



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:55 PM UTC

PDB ID : 6VMJ / pdb_00006vmj
Title : Crystal structure of human Complement Factor D with anti-Factor D Fab 20D12
Authors : Wu, P.; Harris, S.F.; Eigenbrot, C.
Deposited on : 2020-01-28
Resolution : 2.95 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

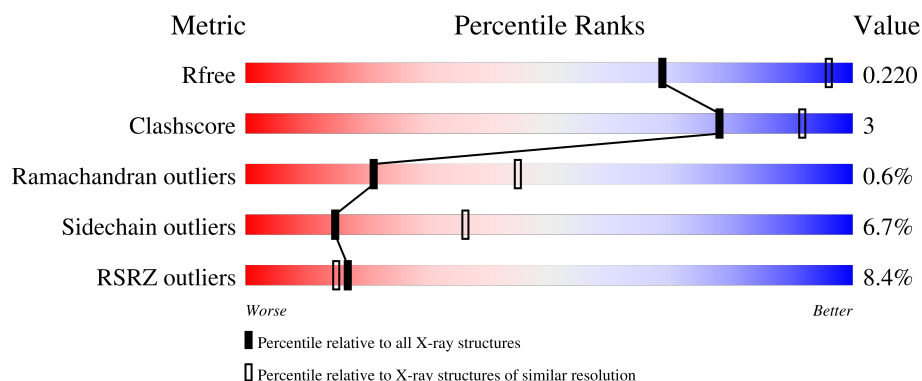
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	214	20% 87% 12%
1	E	214	25% 84% 14% .
1	I	214	4% 81% 17% .
1	L	214	83% 15% .
2	B	223	25% 83% 11% 5%

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Mol	Chain	Length	Quality of chain
2	F	223	16% 78% 15% • 5%
2	J	223	4% 80% 14% • 5%
2	M	223	2% 83% 12% • •
3	W	228	% 89% 11% •
3	X	228	% 84% 14% •
3	Y	228	% 86% 14% •
3	Z	228	% 89% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19932 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 Fab20D12 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1635	1020	274	336	5			
1	E	213	Total	C	N	O	S	0	0	0
			1635	1020	274	336	5			
1	I	213	Total	C	N	O	S	0	0	0
			1635	1020	274	336	5			
1	L	213	Total	C	N	O	S	0	0	0
			1635	1020	274	336	5			

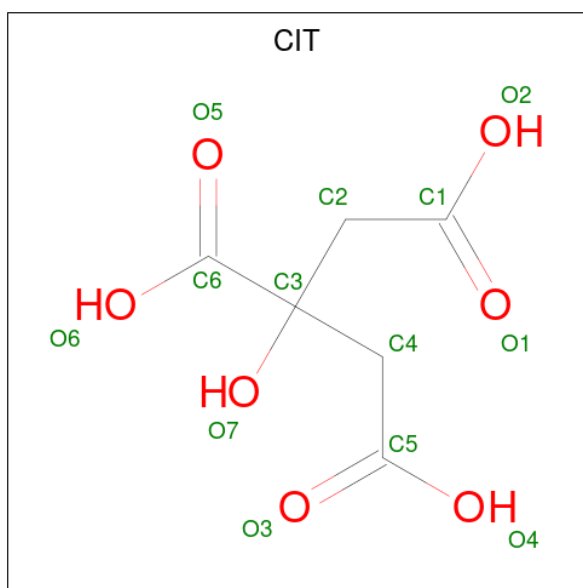
- Molecule 2 is a protein called Fab20D12 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1574	997	257	315	5			
2	F	211	Total	C	N	O	S	0	0	0
			1574	997	257	315	5			
2	J	211	Total	C	N	O	S	0	0	0
			1574	997	257	315	5			
2	M	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			

- Molecule 3 is a protein called Complement factor D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
3	X	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
3	Y	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
3	Z	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		
4	F	1	Total	C	O	0	0
			13	6	7		
4	J	1	Total	C	O	0	0
			13	6	7		
4	M	1	Total	C	O	0	0
			13	6	7		
4	W	1	Total	C	O	0	0
			13	6	7		
4	X	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	E	6	Total	O	0	0
			6	6		
5	F	6	Total	O	0	0
			6	6		
5	I	5	Total	O	0	0
			5	5		
5	J	15	Total	O	0	0
			15	15		

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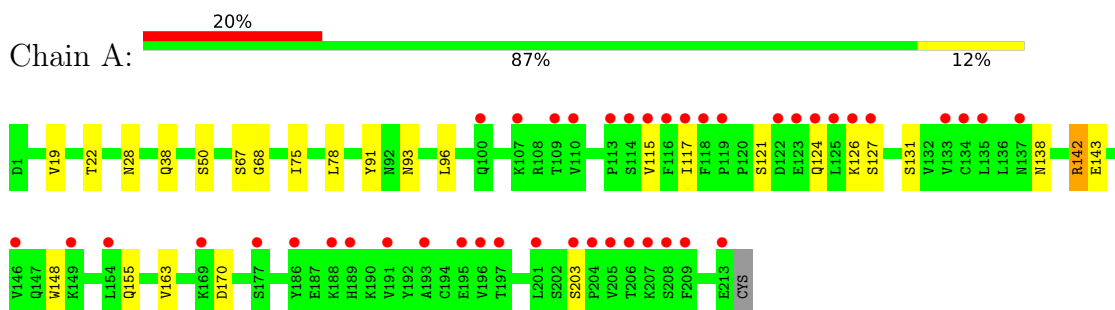
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	21	Total 21	O 21	0	0
5	M	13	Total 13	O 13	0	0
5	W	23	Total 23	O 23	0	0
5	X	27	Total 27	O 27	0	0
5	Y	13	Total 13	O 13	0	0
5	Z	14	Total 14	O 14	0	0

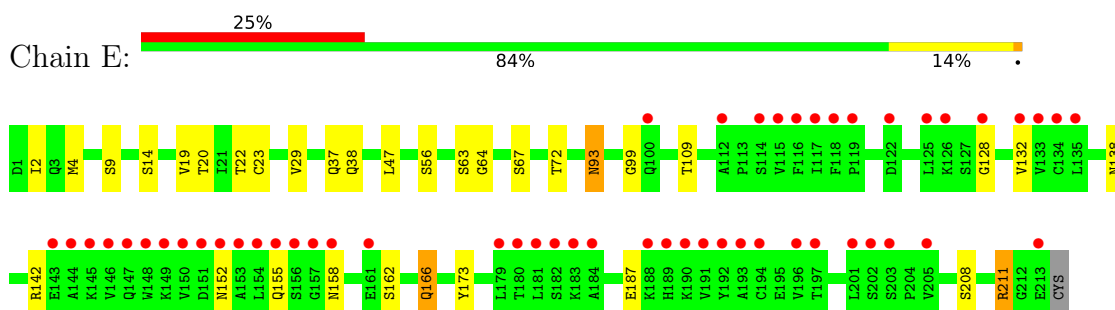
3 Residue-property plots [i](#)

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.

