Full wwPDB X-ray Structure Validation Report (i)

Oct 6, 2022 – 12:31 PM EDT

PDB ID	:	7T99
Title	:	Crystal structure of engineered CYS-CYS fab dimer CL-205 (LC25)
Authors	:	Harris, S.F.; Boenig, G.D.L.
Deposited on	:	2021-12-18
Resolution	:	2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

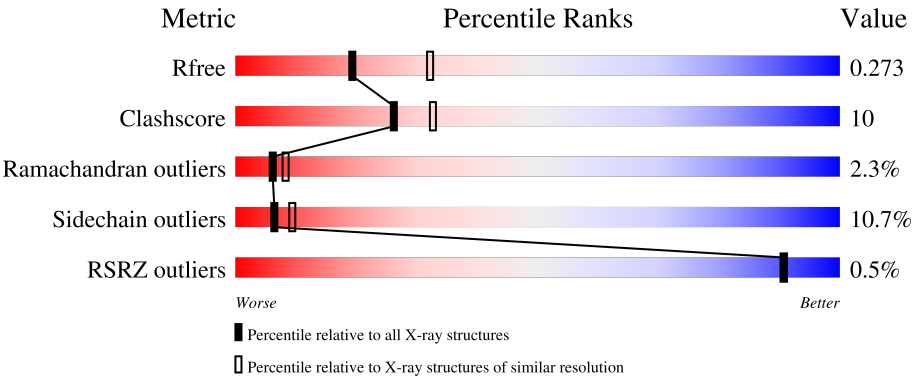
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	228	70% 24%
1	C	228	67% 25%
1	E	228	74% 21%
1	H	228	65% 30%
2	B	214	67% 30%

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Mol	Chain	Length	Quality of chain
2	D	214	
2	F	214	
2	L	214	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13261 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.

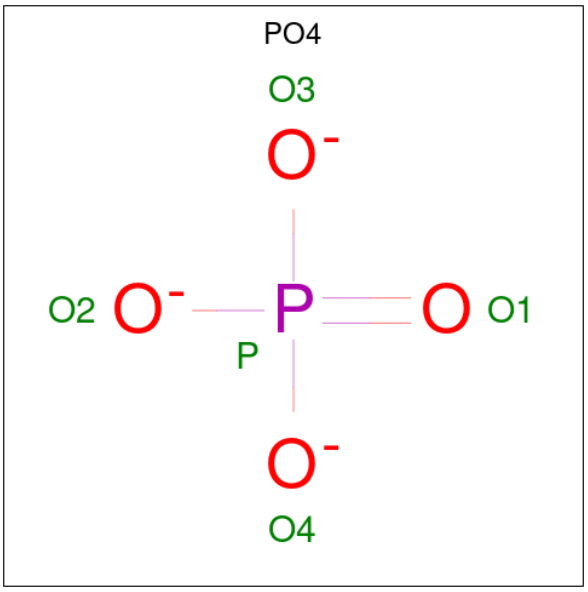
- Molecule 1 is a protein called FAB Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	3	0
			1655	1047	279	321	8			
1	C	220	Total	C	N	O	S	0	3	0
			1655	1047	279	321	8			
1	E	220	Total	C	N	O	S	0	3	0
			1655	1047	279	321	8			
1	H	220	Total	C	N	O	S	0	3	0
			1655	1047	279	321	8			

- Molecule 2 is a protein called FAB Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	2	0
			1640	1028	275	329	8			
2	D	212	Total	C	N	O	S	0	2	0
			1640	1028	275	329	8			
2	F	212	Total	C	N	O	S	0	2	0
			1640	1028	275	329	8			
2	L	212	Total	C	N	O	S	0	2	0
			1640	1028	275	329	8			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

