



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2021 – 12:08 PM EST

PDB ID : 6VMJ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

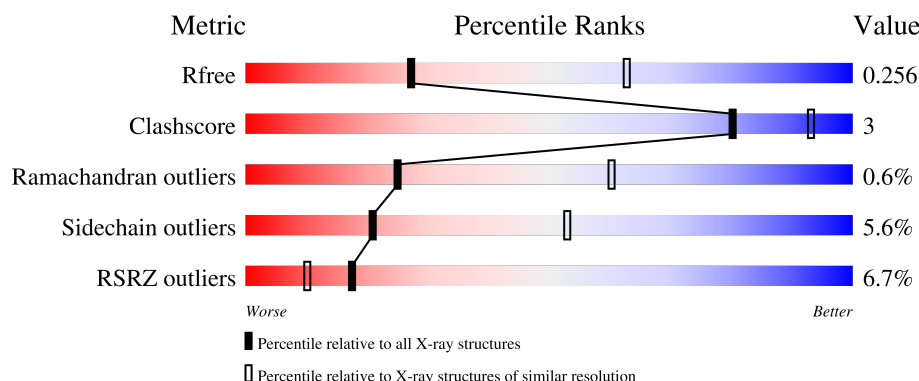
1 Overall quality at a glance

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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	<div> <div>21%</div> <div>89%</div> <div>10%</div> </div>
1	E	214	<div> <div>23%</div> <div>88%</div> <div>11%</div> </div>
1	I	214	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	L	214	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	B	223	<div> <div>19%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	223	
2	J	223	
2	M	223	
3	W	228	
3	X	228	
3	Y	228	
3	Z	228	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	F	301	-	-	-	X

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			

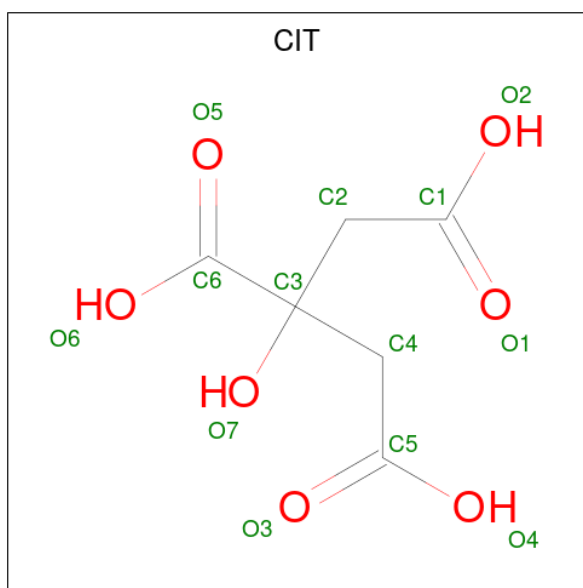
- Molecule 2 is a protein called Fab20D12 heavy chain.

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 (three-letter code: 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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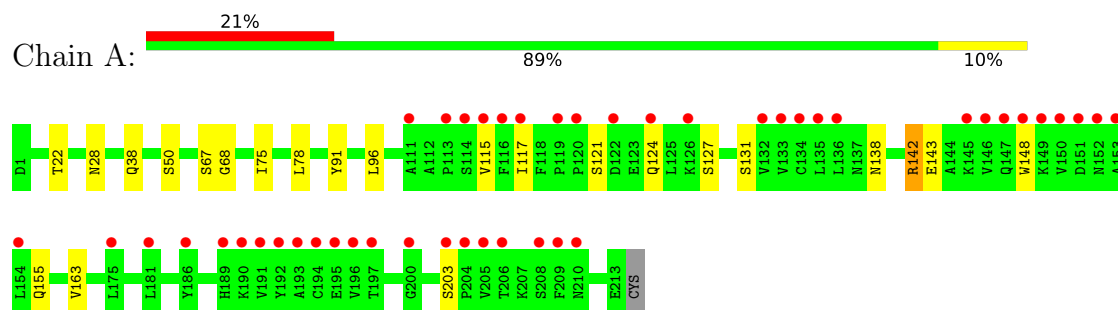
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	21	Total 21	O 21	0	0
5	M	13	Total 13	O 13	0	0
5	W	23	Total 23	O 23	0	0
5	X	27	Total 27	O 27	0	0
5	Y	13	Total 13	O 13	0	0
5	Z	14	Total 14	O 14	0	0