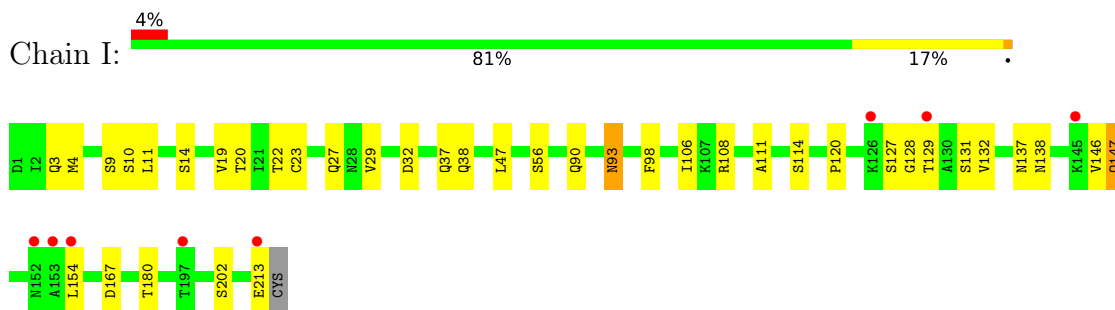
- Molecule 1: Fab20D12 Light Chain



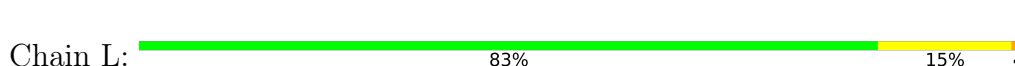
- Molecule 1: Fab20D12 Light Chain

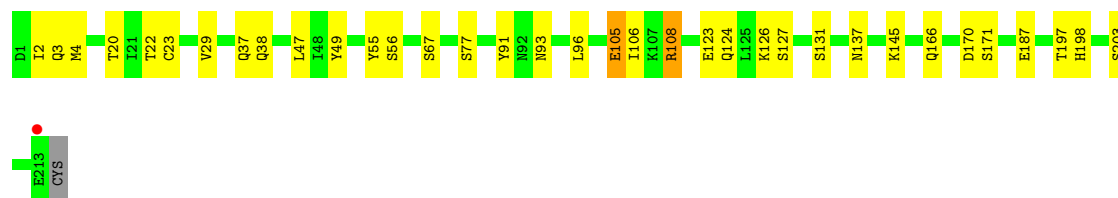


- Molecule 1: Fab20D12 Light Chain

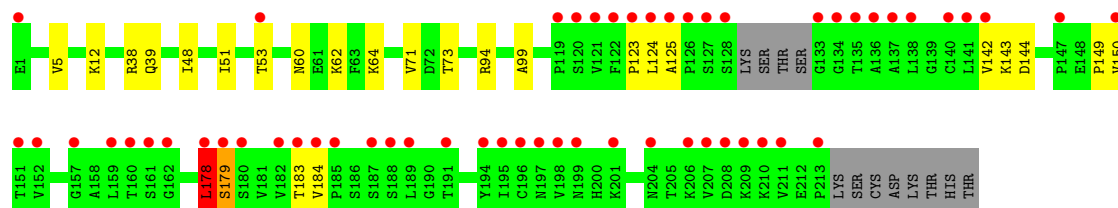
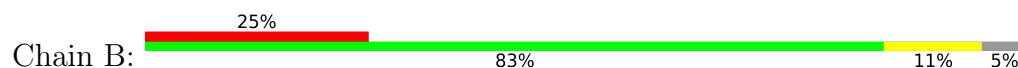


- Molecule 1: Fab20D12 Light Chain

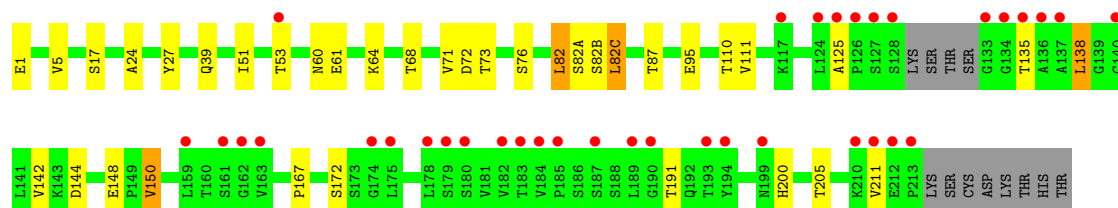
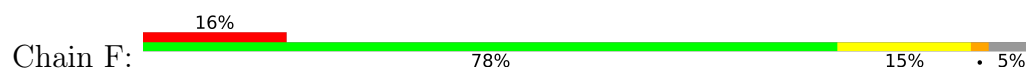




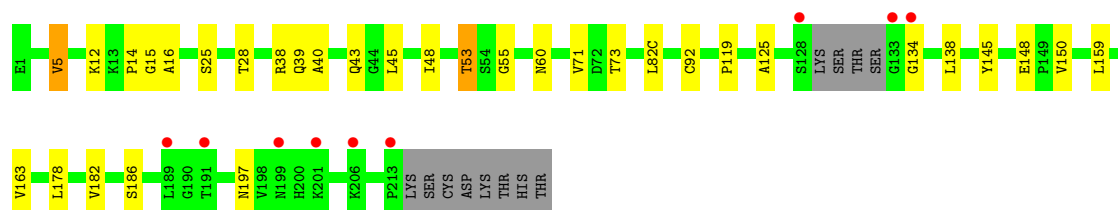
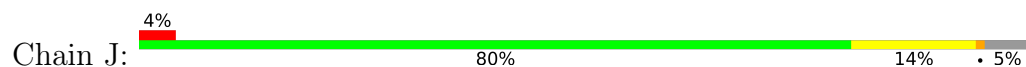
- Molecule 2: Fab20D12 heavy chain



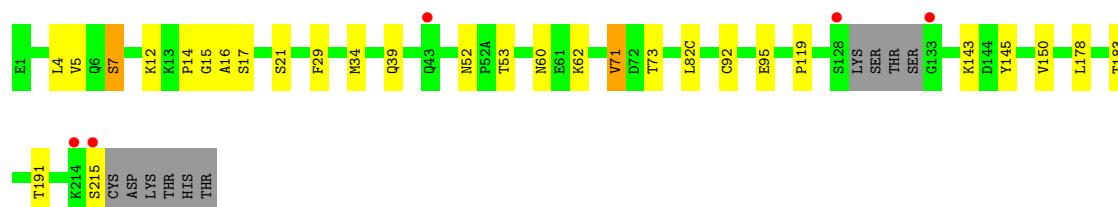
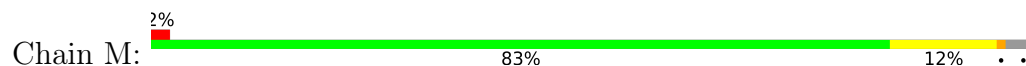
- Molecule 2: Fab20D12 heavy chain