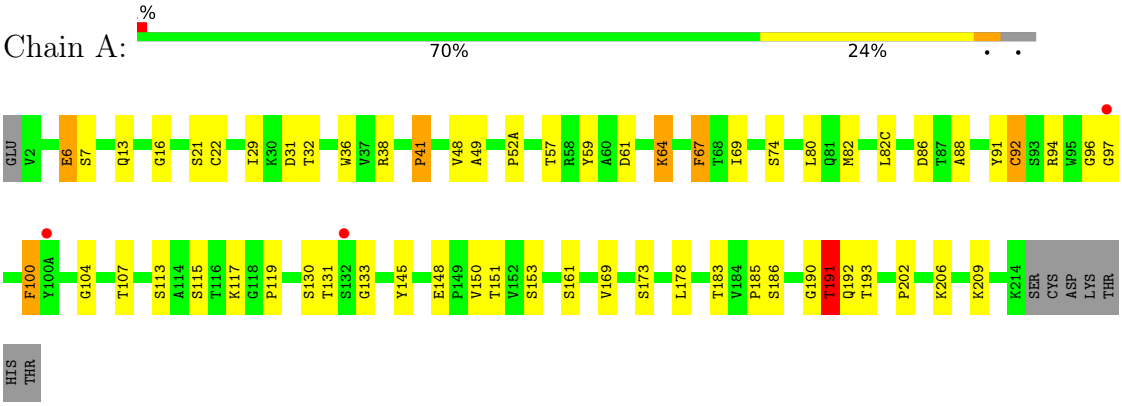
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	16	Total O 16 16	0	0
4	C	4	Total O 4 4	0	0
4	D	11	Total O 11 11	0	0
4	E	2	Total O 2 2	0	0
4	F	13	Total O 13 13	0	0
4	H	8	Total O 8 8	0	0
4	L	10	Total O 10 10	0	0

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.

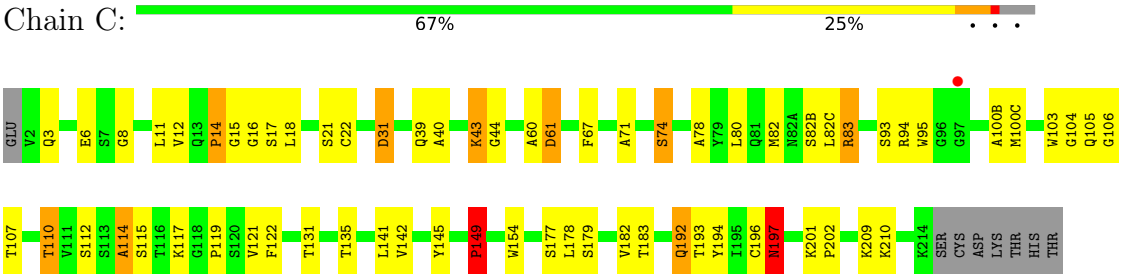
• Molecule 1: FAB Heavy Chain

Chain A:



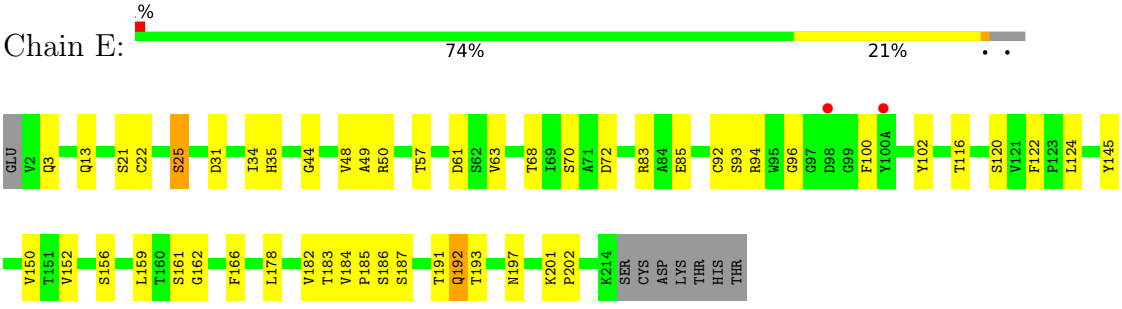
• Molecule 1: FAB Heavy Chain

Chain C:



