25:GLY:CA	2.50	0.41
1:H:51:ILE:HD12	1:H:57:THR:HG22	2.02	0.41
1:H:12:VAL:O	1:H:111:VAL:HA	2.21	0.40
2:L:62:PHE:CE2	2:L:75:ILE:HG12	2.56	0.40
1:A:71:ARG:HD2	1:A:73:ASN:OD1	2.20	0.40
1:A:121:VAL:O	1:A:209:LYS:HE3	2.21	0.40
1:H:93:ALA:HB1	1:H:100(B):SER:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:GLU:OE1	6:E:471:HOH:O[2_655]	1.79	0.41

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	208/226 (92%)	204 (98%)	3 (1%)	1 (0%)	24	16
1	C	208/226 (92%)	203 (98%)	3 (1%)	2 (1%)	12	5
1	E	206/226 (91%)	203 (98%)	3 (2%)	0	100	100
1	H	207/226 (92%)	203 (98%)	4 (2%)	0	100	100
2	B	210/217 (97%)	202 (96%)	7 (3%)	1 (0%)	24	16
2	D	210/217 (97%)	201 (96%)	8 (4%)	1 (0%)	24	16
2	F	210/217 (97%)	200 (95%)	7 (3%)	3 (1%)	9	3
2	L	210/217 (97%)	200 (95%)	10 (5%)	0	100	100
All	All	1669/1772 (94%)	1616 (97%)	45 (3%)	8 (0%)	24	16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	169	SER
1	C	189	LEU
1	A	62	SER
1	C	187	SER
2	F	168	GLN
2	B	51	VAL
2	D	51	VAL
2	F	51	VAL

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	176/189 (93%)	166 (94%)	10 (6%)	18	8
1	C	176/189 (93%)	164 (93%)	12 (7%)	14	5
1	E	174/189 (92%)	168 (97%)	6 (3%)	32	23
1	H	175/189 (93%)	165 (94%)	10 (6%)	18	8
2	B	177/182 (97%)	169 (96%)	8 (4%)	24	14
2	D	177/182 (97%)	173 (98%)	4 (2%)	44	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	177/182 (97%)	168 (95%)	9 (5%)	21	10
2	L	177/182 (97%)	173 (98%)	4 (2%)	44	38
All	All	1409/1484 (95%)	1346 (96%)	63 (4%)	24	14

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLU
1	H	13	GLN
1	H	63	VAL
1	H	105	GLN
1	H	135	THR
1	H	138	LEU
1	H	150	VAL
1	H	178	LEU
1	H	191	THR
1	H	212	GLU
2	L	51	VAL
2	L	115	SER
2	L	147	VAL
2	L	210	THR
1	A	18	LEU
1	A	19	ARG
1	A	31	THR
1	A	63	VAL
1	A	117	LYS
1	A	135	THR
1	A	169	VAL
1	A	172	SER
1	A	178	LEU
1	A	204	ASN
2	B	51	VAL
2	B	78	LEU
2	B	96	ARG
2	B	107	ARG
2	B	157	LYS
2	B	181	LEU
2	B	197	THR
2	B	199	GLU
1	C	1	GLU
1	C	18	LEU

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Mol	Chain	Res	Type
1	C	19	ARG
1	C	31	THR
1	C	96	LEU
1	C	116	THR
1	C	138	LEU
1	C	171	GLN
1	C	178	LEU
1	C	181	VAL
1	C	186	SER
1	C	191	THR
2	D	19	ILE
2	D	51	VAL
2	D	147	VAL
2	D	181	LEU
1	E	41	PRO
1	E	105	GLN
1	E	169	VAL
1	E	191	THR
1	E	193	THR
1	E	201	LYS
2	F	42	LYS
2	F	51	VAL
2	F	139	ASP
2	F	145	VAL
2	F	146	THR
2	F	157	LYS
2	F	161	GLU
2	F	168	GLN
2	F	169	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	37	GLN
2	L	109	GLN
2	L	195	GLN
1	A	82(A)	ASN
2	B	37	GLN
1	C	56	ASN
1	C	192	GLN
2	D	37	GLN
2	D	69	ASN