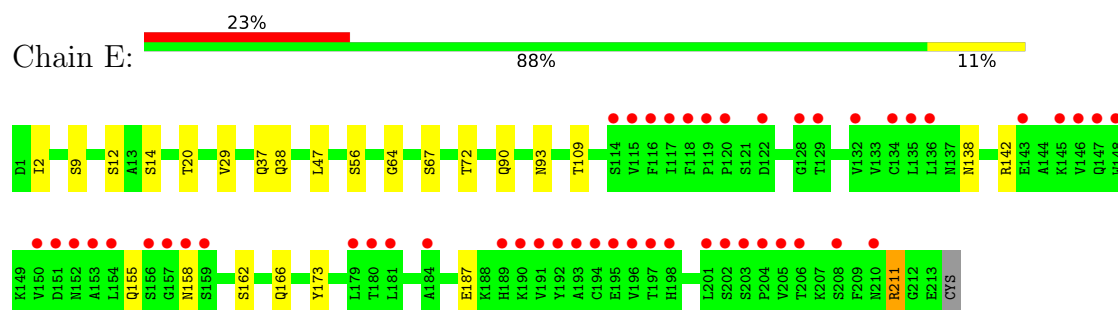
3 Residue-property plots [i](#)

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.

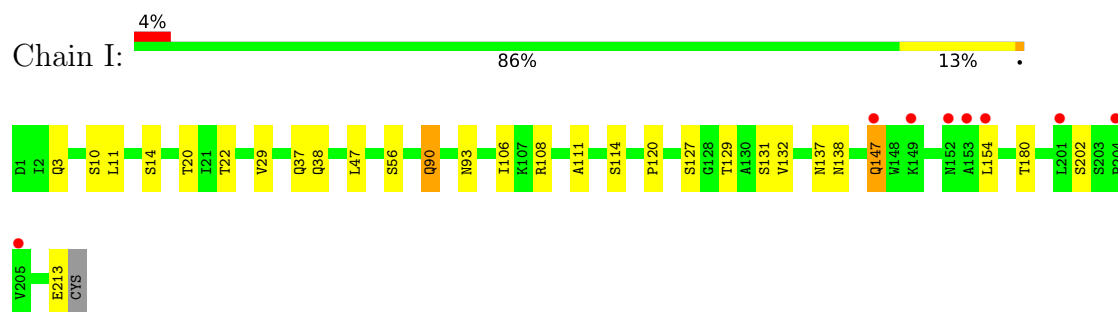
• Molecule 1: Fab20D12 Light Chain



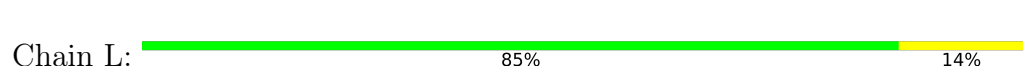
• Molecule 1: Fab20D12 Light Chain

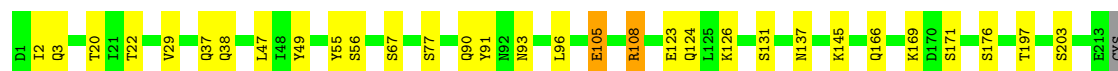


• Molecule 1: Fab20D12 Light Chain

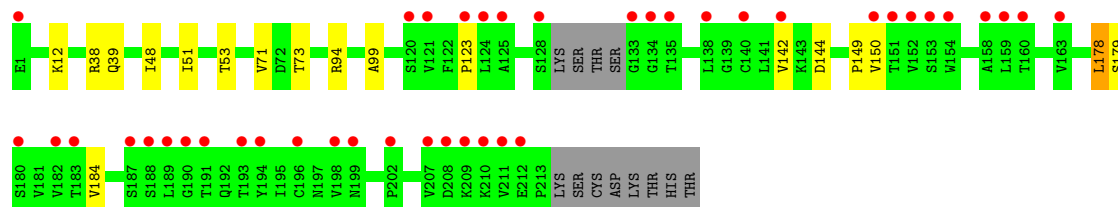
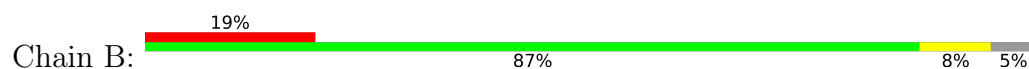


• Molecule 1: Fab20D12 Light Chain

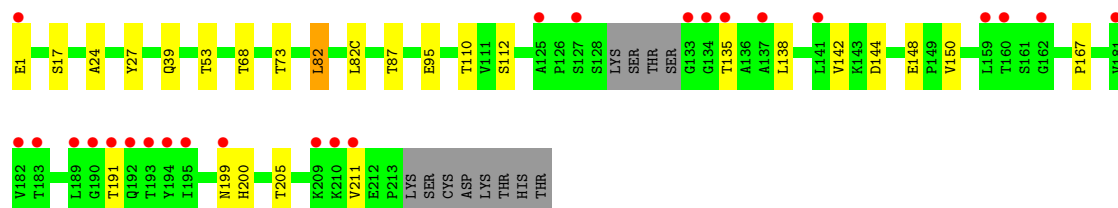
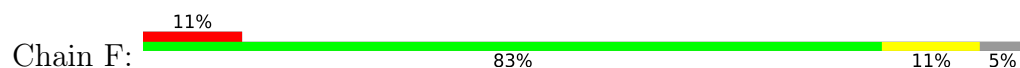