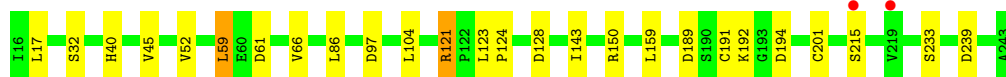
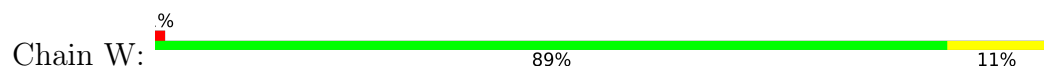
- Molecule 2: Fab20D12 heavy chain



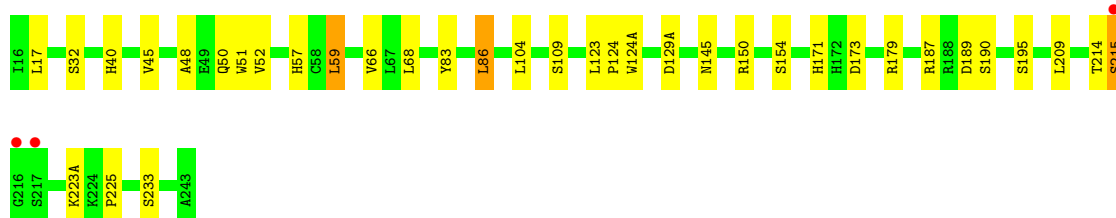
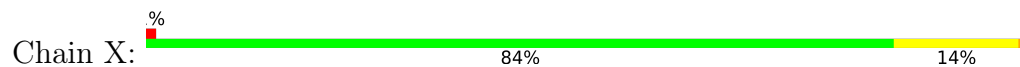
- Molecule 2: Fab20D12 heavy chain



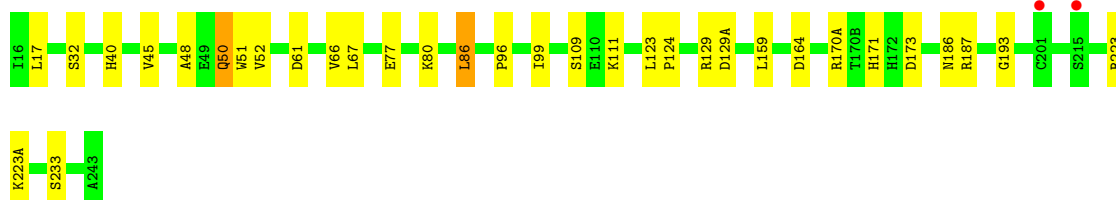
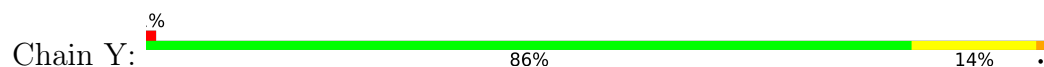
- Molecule 3: Complement factor D



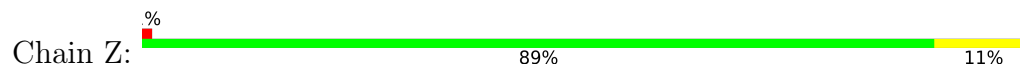
- Molecule 3: Complement factor D



- Molecule 3: Complement factor D



- Molecule 3: Complement factor D



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	180.84Å 180.84Å 304.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.24 – 2.95 47.24 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.24-2.95) 99.3 (47.24-2.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.217 , 0.265 (Not available) , 0.220	Depositor DCC
R_{free} test set	1050 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19932	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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 i