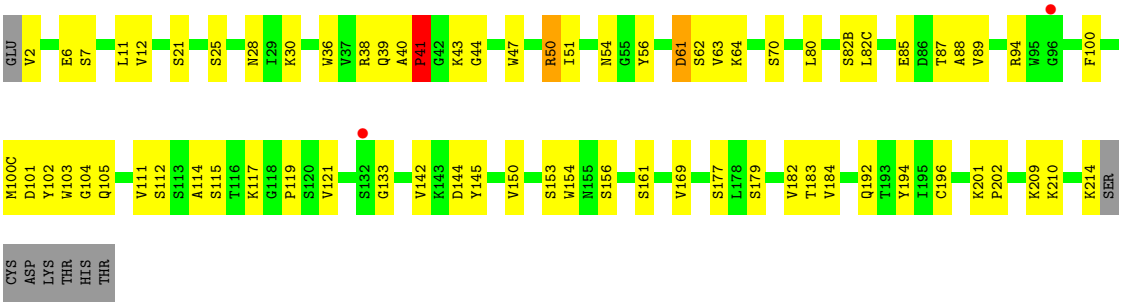
• Molecule 1: FAB Heavy Chain

Chain E:



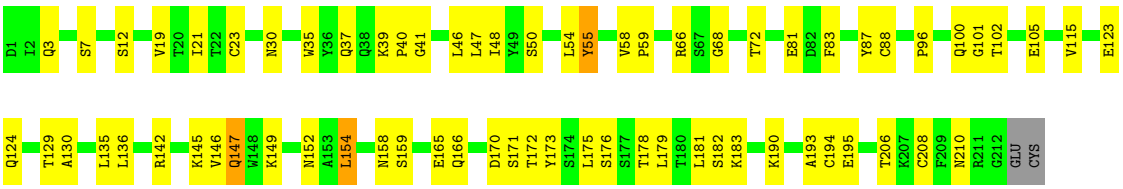
• Molecule 1: FAB Heavy Chain

Chain H:



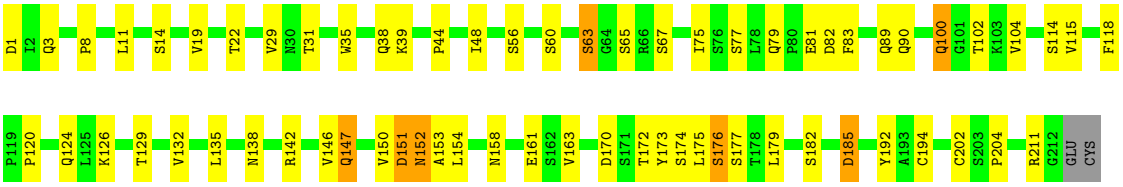
• Molecule 2: FAB Light Chain

Chain B:



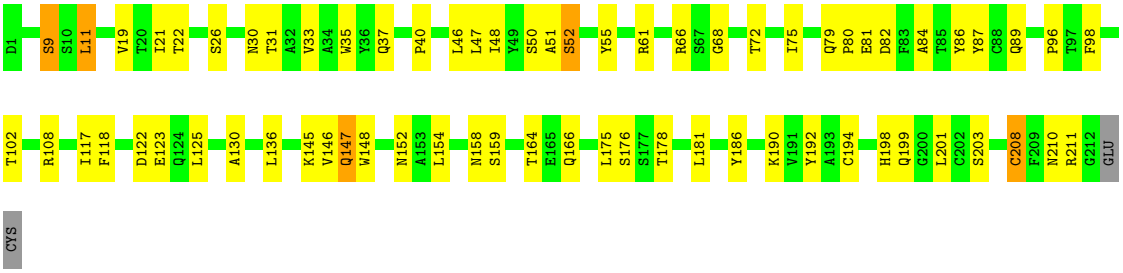
• Molecule 2: FAB Light Chain

Chain D:



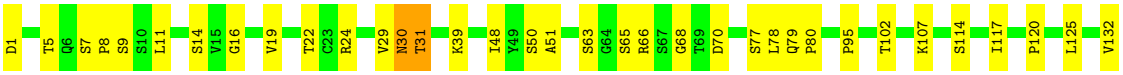
• Molecule 2: FAB Light Chain

Chain F:



• Molecule 2: FAB Light Chain

Chain L:




V133
C134
L135
L136
N137
N138
R142
K145
W148
K149
V150
D151
N152
A153
L154
N158
S159
D170
Y173
S176
S177
T178
L179
Y186
H189
K190
V191
Y192
A193
C194
E195
V196
T197
S203
P204
N210
R211
G212
GLU
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	52.82Å 62.45Å 124.02Å 89.99° 98.37° 89.89°	Depositor
Resolution (Å)	62.45 – 2.65 62.45 – 2.65	Depositor EDS
% Data completeness (in resolution range)	82.4 (62.45-2.65) 95.7 (62.45-2.65)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.184 , 0.265 0.196 , 0.273	Depositor DCC
R_{free} test set	1670 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å^2)	62.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.247 for -h,k,-l	Xtriage
Reported twinning fraction	0.631 for H, K, L 0.369 for -H, K, -L	Depositor
Outliers	0 of 43584 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13261	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 74.62 % 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 1.4770e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4

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	0.74	1/1703 (0.1%)	0.99	0/2321
1	C	0.74	0/1703	0.96	1/2321 (0.0%)
1	E	0.72	0/1703	0.96	0/2321
1	H	0.74	0/1703	0.94	0/2321
2	B	0.78	1/1683 (0.1%)	0.99	0/2288
2	D	0.79	0/1683	1.01	0/2288
2	F	0.76	0/1683	0.98	0/2288
2	L	0.78	0/1683	0.98	0/2288
All	All	0.76	2/13544 (0.0%)	0.98	1/18436 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	195	GLU	CD-OE2	5.25	1.31	1.25
1	A	148	GLU	CD-OE1	5.09	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	149	PRO	N-CA-CB	-5.34	96.72	102.60

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	1655	0	1618	31	0
1	C	1655	0	1618	40	0
1	E	1655	0	1618	22	0
1	H	1655	0	1618	36	0
2	B	1640	0	1596	44	0
2	D	1640	0	1597	34	0
2	F	1640	0	1597	41	0
2	L	1640	0	1596	30	0
3	C	5	0	0	0	0
3	H	5	0	0	0	0
4	A	7	0	0	4	0
4	B	16	0	0	5	0
4	C	4	0	0	2	0
4	D	11	0	0	5	0
4	E	2	0	0	1	0
4	F	13	0	0	8	0
4	H	8	0	0	4	0
4	L	10	0	0	1	0
All	All	13261	0	12858	270	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 10.