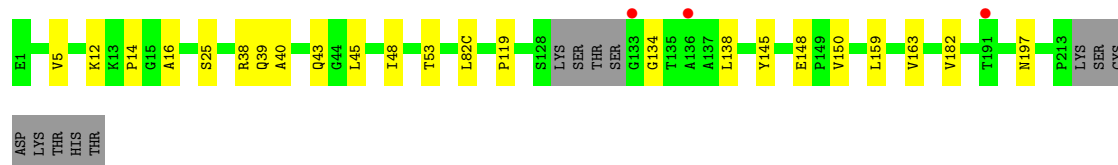
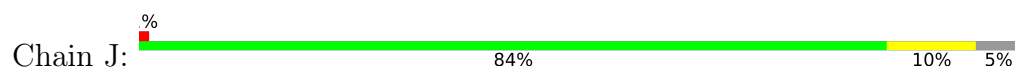
- Molecule 2: Fab20D12 heavy chain



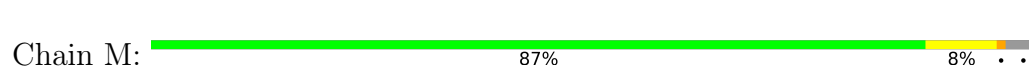
- Molecule 2: Fab20D12 heavy chain



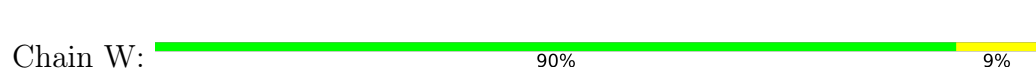
- Molecule 2: Fab20D12 heavy chain



- Molecule 2: Fab20D12 heavy chain



- Molecule 3: Complement factor D



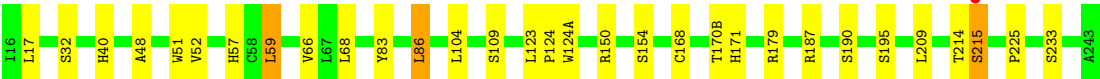
- Molecule 3: Complement factor D

Chain X:

86%

12%

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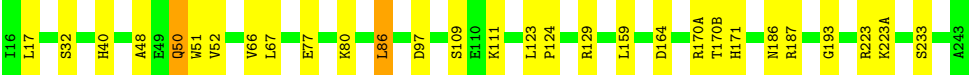
• Molecule 3: Complement factor D