5.1 Standard geometry i

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

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	0.83	0/1670	1.21	3/2267 (0.1%)
1	E	0.85	0/1670	1.27	6/2267 (0.3%)
1	I	0.76	0/1670	1.23	6/2267 (0.3%)
1	L	0.82	0/1670	1.21	5/2267 (0.2%)
2	B	0.80	0/1612	1.23	10/2198 (0.5%)
2	F	0.82	0/1612	1.29	10/2198 (0.5%)
2	J	0.79	0/1612	1.24	13/2198 (0.6%)
2	M	0.81	0/1627	1.23	4/2217 (0.2%)
3	W	0.85	0/1753	1.25	4/2385 (0.2%)
3	X	0.86	0/1753	1.24	4/2385 (0.2%)
3	Y	0.81	0/1753	1.25	4/2385 (0.2%)
3	Z	0.83	0/1753	1.22	5/2385 (0.2%)
All	All	0.82	0/20155	1.24	74/27419 (0.3%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	93	ASN	CA-CB-CG	8.94	121.54	112.60
1	I	128	GLY	N-CA-C	7.81	123.07	114.40
3	X	129(A)	ASP	CA-CB-CG	7.80	120.40	112.60
3	X	189	ASP	CA-CB-CG	7.38	119.98	112.60
1	E	128	GLY	N-CA-C	7.30	122.98	113.27
2	M	15	GLY	CA-C-N	6.61	134.16	121.54
2	M	15	GLY	C-N-CA	6.61	134.16	121.54
2	B	60	ASN	N-CA-C	-6.49	98.69	109.46
3	X	173	ASP	CA-CB-CG	6.24	118.84	112.60
3	Z	173	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	170	ASP	CA-CB-CG	6.19	118.79	112.60
3	Z	189	ASP	CA-CB-CG	6.19	118.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	189	ASP	CA-CB-CG	6.17	118.77	112.60
2	F	172	SER	CA-C-N	6.17	129.17	120.28
2	F	172	SER	C-N-CA	6.17	129.17	120.28
2	F	60	ASN	N-CA-C	-6.08	99.30	108.96
2	M	60	ASN	N-CA-C	-6.04	99.35	108.96
2	F	72	ASP	CA-C-N	6.03	129.19	120.38
2	F	72	ASP	C-N-CA	6.03	129.19	120.38
2	B	124	LEU	CA-C-N	6.03	128.85	120.65
2	B	124	LEU	C-N-CA	6.03	128.85	120.65
2	F	64	LYS	CA-C-N	6.03	128.68	120.54
2	F	64	LYS	C-N-CA	6.03	128.68	120.54
1	A	93	ASN	CA-CB-CG	5.96	118.56	112.60
1	I	93	ASN	CA-CB-CG	5.82	118.42	112.60
1	I	167	ASP	CA-C-N	5.76	128.00	120.28
1	I	167	ASP	C-N-CA	5.76	128.00	120.28
2	J	28	THR	CA-C-N	5.66	127.80	120.44
2	J	28	THR	C-N-CA	5.66	127.80	120.44
2	J	186	SER	CA-C-N	5.64	128.10	120.38
2	J	186	SER	C-N-CA	5.64	128.10	120.38
1	I	98	PHE	CA-CB-CG	5.63	119.43	113.80
2	M	92	CYS	N-CA-C	-5.62	100.54	109.76
3	Z	164	ASP	CA-C-N	5.60	128.10	120.54
3	Z	164	ASP	C-N-CA	5.60	128.10	120.54
2	F	125	ALA	N-CA-C	5.57	116.00	109.60
2	J	55	GLY	CA-C-N	5.57	125.39	120.10
2	J	55	GLY	C-N-CA	5.57	125.39	120.10
1	L	187	GLU	CB-CG-CD	5.56	122.05	112.60
2	B	143	LYS	CA-C-N	5.53	132.11	121.54
2	B	143	LYS	C-N-CA	5.53	132.11	121.54
2	J	60	ASN	N-CA-C	-5.52	100.99	109.76
1	L	170	ASP	CA-CB-CG	5.49	118.09	112.60
3	W	128	ASP	CA-CB-CG	5.47	118.07	112.60
1	E	99	GLY	N-CA-C	-5.46	105.29	112.82
3	Y	173	ASP	CA-CB-CG	5.37	117.97	112.60
3	Y	96	PRO	CA-C-N	5.36	128.00	120.28
3	Y	96	PRO	C-N-CA	5.36	128.00	120.28
2	J	125	ALA	N-CA-C	5.33	115.73	109.60
1	A	126	LYS	N-CA-C	-5.32	105.56	111.36
1	L	127	SER	N-CA-C	-5.28	103.07	110.35
2	F	61	GLU	CA-C-N	5.27	127.60	120.38
2	F	61	GLU	C-N-CA	5.27	127.60	120.38
2	J	5	VAL	N-CA-CB	5.26	118.09	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	9	SER	N-CA-C	-5.21	105.67	112.23
2	B	125	ALA	N-CA-C	5.17	116.93	109.48
3	Y	61	ASP	CA-CB-CG	5.17	117.77	112.60
2	B	178	LEU	CA-C-N	5.17	131.40	121.54
2	B	178	LEU	C-N-CA	5.17	131.40	121.54
1	L	198	HIS	CA-C-N	5.16	127.45	120.38
1	L	198	HIS	C-N-CA	5.16	127.45	120.38
2	J	53	THR	N-CA-C	-5.12	106.72	113.12
3	X	145	ASN	CA-CB-CG	5.11	117.71	112.60
1	E	166	GLN	CA-C-N	5.10	128.35	121.05
1	E	166	GLN	C-N-CA	5.10	128.35	121.05
3	W	61	ASP	CA-CB-CG	5.10	117.70	112.60
2	J	92	CYS	N-CA-C	-5.09	101.40	109.76
2	B	64	LYS	CA-C-N	5.06	127.02	120.44
2	B	64	LYS	C-N-CA	5.06	127.02	120.44
1	E	208	SER	N-CA-C	5.06	115.72	108.74
2	J	15	GLY	CA-C-N	5.06	131.20	121.54
2	J	15	GLY	C-N-CA	5.06	131.20	121.54
3	Z	170(B)	THR	CB-CA-C	-5.04	102.42	110.79
3	W	239	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1635	0	1578	10	0
1	E	1635	0	1578	10	0
1	I	1635	0	1578	12	0
1	L	1635	0	1578	16	0
2	B	1574	0	1536	5	0
2	F	1574	0	1536	9	0
2	J	1574	0	1536	10	0
2	M	1589	0	1554	7	0
3	W	1713	0	1696	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	1713	0	1696	15	0
3	Y	1713	0	1696	13	0
3	Z	1713	0	1696	7	0
4	B	13	0	5	1	0
4	F	13	0	5	0	0
4	J	13	0	5	0	0
4	M	13	0	5	0	0
4	W	13	0	5	0	0
4	X	13	0	5	0	0
5	A	8	0	0	0	0
5	E	6	0	0	0	0
5	F	6	0	0	0	0
5	I	5	0	0	0	0
5	J	15	0	0	0	0
5	L	21	0	0	0	0
5	M	13	0	0	0	0
5	W	23	0	0	0	0
5	X	27	0	0	0	0
5	Y	13	0	0	0	0
5	Z	14	0	0	0	0
All	All	19932	0	19288	109	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 3.