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Mol	Chain	Res	Type
2	D	129	ASN
1	E	39	GLN
1	E	199	ASN
2	F	38	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 24 ligands modelled in this entry, 14 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	D	215	-	4,4,4	0.19	0	6,6,6	0.21	0
3	SO4	H	221	-	4,4,4	0.24	0	6,6,6	0.51	0
4	GOL	L	215	-	5,5,5	0.65	0	5,5,5	1.17	0
3	SO4	H	222	-	4,4,4	0.25	0	6,6,6	0.23	0
3	SO4	L	214	-	4,4,4	0.26	0	6,6,6	0.49	0
3	SO4	D	214	-	4,4,4	0.34	0	6,6,6	0.81	0
3	SO4	F	215	-	4,4,4	0.29	0	6,6,6	0.39	0
3	SO4	B	214	-	4,4,4	0.25	0	6,6,6	0.30	0
3	SO4	F	214	-	4,4,4	0.19	0	6,6,6	0.34	0
4	GOL	H	223	-	5,5,5	0.57	0	5,5,5	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	223	-	-	4/4/4/4	-
4	GOL	L	215	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	215	GOL	C1-C2-C3-O3
4	H	223	GOL	O1-C1-C2-C3
4	H	223	GOL	C1-C2-C3-O3
4	H	223	GOL	O1-C1-C2-O2
4	H	223	GOL	O2-C2-C3-O3
4	L	215	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	215	GOL	3	0
3	H	222	SO4	1	0
3	B	214	SO4	1	0

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	212/226 (93%)	0.09	1 (0%) 87 90	27, 42, 56, 66	0
1	C	212/226 (93%)	0.28	4 (1%) 66 74	31, 44, 65, 82	0
1	E	210/226 (92%)	-0.17	1 (0%) 87 90	21, 32, 53, 63	0
1	H	211/226 (93%)	-0.11	1 (0%) 87 90	21, 33, 54, 59	0
2	B	212/217 (97%)	-0.00	2 (0%) 81 85	24, 39, 50, 59	0
2	D	212/217 (97%)	0.14	3 (1%) 73 79	26, 42, 52, 58	0
2	F	212/217 (97%)	-0.13	3 (1%) 73 79	21, 34, 51, 69	0
2	L	212/217 (97%)	-0.08	0 100 100	22, 34, 53, 62	0
All	All	1693/1772 (95%)	0.00	15 (0%) 81 85	21, 38, 55, 82	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	160	THR	3.6
1	C	190	GLY	3.1
2	F	168	GLN	3.0
2	F	170	ASN	2.8
2	B	4	ALA	2.6
2	B	108	GLY	2.5
2	D	32	PHE	2.5
2	D	108	GLY	2.5
2	F	169	SER	2.4
1	A	134	GLY	2.3
1	C	186	SER	2.3
1	C	191	THR	2.3
1	C	189	LEU	2.2
1	E	134	GLY	2.2
2	D	210	THR	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
4	GOL	L	215	6/6	0.71	0.16	51,52,53,57	0
3	SO4	B	214	5/5	0.75	0.11	93,94,95,95	0
3	SO4	F	215	5/5	0.79	0.11	78,79,81,82	0
3	SO4	H	222	5/5	0.80	0.09	89,89,90,90	0
3	SO4	D	215	5/5	0.85	0.08	86,87,87,89	0
3	SO4	L	214	5/5	0.86	0.10	67,68,69,70	0
5	CL	B	216	1/1	0.88	0.12	73,73,73,73	0
3	SO4	H	221	5/5	0.89	0.11	59,59,62,62	0
4	GOL	H	223	6/6	0.90	0.12	49,51,52,53	0
5	CL	E	222	1/1	0.90	0.11	68,68,68,68	0
5	CL	D	216	1/1	0.91	0.13	86,86,86,86	0
3	SO4	F	214	5/5	0.92	0.08	71,71,72,72	0
5	CL	E	223	1/1	0.92	0.13	63,63,63,63	0
5	CL	H	225	1/1	0.93	0.07	75,75,75,75	0
5	CL	E	221	1/1	0.93	0.19	60,60,60,60	0
5	CL	H	224	1/1	0.94	0.12	72,72,72,72	0
3	SO4	D	214	5/5	0.94	0.08	42,45,49,50	0
5	CL	L	216	1/1	0.94	0.21	68,68,68,68	0
5	CL	L	217	1/1	0.94	0.12	68,68,68,68	0
5	CL	A	221	1/1	0.94	0.19	66,66,66,66	0
5	CL	F	216	1/1	0.95	0.19	63,63,63,63	0
5	CL	D	1	1/1	0.96	0.17	59,59,59,59	0
5	CL	B	215	1/1	0.96	0.22	63,63,63,63	0
5	CL	F	217	1/1	0.99	0.03	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.