All (270) 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:11:LEU:HA	4:F:304:HOH:O	1.71	0.89
1:C:39:GLN:HG3	1:C:44:GLY:O	1.76	0.85
2:F:87:TYR:HE1	4:F:307:HOH:O	1.62	0.82
1:H:47:TRP:HZ2	1:H:50:ARG:HB3	1.43	0.81
2:B:96:PRO:HD3	4:B:311:HOH:O	1.80	0.79
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.66	0.77
1:H:2:VAL:HG11	1:H:94:ARG:NH1	2.00	0.76
2:B:170:ASP:OD1	2:B:172:THR:OG1	2.04	0.75
2:F:146:VAL:HG13	2:F:194[B]:CYS:SG	2.29	0.72
1:A:31:ASP:O	1:A:32:THR:HG23	1.89	0.72
1:E:166:PHE:CE1	2:F:176:SER:HB3	2.25	0.71
1:A:145:TYR:CE1	1:A:150:VAL:HG23	2.25	0.70
1:C:82(B):SER:O	1:C:83:ARG:HD2	1.92	0.69
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:SER:HA	4:A:304:HOH:O	1.92	0.68
1:A:6:GLU:N	1:A:6:GLU:OE1	2.25	0.68
2:F:50:SER:O	2:F:52:SER:N	2.24	0.67
2:B:158:ASN:O	2:B:179:LEU:HD12	1.95	0.66
1:E:145:TYR:CE1	1:E:150:VAL:HG23	2.31	0.66
2:F:21:ILE:HG12	2:F:102:THR:HG21	1.76	0.66
2:D:100:GLN:HA	4:D:305:HOH:O	1.93	0.66
2:D:202:CYS:HG	2:F:208:CYS:CB	2.09	0.66
2:B:182:SER:HA	4:B:306:HOH:O	1.96	0.65
1:C:178:LEU:HD12	1:C:178:LEU:C	2.16	0.65
1:C:6:GLU:OE1	1:C:104:GLY:HA3	1.97	0.65
2:B:166:GLN:HB2	2:B:173:TYR:CZ	2.32	0.64
2:D:147:GLN:HG2	2:D:154:LEU:HD11	1.79	0.64
2:D:158:ASN:O	2:D:179:LEU:HA	1.98	0.64
2:D:63:SER:HB3	4:D:309:HOH:O	1.99	0.63
2:B:190:LYS:O	2:B:210:ASN:HA	2.00	0.61
1:E:3:GLN:N	1:E:25:SER:O	2.34	0.60
2:B:146:VAL:HG13	2:B:194[B]:CYS:SG	2.41	0.60
2:B:66:ARG:NH1	2:B:68:GLY:O	2.35	0.60
2:L:189:HIS:O	2:L:211:ARG:NE	2.24	0.60
1:H:210:LYS:N	4:H:401:HOH:O	2.34	0.59
1:H:209:LYS:HA	4:H:401:HOH:O	2.02	0.59
1:A:48:VAL:O	1:A:49:ALA:HB2	2.01	0.59
1:H:94:ARG:O	1:H:100(C):MET:HA	2.03	0.59
2:B:175:LEU:HD23	2:B:175:LEU:C	2.23	0.59
2:L:66:ARG:NH1	2:L:68:GLY:O	2.35	0.58
2:F:35:TRP:HB2	2:F:48:ILE:HB	1.85	0.58
1:E:35:HIS:HB2	1:E:93:SER:OG	2.02	0.58
1:E:44:GLY:HA3	4:F:307:HOH:O	2.02	0.58
2:D:124:GLN:HG2	2:D:129:THR:OG1	2.03	0.58
1:H:38:ARG:HA	1:H:89:VAL:O	2.03	0.57
2:B:21:ILE:HG12	2:B:102:THR:HG21	1.87	0.57
1:E:185:PRO:O	1:E:187:SER:N	2.36	0.57
1:C:154:TRP:CZ2	1:C:196[B]:CYS:SG	2.97	0.57
2:F:166:GLN:HG3	4:F:310:HOH:O	2.06	0.56
2:D:38:GLN:HA	4:D:306:HOH:O	2.06	0.56
2:L:8:PRO:O	2:L:102:THR:OG1	2.15	0.56
1:A:191:THR:HG23	2:F:199:GLN:HG3	1.88	0.56
1:C:192:GLN:HB3	1:C:194:TYR:CE1	2.41	0.55
2:F:33:VAL:HA	2:F:89:GLN:O	2.07	0.55
1:C:8:GLY:O	1:C:18:LEU:HD22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:ALA:O	1:H:43:LYS:HB2	2.07	0.55
1:E:166:PHE:CZ	2:F:176:SER:HB3	2.42	0.55
2:F:82:ASP:O	2:F:86:TYR:OH	2.17	0.55
2:D:163:VAL:HG22	2:D:175:LEU:HD12	1.87	0.54
1:H:145:TYR:CE1	1:H:150:VAL:HG23	2.41	0.54
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.89	0.54