All (109) 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:L:108:ARG:HH21	1:L:108:ARG:HG3	1.30	0.94
1:L:38:GLN:HE22	2:M:39:GLN:HE22	1.23	0.83
1:I:108:ARG:HH12	1:I:111:ALA:HB2	1.44	0.82
1:E:67:SER:HB3	3:X:150:ARG:HG3	1.61	0.79
3:Z:86:LEU:HD13	3:Z:109:SER:HA	1.65	0.78
1:A:38:GLN:HE22	2:B:39:GLN:HE22	1.29	0.77
3:W:123:LEU:HD12	3:W:124:PRO:HD2	1.67	0.75
3:X:123:LEU:HD12	3:X:124:PRO:HD2	1.69	0.74
1:E:38:GLN:HE22	2:F:39:GLN:HE22	1.33	0.74
3:X:86:LEU:HD13	3:X:109:SER:HA	1.73	0.70
2:M:52:ASN:OD1	2:M:53:THR:HB	1.92	0.69
1:A:67:SER:HB3	3:W:150:ARG:HG3	1.78	0.65
3:Y:86:LEU:HD13	3:Y:109:SER:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:32:SER:OG	3:W:40:HIS:HD2	1.80	0.65
1:I:38:GLN:HE22	2:J:39:GLN:HE22	1.45	0.65
2:B:38:ARG:HB2	2:B:48:ILE:HD11	1.78	0.64
3:Y:123:LEU:HD12	3:Y:124:PRO:HD2	1.78	0.63
1:I:147:GLN:HG3	1:I:154:LEU:HD13	1.81	0.62
2:M:4:LEU:HD22	2:M:34:MET:HE1	1.83	0.60
3:Y:52:VAL:HG21	3:Y:66:VAL:HG11	1.82	0.59
2:J:38:ARG:HB3	2:J:48:ILE:HD11	1.85	0.58
1:L:108:ARG:HH21	1:L:108:ARG:CG	2.13	0.58
3:Z:186:ASN:HB2	3:Z:223:ARG:HB3	1.86	0.58
3:W:59:LEU:HD22	3:W:104:LEU:HD21	1.85	0.58
2:F:142:VAL:HG11	2:F:150:VAL:HG11	1.85	0.57
1:E:4:MET:HE3	1:E:23:CYS:SG	2.45	0.57
1:L:108:ARG:HG3	1:L:108:ARG:NH2	2.10	0.56
2:F:87:THR:HG23	2:F:110:THR:HA	1.88	0.56
2:B:142:VAL:HB	2:B:178:LEU:HB3	1.88	0.55
1:L:67:SER:HB3	3:Z:150:ARG:HG3	1.89	0.55
1:A:121:SER:HB3	2:B:123:PRO:HD2	1.88	0.55
1:L:145:LYS:HB3	1:L:197:THR:HB	1.89	0.54
3:Z:52:VAL:HG21	3:Z:66:VAL:HG11	1.90	0.54
1:I:108:ARG:NH1	1:I:111:ALA:HB2	2.19	0.54
1:L:4:MET:HE3	1:L:23:CYS:SG	2.49	0.53
2:F:138:LEU:HB2	2:F:211:VAL:HG11	1.91	0.53
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.92	0.52
2:J:39:GLN:HB2	2:J:45:LEU:HD23	1.91	0.52
3:W:52:VAL:HG21	3:W:66:VAL:HG11	1.91	0.52
1:E:166:GLN:HB3	1:E:173:TYR:CZ	2.46	0.51
3:Z:32:SER:HB3	3:Z:67:LEU:HB3	1.92	0.51
1:L:2:ILE:HD13	1:L:29:VAL:HG12	1.92	0.51
1:L:108:ARG:HD2	1:L:171:SER:HB2	1.93	0.51
1:A:142:ARG:HD2	1:A:163:VAL:HG11	1.92	0.51
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.92	0.51
1:E:155:GLN:HB3	1:E:158:ASN:HD21	1.76	0.50
1:A:91:TYR:HA	1:A:96:LEU:HG	1.94	0.50
3:X:57:HIS:CE1	3:X:214:THR:O	2.65	0.49
1:I:37:GLN:HB2	1:I:47:LEU:HD11	1.95	0.49
2:M:14:PRO:O	2:M:82(C):LEU:O	2.30	0.49
2:J:163:VAL:HG22	2:J:182:VAL:HB	1.95	0.49
3:Y:67:LEU:HD11	3:Y:80:LYS:HG2	1.95	0.49
2:J:14:PRO:O	2:J:82(C):LEU:O	2.31	0.48
3:X:52:VAL:HG21	3:X:66:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLN:HE22	1:A:131:SER:H	1.62	0.48
2:M:7:SER:HB3	2:M:21:SER:H	1.79	0.48
2:B:94:ARG:HH22	4:B:301:CIT:H42	1.79	0.48
3:Z:123:LEU:HD12	3:Z:124:PRO:HD2	1.96	0.47
2:F:95:GLU:OE2	3:Y:170(A):ARG:HD3	2.14	0.47
3:X:32:SER:OG	3:X:40:HIS:HD2	1.96	0.47
3:X:59:LEU:HD22	3:X:104:LEU:HD21	1.96	0.47
2:F:82:LEU:HD22	2:F:82(C):LEU:HD23	1.96	0.47
1:L:2:ILE:HD12	1:L:93:ASN:HB3	1.97	0.46
1:I:4:MET:HE3	1:I:23:CYS:SG	2.56	0.46
1:I:120:PRO:HB3	1:I:131:SER:H	1.81	0.46
1:L:49:TYR:HB3	1:L:55:TYR:CZ	2.51	0.46
1:L:91:TYR:HA	1:L:96:LEU:HG	1.99	0.45
3:W:191:CYS:O	3:W:194:ASP:HB2	2.17	0.45
3:W:32:SER:OG	3:W:40:HIS:CD2	2.65	0.45
3:X:171:HIS:HD2	3:X:225:PRO:HD3	1.81	0.45
1:I:29:VAL:HG11	1:I:90:GLN:HG3	2.00	0.44
2:M:119:PRO:HB3	2:M:145:TYR:HB3	1.98	0.44
3:W:143:ILE:HD12	3:W:192:LYS:HB2	1.99	0.44
1:E:2:ILE:HD13	1:E:29:VAL:HG12	1.99	0.44
2:F:24:ALA:HB1	2:F:27:TYR:CE1	2.53	0.44
1:I:120:PRO:HD3	1:I:132:VAL:HG22	1.99	0.44
1:E:64:GLY:HA2	1:E:72:THR:O	2.17	0.43
1:I:38:GLN:NE2	2:J:39:GLN:HE22	2.12	0.43
3:X:124(A):TRP:HA	3:X:209:LEU:HB3	2.01	0.43
3:Z:171:HIS:HD2	3:Z:223(A):LYS:O	2.01	0.43
3:X:124(A):TRP:HB3	3:X:209:LEU:HD23	2.00	0.43
3:Y:50:GLN:HG3	3:Y:111:LYS:HA	2.00	0.43
1:E:187:GLU:HA	1:E:211:ARG:CZ	2.48	0.43
1:A:75:ILE:HG21	1:A:78:LEU:HD12	2.01	0.43
3:X:86:LEU:HD12	3:X:86:LEU:HA	1.89	0.43
3:Y:40:HIS:HE1	3:Y:193:GLY:O	2.02	0.42
3:Y:77:GLU:HB2	3:Y:80:LYS:HB2	2.00	0.42
3:Y:32:SER:HB3	3:Y:67:LEU:HB3	2.01	0.42
1:E:162:SER:OG	2:F:167:PRO:HD2	2.20	0.42
2:J:159:LEU:HD21	2:J:182:VAL:HG21	2.02	0.42
1:L:105:GLU:HG2	1:L:166:GLN:OE1	2.18	0.42
2:F:200:HIS:HB3	2:F:205:THR:HB	2.01	0.42
3:Y:171:HIS:HD2	3:Y:223(A):LYS:O	2.01	0.42
1:L:123:GLU:HA	1:L:126:LYS:HE3	2.01	0.42
1:I:38:GLN:HE22	2:J:39:GLN:NE2	2.13	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ASN:OD1	1:A:68:GLY:HA2	2.20	0.42
3:X:187:ARG:HH22	3:Y:187:ARG:HH22	1.68	0.42
1:I:32:ASP:CG	3:X:223(A):LYS:HZ1	2.27	0.42
1:A:148:TRP:HB2	1:A:155:GLN:HB2	2.02	0.41
3:Y:48:ALA:HB3	3:Y:51:TRP:HB2	2.03	0.41
1:A:124:GLN:NE2	1:A:131:SER:H	2.19	0.41
2:J:119:PRO:HB3	2:J:145:TYR:HB3	2.02	0.41
2:M:29:PHE:HZ	2:M:71:VAL:HG22	1.85	0.41
3:X:68:LEU:HD12	3:X:83:TYR:CE1	2.56	0.41
2:J:40:ALA:HB3	2:J:43:GLN:HG3	2.03	0.41
3:W:121:ARG:CG	3:W:121:ARG:HH11	2.34	0.41
3:Y:186:ASN:HB2	3:Y:223:ARG:HB3	2.03	0.40
1:L:124:GLN:HE22	1:L:131:SER:HB2	1.85	0.40
3:X:48:ALA:HB3	3:X:51:TRP:HB2	2.02	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	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	24	49
1	E	211/214 (99%)	199 (94%)	10 (5%)	2 (1%)	14	34
1	I	211/214 (99%)	202 (96%)	8 (4%)	1 (0%)	24	49
1	L	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
2	B	207/223 (93%)	190 (92%)	13 (6%)	4 (2%)	6	17
2	F	207/223 (93%)	197 (95%)	9 (4%)	1 (0%)	24	49
2	J	207/223 (93%)	197 (95%)	8 (4%)	2 (1%)	12	32
2	M	209/223 (94%)	199 (95%)	9 (4%)	1 (0%)	24	49
3	W	227/228 (100%)	217 (96%)	9 (4%)	1 (0%)	30	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	X	227/228 (100%)	215 (95%)	11 (5%)	1 (0%)	30	53
3	Y	227/228 (100%)	217 (96%)	10 (4%)	0	100	100
3	Z	227/228 (100%)	215 (95%)	11 (5%)	1 (0%)	30	53
All	All	2582/2660 (97%)	2450 (95%)	117 (4%)	15 (1%)	21	45