Chain Y:

87%

12%

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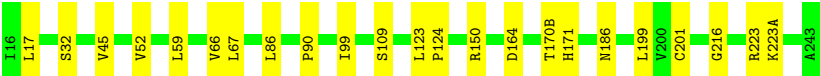
• Molecule 3: Complement factor D

Chain Z:

90%

10%

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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) 99.4 (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 0.209 , 0.256	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)	0.31 , 44.4	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	0.49	0/1670	0.71	0/2267
1	E	0.50	0/1670	0.74	0/2267
1	I	0.46	0/1670	0.74	0/2267
1	L	0.51	0/1670	0.77	0/2267
2	B	0.47	0/1612	0.73	0/2198
2	F	0.48	0/1612	0.75	0/2198
2	J	0.49	0/1612	0.76	0/2198
2	M	0.51	0/1627	0.78	0/2217
3	W	0.52	0/1753	0.71	0/2385
3	X	0.51	0/1753	0.70	0/2385
3	Y	0.48	0/1753	0.69	0/2385
3	Z	0.49	0/1753	0.69	0/2385
All	All	0.49	0/20155	0.73	0/27419

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1635	0	1578	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1635	0	1578	9	0
1	I	1635	0	1578	10	0
1	L	1635	0	1578	15	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	6	0
3	W	1713	0	1696	9	0
3	X	1713	0	1696	14	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	104	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 (104) 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:HG3	1:L:108:ARG:HH21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:59:LEU:HD22	3:X:104:LEU:HD21	1.96	0.47
3:X:32:SER:OG	3:X:40:HIS:HD2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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%)	29	64
1	E	211/214 (99%)	199 (94%)	10 (5%)	2 (1%)	17	51
1	I	211/214 (99%)	202 (96%)	8 (4%)	1 (0%)	29	64
1	L	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
2	B	207/223 (93%)	190 (92%)	13 (6%)	4 (2%)	8	32
2	F	207/223 (93%)	197 (95%)	9 (4%)	1 (0%)	29	64
2	J	207/223 (93%)	197 (95%)	8 (4%)	2 (1%)	15	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	209/223 (94%)	199 (95%)	9 (4%)	1 (0%)	29	64
3	W	227/228 (100%)	217 (96%)	9 (4%)	1 (0%)	34	69
3	X	227/228 (100%)	215 (95%)	11 (5%)	1 (0%)	34	69
3	Y	227/228 (100%)	217 (96%)	10 (4%)	0	100	100
3	Z	227/228 (100%)	215 (95%)	11 (5%)	1 (0%)	34	69
All	All	2582/2660 (97%)	2450 (95%)	117 (4%)	15 (1%)	25	60

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%)	179 (96%)	8 (4%)	29	62
1	E	187/188 (100%)	178 (95%)	9 (5%)	25	59
1	I	187/188 (100%)	169 (90%)	18 (10%)	8	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	187/188 (100%)	175 (94%)	12 (6%)	17	47
2	B	176/188 (94%)	168 (96%)	8 (4%)	27	61
2	F	176/188 (94%)	165 (94%)	11 (6%)	18	48
2	J	176/188 (94%)	168 (96%)	8 (4%)	27	61
2	M	178/188 (95%)	168 (94%)	10 (6%)	21	53
3	W	183/182 (100%)	174 (95%)	9 (5%)	25	58
3	X	183/182 (100%)	172 (94%)	11 (6%)	19	50
3	Y	183/182 (100%)	174 (95%)	9 (5%)	25	58
3	Z	183/182 (100%)	174 (95%)	9 (5%)	25	58
All	All	2186/2232 (98%)	2064 (94%)	122 (6%)	21	53

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	12	LYS
2	B	51	ILE
2	B	53	THR
2	B	71	VAL
2	B	73	THR
2	B	150	VAL
2	B	178	LEU
2	B	184	VAL
1	E	9	SER
1	E	12	SER
1	E	14	SER
1	E	20	THR
1	E	56	SER
1	E	90	GLN
1	E	93	ASN
1	E	109	THR
1	E	142	ARG