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	ALA
1	E	211	ARG
3	X	215	SER
1	A	138	ASN
2	B	144	ASP
2	M	16	ALA
2	F	144	ASP
1	E	138	ASN
1	I	138	ASN
2	J	16	ALA
2	B	179	SER
3	W	215	SER
2	J	134	GLY
3	Z	216	GLY
2	B	149	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	187/188 (100%)	178 (95%)	9 (5%)	23	48
1	E	187/188 (100%)	175 (94%)	12 (6%)	16	38
1	I	187/188 (100%)	167 (89%)	20 (11%)	6	18
1	L	187/188 (100%)	177 (95%)	10 (5%)	20	45
2	B	176/188 (94%)	164 (93%)	12 (7%)	14	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	176/188 (94%)	157 (89%)	19 (11%)	6	18
2	J	176/188 (94%)	165 (94%)	11 (6%)	16	38
2	M	178/188 (95%)	164 (92%)	14 (8%)	11	29
3	W	183/182 (100%)	174 (95%)	9 (5%)	22	48
3	X	183/182 (100%)	172 (94%)	11 (6%)	17	40
3	Y	183/182 (100%)	173 (94%)	10 (6%)	19	43
3	Z	183/182 (100%)	174 (95%)	9 (5%)	22	48
All	All	2186/2232 (98%)	2040 (93%)	146 (7%)	15	36

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	22	THR
1	A	50	SER
1	A	115	VAL
1	A	117	ILE
1	A	127	SER
1	A	142	ARG
1	A	143	GLU
1	A	203	SER
2	B	5	VAL
2	B	12	LYS
2	B	51	ILE
2	B	53	THR
2	B	62	LYS
2	B	71	VAL
2	B	73	THR
2	B	150	VAL
2	B	178	LEU
2	B	179	SER
2	B	183	THR
2	B	184	VAL
1	E	9	SER
1	E	14	SER
1	E	19	VAL
1	E	20	THR
1	E	22	THR
1	E	56	SER
1	E	63	SER

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Mol	Chain	Res	Type
1	E	93	ASN
1	E	109	THR
1	E	132	VAL
1	E	142	ARG
1	E	152	ASN
2	F	1	GLU
2	F	5	VAL
2	F	17	SER
2	F	51	ILE
2	F	53	THR
2	F	68	THR
2	F	71	VAL
2	F	73	THR
2	F	76	SER
2	F	82	LEU
2	F	82(A)	SER
2	F	82(B)	SER
2	F	82(C)	LEU
2	F	111	VAL
2	F	135	THR
2	F	138	LEU
2	F	148	GLU
2	F	150	VAL
2	F	191	THR
1	I	3	GLN
1	I	10	SER
1	I	11	LEU
1	I	14	SER
1	I	19	VAL
1	I	20	THR
1	I	22	THR
1	I	27	GLN
1	I	56	SER
1	I	93	ASN
1	I	106	ILE
1	I	114	SER
1	I	127	SER
1	I	129	THR
1	I	137	ASN
1	I	146	VAL
1	I	147	GLN
1	I	180	THR

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Mol	Chain	Res	Type
1	I	202	SER
1	I	213	GLU
2	J	5	VAL
2	J	12	LYS
2	J	25	SER
2	J	53	THR
2	J	71	VAL
2	J	73	THR
2	J	138	LEU
2	J	148	GLU
2	J	150	VAL
2	J	178	LEU
2	J	197	ASN
1	L	3	GLN
1	L	20	THR
1	L	22	THR
1	L	56	SER
1	L	77	SER
1	L	105	GLU
1	L	106	ILE
1	L	108	ARG
1	L	137	ASN
1	L	203	SER
2	M	5	VAL
2	M	7	SER
2	M	12	LYS
2	M	17	SER
2	M	62	LYS
2	M	71	VAL
2	M	73	THR
2	M	95	GLU
2	M	143	LYS
2	M	150	VAL
2	M	178	LEU
2	M	183	THR
2	M	191	THR
2	M	215	SER
3	W	17	LEU
3	W	45	VAL
3	W	59	LEU
3	W	86	LEU
3	W	97	ASP

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Mol	Chain	Res	Type
3	W	121	ARG
3	W	159	LEU
3	W	201	CYS
3	W	233	SER
3	X	17	LEU
3	X	45	VAL
3	X	50	GLN
3	X	59	LEU
3	X	86	LEU
3	X	154	SER
3	X	179	ARG
3	X	190	SER
3	X	195	SER
3	X	215	SER
3	X	233	SER
3	Y	17	LEU
3	Y	45	VAL
3	Y	50	GLN
3	Y	86	LEU
3	Y	99	ILE
3	Y	129	ARG
3	Y	129(A)	ASP
3	Y	159	LEU
3	Y	164	ASP
3	Y	233	SER
3	Z	17	LEU
3	Z	45	VAL
3	Z	59	LEU
3	Z	86	LEU
3	Z	99	ILE
3	Z	138	VAL
3	Z	143	ILE
3	Z	159	LEU
3	Z	201	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	124	GLN
1	A	210	ASN
2	B	171	GLN

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Mol	Chain	Res	Type
2	B	204	ASN
1	E	3	GLN
1	E	38	GLN
1	E	147	GLN
2	F	171	GLN
1	I	137	ASN
1	I	138	ASN
1	I	147	GLN
2	J	3	GLN
2	J	39	GLN
2	J	58	ASN
2	J	164	HIS
2	J	199	ASN
1	L	38	GLN
1	L	92	ASN
1	L	93	ASN
1	L	124	GLN
1	L	137	ASN
1	L	138	ASN
1	L	199	GLN
2	M	58	ASN
2	M	171	GLN
2	M	199	ASN
3	W	40	HIS
3	W	222	ASN
3	X	34	GLN
3	X	40	HIS
3	X	50	GLN
3	X	107	GLN
3	X	171	HIS
3	X	222	ASN
3	Y	40	HIS
3	Y	75	GLN
3	Y	95	GLN
3	Y	107	GLN
3	Y	146	HIS
3	Y	171	HIS
3	Z	34	GLN
3	Z	40	HIS
3	Z	50	GLN
3	Z	75	GLN
3	Z	107	GLN

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Mol	Chain	Res	Type
3	Z	171	HIS

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](#)

6 ligands are modelled in this entry.