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Mol	Chain	Res	Type
2	F	1	GLU
2	F	17	SER
2	F	53	THR
2	F	68	THR
2	F	73	THR
2	F	82	LEU
2	F	112	SER
2	F	135	THR
2	F	148	GLU
2	F	191	THR
2	F	199	ASN
1	I	3	GLN
1	I	10	SER
1	I	11	LEU
1	I	14	SER
1	I	20	THR
1	I	22	THR
1	I	56	SER
1	I	90	GLN
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	147	GLN
1	I	180	THR
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	138	LEU
2	J	148	GLU
2	J	150	VAL
2	J	197	ASN
1	L	3	GLN
1	L	20	THR
1	L	22	THR
1	L	56	SER
1	L	77	SER

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Mol	Chain	Res	Type
1	L	90	GLN
1	L	105	GLU
1	L	108	ARG
1	L	137	ASN
1	L	169	LYS
1	L	176	SER
1	L	203	SER
2	M	7	SER
2	M	12	LYS
2	M	17	SER
2	M	71	VAL
2	M	73	THR
2	M	82(B)	SER
2	M	150	VAL
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	97	ASP
3	W	121	ARG
3	W	159	LEU
3	W	168	CYS
3	W	201	CYS
3	W	233	SER
3	X	17	LEU
3	X	59	LEU
3	X	86	LEU
3	X	154	SER
3	X	168	CYS
3	X	170(B)	THR
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	50	GLN
3	Y	86	LEU
3	Y	97	ASP
3	Y	129	ARG

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Mol	Chain	Res	Type
3	Y	159	LEU
3	Y	164	ASP
3	Y	170(B)	THR
3	Y	233	SER
3	Z	17	LEU
3	Z	45	VAL
3	Z	59	LEU
3	Z	90	PRO
3	Z	99	ILE
3	Z	164	ASP
3	Z	170(B)	THR
3	Z	199	LEU
3	Z	201	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	137	ASN
1	A	138	ASN
2	B	39	GLN
2	B	164	HIS
2	B	171	GLN
1	E	38	GLN
2	F	171	GLN
1	I	92	ASN
1	I	137	ASN
1	I	138	ASN
1	I	147	GLN
2	J	3	GLN
2	J	39	GLN
2	J	164	HIS
1	L	38	GLN
1	L	124	GLN
1	L	199	GLN
2	M	171	GLN
2	M	199	ASN
3	W	34	GLN
3	W	40	HIS
3	W	50	GLN
3	X	40	HIS
3	X	50	GLN

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Mol	Chain	Res	Type
3	Y	40	HIS
3	Y	171	HIS
3	Z	40	HIS
3	Z	50	GLN
3	Z	171	HIS

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	3,12,12	0.47	0	3,17,17	1.70	1 (33%)
4	CIT	M	301	-	3,12,12	0.55	0	3,17,17	1.67	1 (33%)
4	CIT	J	301	-	3,12,12	0.41	0	3,17,17	2.01	2 (66%)
4	CIT	X	301	-	3,12,12	0.46	0	3,17,17	0.85	0
4	CIT	W	301	-	3,12,12	0.50	0	3,17,17	0.61	0
4	CIT	F	301	-	3,12,12	0.43	0	3,17,17	1.28	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	CIT	B	301	-	-	0/6/16/16	-
4	CIT	M	301	-	-	0/6/16/16	-
4	CIT	J	301	-	-	2/6/16/16	-
4	CIT	X	301	-	-	2/6/16/16	-
4	CIT	W	301	-	-	0/6/16/16	-
4	CIT	F	301	-	-	0/6/16/16	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	CIT	C3-C4-C5	2.81	119.48	114.98
4	J	301	CIT	C3-C2-C1	2.79	119.45	114.98
4	M	301	CIT	C3-C4-C5	2.34	118.73	114.98
4	J	301	CIT	C3-C4-C5	2.05	118.27	114.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	301	CIT	C1-C2-C3-C6
4	X	301	CIT	C1-C2-C3-C6
4	J	301	CIT	C1-C2-C3-O7
4	X	301	CIT	C1-C2-C3-O7

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	213/214 (99%)	0.84	46 (21%) 0 0	28, 75, 122, 142	0
1	E	213/214 (99%)	0.79	50 (23%) 0 0	27, 70, 126, 141	0
1	I	213/214 (99%)	0.20	8 (3%) 40 26	23, 51, 98, 117	0
1	L	213/214 (99%)	-0.26	0 100 100	22, 33, 53, 82	0
2	B	211/223 (94%)	0.66	42 (19%) 1 0	38, 67, 137, 145	0
2	F	211/223 (94%)	0.42	25 (11%) 4 2	31, 65, 119, 139	0
2	J	211/223 (94%)	-0.07	3 (1%) 75 59	23, 44, 83, 110	0
2	M	213/223 (95%)	-0.30	1 (0%) 91 81	20, 33, 55, 88	0
3	W	228/228 (100%)	-0.32	0 100 100	18, 33, 55, 74	0
3	X	228/228 (100%)	-0.33	1 (0%) 92 84	21, 32, 57, 69	0
3	Y	228/228 (100%)	-0.26	0 100 100	32, 46, 69, 84	0
3	Z	228/228 (100%)	-0.30	0 100 100	24, 43, 63, 74	0
All	All	2610/2660 (98%)	0.08	176 (6%) 17 10	18, 44, 112, 145	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	GLU	7.8
2	B	194	TYR	5.8
1	E	147	GLN	5.6
1	A	152	ASN	5.5
2	B	193	THR	5.5
1	E	115	VAL	5.5
2	B	159	LEU	5.1
1	E	192	TYR	5.1
1	E	203	SER	5.0
1	E	154	LEU	4.8
2	B	207	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	125	ALA	4.6
1	E	150	VAL	4.6
1	A	149	LYS	4.6
1	A	208	SER	4.5
2	F	193	THR	4.4
2	B	182	VAL	4.4
1	E	194	CYS	4.4
1	A	147	GLN	4.2
2	B	191	THR	4.2
1	A	126	LYS	4.2
1	A	193	ALA	4.2
1	E	134	CYS	4.2
1	E	151	ASP	4.1
2	B	189	LEU	4.1
1	A	132	VAL	4.0
2	B	198	VAL	4.0
1	E	132	VAL	4.0
1	A	210	ASN	4.0
1	E	153	ALA	3.9
1	A	203	SER	3.9
2	F	183	THR	3.9
2	F	194	TYR	3.9
1	A	197	THR	3.9
2	F	1	GLU	3.9
2	B	120	SER	3.9
2	B	187	SER	3.9
1	E	202	SER	3.9
1	E	148	TRP	3.8
1	A	134	CYS	3.8
2	F	190	GLY	3.8
2	F	210	LYS	3.7
1	A	204	PRO	3.7
1	E	117	ILE	3.7
1	E	128	GLY	3.7
1	E	210	ASN	3.7
2	B	190	GLY	3.7
1	A	119	PRO	3.7
2	F	191	THR	3.7
2	F	133	GLY	3.6
1	I	152	ASN	3.6
1	A	113	PRO	3.6
1	A	122	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	J	133	GLY	3.6
1	A	190	LYS	3.6
1	A	146	VAL	3.6
2	B	154	TRP	3.5
2	B	138	LEU	3.5
1	E	201	LEU	3.5
2	F	127	SER	3.5
1	E	204	PRO	3.5
1	A	153	ALA	3.4
1	E	152	ASN	3.4
2	F	189	LEU	3.4
1	E	122	ASP	3.4
2	F	135	THR	3.4
1	A	205	VAL	3.3
1	A	209	PHE	3.3
1	E	208	SER	3.3
2	B	133	GLY	3.3
1	A	115	VAL	3.3
1	E	116	PHE	3.3
2	F	125	ALA	3.3
2	B	128	SER	3.3
1	A	133	VAL	3.3
2	B	210	LYS	3.2
2	B	211	VAL	3.2