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	$\# Z > 2$
4	CIT	B	301	-	12,12,12	0.36	0	17,17,17	0.69	1 (5%)
4	CIT	F	301	-	12,12,12	0.29	0	17,17,17	0.53	0
4	CIT	W	301	-	12,12,12	1.99	6 (50%)	17,17,17	2.13	6 (35%)
4	CIT	X	301	-	12,12,12	1.92	6 (50%)	17,17,17	2.24	6 (35%)
4	CIT	J	301	-	12,12,12	0.51	0	17,17,17	0.77	1 (5%)
4	CIT	M	301	-	12,12,12	1.59	4 (33%)	17,17,17	2.03	4 (23%)

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	CIT	B	301	-	-	0/16/16/16	-
4	CIT	F	301	-	-	0/16/16/16	-
4	CIT	W	301	-	-	2/16/16/16	-
4	CIT	X	301	-	-	5/16/16/16	-
4	CIT	J	301	-	-	2/16/16/16	-
4	CIT	M	301	-	-	6/16/16/16	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	301	CIT	O5-C6	3.27	1.32	1.22
4	X	301	CIT	O4-C5	-3.22	1.20	1.30
4	W	301	CIT	O3-C5	3.16	1.32	1.22
4	M	301	CIT	O5-C6	3.12	1.31	1.22
4	X	301	CIT	O5-C6	3.05	1.31	1.22
4	M	301	CIT	O1-C1	2.97	1.31	1.22
4	X	301	CIT	O1-C1	2.91	1.31	1.22
4	W	301	CIT	O1-C1	2.82	1.31	1.22
4	W	301	CIT	O2-C1	-2.54	1.22	1.30
4	M	301	CIT	O6-C6	-2.45	1.21	1.30
4	W	301	CIT	O6-C6	-2.43	1.21	1.30
4	X	301	CIT	O2-C1	-2.41	1.22	1.30
4	X	301	CIT	O3-C5	2.37	1.29	1.22
4	W	301	CIT	O4-C5	-2.36	1.23	1.30
4	M	301	CIT	O2-C1	-2.30	1.23	1.30
4	X	301	CIT	O6-C6	-2.08	1.23	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	301	CIT	O6-C6-C3	4.95	122.63	113.14
4	M	301	CIT	O6-C6-C3	4.85	122.44	113.14
4	W	301	CIT	O6-C6-C3	4.68	122.12	113.14
4	W	301	CIT	O5-C6-C3	-4.30	113.77	122.09
4	M	301	CIT	O5-C6-C3	-4.21	113.93	122.09
4	X	301	CIT	O5-C6-C3	-4.18	114.00	122.09
4	M	301	CIT	O1-C1-C2	-3.64	112.65	122.95
4	X	301	CIT	O1-C1-C2	-3.57	112.84	122.95
4	W	301	CIT	O3-C5-C4	-3.27	113.69	122.95
4	W	301	CIT	O1-C1-C2	-3.27	113.70	122.95
4	X	301	CIT	O3-C5-C4	-3.26	113.71	122.95
4	X	301	CIT	O2-C1-C2	2.86	123.41	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	301	CIT	O4-C5-C4	2.76	123.11	114.35
4	M	301	CIT	O2-C1-C2	2.70	122.89	114.35
4	W	301	CIT	O2-C1-C2	2.69	122.87	114.35
4	W	301	CIT	O4-C5-C4	2.67	122.82	114.35
4	B	301	CIT	C3-C4-C5	2.03	119.48	113.92
4	J	301	CIT	C3-C2-C1	2.02	119.45	113.92