1	A	114	SER	3.2
1	I	153	ALA	3.2
1	E	119	PRO	3.1
1	E	197	THR	3.1
1	E	157	GLY	3.1
1	E	196	VAL	3.0
2	B	123	PRO	3.0
1	A	145	LYS	3.0
2	B	196	CYS	3.0
2	M	133	GLY	3.0
1	E	205	VAL	2.9
1	I	154	LEU	2.9
1	E	180	THR	2.9
1	A	151	ASP	2.9
1	A	196	VAL	2.9
1	A	192	TYR	2.9
1	E	181	LEU	2.9
2	F	159	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	129	THR	2.8
2	B	158	ALA	2.8
1	E	189	HIS	2.8
1	E	118	PHE	2.7
1	A	181	LEU	2.7
2	B	140	CYS	2.7
2	B	208	ASP	2.7
1	A	154	LEU	2.7
2	B	199	ASN	2.7
1	E	114	SER	2.7
1	E	191	VAL	2.7
1	A	116	PHE	2.7
1	A	111	ALA	2.7
1	E	156	SER	2.6
1	A	124	GLN	2.6
2	B	163	VAL	2.6
2	B	135	THR	2.6
1	A	135	LEU	2.6
2	F	211	VAL	2.6
1	E	145	LYS	2.6
2	B	1	GLU	2.6
1	A	175	LEU	2.6
2	B	212	GLU	2.5
2	F	162	GLY	2.5
2	F	141	LEU	2.5
2	F	192	GLN	2.5
1	A	148	TRP	2.5
1	E	179	LEU	2.5
2	B	150	VAL	2.5
2	F	182	VAL	2.5
1	A	117	ILE	2.5
2	F	209	LYS	2.4
1	A	206	THR	2.4
1	A	194	CYS	2.4
1	I	147	GLN	2.4
1	E	206	THR	2.4
2	B	134	GLY	2.4
2	J	191	THR	2.4
1	E	193	ALA	2.4
1	A	191	VAL	2.4
1	E	190	LYS	2.4
2	B	142	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	204	PRO	2.3
1	E	146	VAL	2.3
2	B	160	THR	2.3
1	A	150	VAL	2.3
1	A	186	TYR	2.3
1	E	135	LEU	2.3
1	E	120	PRO	2.3
1	E	184	ALA	2.3
1	A	200	GLY	2.2
2	B	202	PRO	2.2
1	E	136	LEU	2.2
2	F	134	GLY	2.2
2	F	195	ILE	2.2
1	E	143	GLU	2.2
1	I	201	LEU	2.2
1	E	158	ASN	2.2
1	A	189	HIS	2.2
1	E	159	SER	2.2
2	B	121	VAL	2.1
2	F	181	VAL	2.1
2	B	152	VAL	2.1
1	E	195	GLU	2.1
1	A	120	PRO	2.1
2	B	183	THR	2.1
1	I	205	VAL	2.1
1	A	136	LEU	2.1
2	B	180	SER	2.1
1	I	149	LYS	2.1
2	B	151	THR	2.1
2	B	124	LEU	2.0
2	B	153	SER	2.0
2	B	188	SER	2.0
3	X	215	SER	2.0
2	F	199	ASN	2.0
2	F	137	ALA	2.0
1	E	198	HIS	2.0
2	F	160	THR	2.0
2	J	136	ALA	2.0
2	B	209	LYS	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 monosaccharides 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(\AA^2)	Q<0.9
4	CIT	J	301	13/13	0.72	0.32	82,92,100,100	0
4	CIT	F	301	13/13	0.76	0.41	103,110,116,118	0
4	CIT	B	301	13/13	0.81	0.37	89,92,100,102	0
4	CIT	M	301	13/13	0.81	0.31	68,84,91,94	0
4	CIT	W	301	13/13	0.83	0.25	61,84,92,93	0
4	CIT	X	301	13/13	0.86	0.30	70,88,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.