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	301	CIT	C2-C3-C6-O5
4	X	301	CIT	C2-C3-C6-O6
4	X	301	CIT	O7-C3-C6-O5
4	X	301	CIT	O7-C3-C6-O6
4	M	301	CIT	C2-C3-C6-O5
4	M	301	CIT	C2-C3-C6-O6
4	M	301	CIT	C4-C3-C6-O6
4	X	301	CIT	C4-C3-C6-O6
4	J	301	CIT	C1-C2-C3-C6
4	M	301	CIT	C4-C3-C6-O5
4	J	301	CIT	C1-C2-C3-O7
4	M	301	CIT	O7-C3-C6-O5
4	M	301	CIT	O7-C3-C6-O6
4	W	301	CIT	O1-C1-C2-C3
4	W	301	CIT	O2-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	CIT	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	213/214 (99%)	0.88	43 (20%) 3 2	28, 75, 122, 142	0
1	E	213/214 (99%)	0.99	53 (24%) 2 1	27, 70, 126, 141	0
1	I	213/214 (99%)	0.15	8 (3%) 44 36	23, 51, 98, 117	0
1	L	213/214 (99%)	-0.39	1 (0%) 87 83	22, 33, 53, 82	0
2	B	211/223 (94%)	1.22	56 (26%) 1 1	38, 67, 137, 145	0
2	F	211/223 (94%)	0.81	36 (17%) 4 3	31, 65, 119, 139	0
2	J	211/223 (94%)	0.08	9 (4%) 40 32	23, 44, 83, 110	0
2	M	213/223 (95%)	-0.31	5 (2%) 61 53	20, 33, 55, 88	0
3	W	228/228 (100%)	-0.39	2 (0%) 81 76	18, 33, 55, 74	1 (0%)
3	X	228/228 (100%)	-0.39	3 (1%) 75 69	21, 32, 57, 69	1 (0%)
3	Y	228/228 (100%)	-0.09	2 (0%) 81 76	32, 46, 69, 84	1 (0%)
3	Z	228/228 (100%)	-0.19	2 (0%) 81 76	24, 43, 63, 74	1 (0%)
All	All	2610/2660 (98%)	0.19	220 (8%) 17 15	18, 44, 112, 145	4 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	LYS	5.9
1	E	191	VAL	5.9
2	F	127	SER	5.5
3	X	215	SER	5.3
2	J	128	SER	5.3
2	B	159	LEU	5.3
2	B	128	SER	5.3
2	B	161	SER	5.2
2	M	128	SER	5.2
2	B	189	LEU	5.1
2	F	189	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
3	W	215	SER	4.9
1	E	133	VAL	4.8
2	F	128	SER	4.6
1	E	119	PRO	4.5
1	E	184	ALA	4.5
1	E	154	LEU	4.4
2	B	213	PRO	4.4
2	F	162	GLY	4.3
2	J	133	GLY	4.2
2	B	123	PRO	4.2
2	B	151	THR	4.2
1	E	114	SER	4.1
1	E	213	GLU	4.1
2	B	120	SER	4.1
1	A	197	THR	4.0
2	F	134	GLY	4.0
1	E	205	VAL	4.0
1	E	181	LEU	4.0
2	F	213	PRO	4.0
2	M	133	GLY	3.9
2	B	194	TYR	3.9
1	A	146	VAL	3.9
2	B	126	PRO	3.9
1	A	127	SER	3.9
1	A	114	SER	3.8
2	F	183	THR	3.8
2	B	179	SER	3.7
2	B	185	PRO	3.7
3	Y	215	SER	3.7
1	E	192	TYR	3.7
1	E	197	THR	3.7
2	B	207	VAL	3.7
2	F	133	GLY	3.6
2	B	180	SER	3.6
1	E	148	TRP	3.6
1	A	154	LEU	3.6
2	F	194	TYR	3.6
2	M	215	SER	3.5
2	B	210	LYS	3.5
1	E	147	GLN	3.5
1	A	205	VAL	3.5
2	B	150	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	125	ALA	3.5
1	A	203	SER	3.5
2	B	187	SER	3.5
1	E	151	ASP	3.5
1	E	196	VAL	3.4
1	A	119	PRO	3.4
1	E	128	GLY	3.4
2	B	157	GLY	3.4
1	A	125	LEU	3.4
1	A	135	LEU	3.4
1	E	193	ALA	3.4
1	E	194	CYS	3.3
1	E	180	THR	3.3
2	B	191	THR	3.3
2	B	133	GLY	3.3
2	B	137	ALA	3.3
2	B	160	THR	3.3
2	B	184	VAL	3.3
1	E	158	ASN	3.3
2	F	210	LYS	3.3
2	B	121	VAL	3.3
2	B	182	VAL	3.3
1	E	134	CYS	3.3
2	B	183	THR	3.3
1	E	156	SER	3.3
1	E	126	LYS	3.2
2	B	195	ILE	3.2
2	B	125	ALA	3.2
2	B	136	ALA	3.2
1	A	195	GLU	3.2
2	F	185	PRO	3.2
1	E	125	LEU	3.2
1	E	153	ALA	3.2
1	I	126	LYS	3.2
2	J	191	THR	3.2
2	B	209	LYS	3.2
2	B	201	LYS	3.1
2	J	213	PRO	3.1
2	B	178	LEU	3.1
1	E	145	LYS	3.1
2	F	182	VAL	3.1
1	A	201	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	183	LYS	3.1
1	E	188	LYS	3.1
1	A	213	GLU	3.1
1	E	150	VAL	3.0
3	Y	201	CYS	3.0
2	F	124	LEU	3.0
3	Z	219	VAL	3.0
1	E	182	SER	3.0
3	Z	97	ASP	3.0
1	E	117	ILE	2.9
2	F	190	GLY	2.9
1	E	112	ALA	2.9
1	E	144	ALA	2.9
2	B	138	LEU	2.9
2	F	159	LEU	2.9
1	A	116	PHE	2.9
2	B	122	PHE	2.9
2	B	140	CYS	2.9
1	E	157	GLY	2.8
1	A	113	PRO	2.8
2	B	198	VAL	2.8
1	E	203	SER	2.8
1	E	135	LEU	2.8
2	F	135	THR	2.8
2	B	141	LEU	2.8
1	E	190	LYS	2.8
3	W	219	VAL	2.8
2	F	161	SER	2.8
1	A	208	SER	2.8
2	F	137	ALA	2.7
1	E	122	ASP	2.7
2	F	179	SER	2.7
1	A	191	VAL	2.7
1	A	196	VAL	2.7
2	M	214	LYS	2.7
1	I	213	GLU	2.7
2	B	135	THR	2.7
1	I	152	ASN	2.7
1	A	124	GLN	2.7
1	L	213	GLU	2.6
2	B	124	LEU	2.6
1	E	202	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	115	VAL	2.6
1	E	116	PHE	2.6
2	B	197	ASN	2.6
1	E	146	VAL	2.5
1	A	209	PHE	2.5
1	A	134	CYS	2.5
1	E	189	HIS	2.5
2	B	206	LYS	2.5
2	J	206	LYS	2.5
1	E	201	LEU	2.5
2	J	189	LEU	2.5
1	A	204	PRO	2.5
1	A	193	ALA	2.5
2	F	53	THR	2.5
2	B	196	CYS	2.5
2	B	127	SER	2.4
3	X	217	SER	2.4
1	A	207	LYS	2.4
2	F	174	GLY	2.4
2	B	188	SER	2.4
1	E	118	PHE	2.4
1	A	133	VAL	2.4
2	J	134	GLY	2.4
2	B	142	VAL	2.4
2	B	211	VAL	2.4
1	I	197	THR	2.4
1	E	179	LEU	2.3
2	B	53	THR	2.3
1	I	145	LYS	2.3
2	F	211	VAL	2.3
2	B	134	GLY	2.3
2	B	162	GLY	2.3
2	B	199	ASN	2.3
1	A	118	PHE	2.3
1	I	153	ALA	2.3
2	B	1	GLU	2.3
2	F	193	THR	2.3
1	A	122	ASP	2.3
3	X	216	GLY	2.3
2	F	199	ASN	2.3
1	A	123	GLU	2.3
1	E	155	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	169	LYS	2.3
2	F	140	CYS	2.3
2	F	212	GLU	2.2
1	E	149	LYS	2.2
2	B	147	PRO	2.2
2	B	152	VAL	2.2
2	F	126	PRO	2.2
1	E	143	GLU	2.2
2	F	136	ALA	2.2
2	F	175	LEU	2.2
2	J	201	LYS	2.2
1	A	188	LYS	2.2
2	F	178	LEU	2.2
1	A	100	GLN	2.2
1	A	110	VAL	2.1
1	E	132	VAL	2.1
1	A	109	THR	2.1
1	A	117	ILE	2.1
2	M	43	GLN	2.1
1	A	137	ASN	2.1
1	A	115	VAL	2.1
2	F	184	VAL	2.1
1	A	177	SER	2.1
1	A	189	HIS	2.1
1	E	152	ASN	2.1
2	J	199	ASN	2.1
1	I	154	LEU	2.1
1	A	186	TYR	2.1
1	A	107	LYS	2.1
2	B	119	PRO	2.1
1	A	206	THR	2.1
2	F	180	SER	2.0
2	F	117	LYS	2.0
1	E	100	GLN	2.0
2	F	187	SER	2.0
2	B	204	ASN	2.0
1	I	129	THR	2.0
1	A	149	LYS	2.0
1	E	161	GLU	2.0
2	B	208	ASP	2.0
2	F	163	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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	CIT	F	301	13/13	0.61	0.21	103,110,116,118	0
4	CIT	J	301	13/13	0.65	0.20	82,92,100,100	0
4	CIT	B	301	13/13	0.68	0.18	89,92,100,102	0
4	CIT	M	301	13/13	0.76	0.18	68,84,91,94	0
4	CIT	X	301	13/13	0.81	0.15	70,88,98,98	0
4	CIT	W	301	13/13	0.88	0.13	61,84,92,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.