2:L:31:THR:O	2:L:50:SER:HA	2.08	0.54
1:A:22:CYS:HB2	1:A:36:TRP:CZ2	2.43	0.53
1:C:201:LYS:N	1:C:202:PRO:HD2	2.22	0.53
2:D:158:ASN:O	2:D:179:LEU:HD12	2.09	0.53
1:A:36:TRP:HD1	1:A:69:ILE:HD12	1.72	0.53
2:F:87:TYR:CE1	4:F:307:HOH:O	2.47	0.53
2:L:150:VAL:HG13	2:L:192:TYR:CE2	2.44	0.53
2:F:186:TYR:O	2:F:192:TYR:OH	2.20	0.53
2:L:125:LEU:HD21	2:L:186:TYR:CD2	2.43	0.53
1:A:57:THR:HG1	1:A:59:TYR:HE1	1.53	0.53
2:B:83:PHE:HE1	4:B:312:HOH:O	1.92	0.53
1:H:47:TRP:CZ2	1:H:50:ARG:HB3	2.33	0.53
2:B:35:TRP:HB2	2:B:48:ILE:HB	1.91	0.53
1:C:12:VAL:HG11	1:C:82(C):LEU:HD13	1.91	0.53
1:C:44:GLY:HA3	4:C:402:HOH:O	2.09	0.53
1:H:11:LEU:HD11	1:H:112:SER:HB3	1.91	0.52
2:L:145:LYS:HB3	2:L:197:THR:HB	1.92	0.52
2:B:146:VAL:CG1	2:B:194[B]:CYS:SG	2.97	0.52
2:B:170:ASP:OD1	2:B:172:THR:HG23	2.10	0.52
2:F:136:LEU:N	2:F:136:LEU:HD12	2.25	0.52
1:H:2:VAL:HG11	1:H:94:ARG:HH12	1.75	0.52
1:C:94:ARG:O	1:C:100(C):MET:HA	2.09	0.52
2:F:66:ARG:NH1	2:F:68:GLY:O	2.43	0.52
1:A:6:GLU:OE2	1:A:104:GLY:HA3	2.09	0.51
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.92	0.51
1:C:122:PHE:CE2	2:D:124:GLN:HG3	2.46	0.51
2:D:142:ARG:NH1	4:D:301:HOH:O	2.42	0.51
2:L:189:HIS:HB2	2:L:192:TYR:CZ	2.46	0.51
2:F:158:ASN:OD1	2:F:158:ASN:N	2.42	0.51
2:B:83:PHE:HZ	2:B:165:GLU:HB3	1.75	0.51
2:L:16:GLY:N	2:L:78:LEU:O	2.42	0.51
1:E:44:GLY:CA	4:F:307:HOH:O	2.59	0.51
2:L:136:LEU:HD21	2:L:196:VAL:HG13	1.92	0.51
1:A:178:LEU:HD12	1:A:178:LEU:C	2.31	0.51
1:C:95:TRP:HA	1:C:100(B):ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:GLY:O	1:E:182:VAL:HA	2.11	0.51
2:B:83:PHE:CZ	2:B:165:GLU:HB3	2.46	0.50
2:B:54:LEU:O	2:B:55:TYR:O	2.29	0.50
1:C:201:LYS:N	1:C:202:PRO:CD	2.74	0.50
1:E:48:VAL:HG13	1:E:63:VAL:HG11	1.93	0.50
1:H:6:GLU:HA	1:H:21:SER:O	2.11	0.50
2:B:193:ALA:HB1	2:B:206:THR:CG2	2.42	0.49
2:F:96:PRO:HD3	4:F:302:HOH:O	2.10	0.49
1:A:61:ASP:O	1:A:64:LYS:HG2	2.12	0.49
2:B:159:SER:HA	2:B:178:THR:O	2.12	0.49
1:A:36:TRP:O	1:A:48:VAL:HB	2.11	0.49
2:B:105:GLU:OE1	2:B:173:TYR:OH	2.30	0.49
2:B:173:TYR:HE1	4:B:304:HOH:O	1.95	0.49
2:L:150:VAL:HG22	2:L:192:TYR:CD2	2.48	0.49
1:A:32:THR:O	1:A:52(A):PRO:HD2	2.12	0.49
2:F:136:LEU:HD13	2:F:175:LEU:HD22	1.94	0.49
2:L:189:HIS:HB2	2:L:192:TYR:OH	2.11	0.49
1:C:17:SER:HA	1:C:82:MET:O	2.12	0.49
2:B:171:SER:HA	4:B:315:HOH:O	2.13	0.49
2:D:150:VAL:HG13	2:D:192:TYR:CE2	2.48	0.49
2:B:87:TYR:CE1	2:B:101:GLY:HA3	2.48	0.49
2:D:182:SER:OG	2:D:185:ASP:HB2	2.13	0.49
2:L:148:TRP:CE3	2:L:194[B]:CYS:HB2	2.48	0.49
2:B:136:LEU:HD13	2:B:175:LEU:HD22	1.95	0.48
1:E:48:VAL:O	1:E:49:ALA:HB2	2.13	0.48
1:H:61:ASP:O	1:H:63:VAL:N	2.46	0.48
2:D:150:VAL:O	2:D:151:ASP:C	2.51	0.48
2:F:37:GLN:HB2	2:F:86:TYR:CE2	2.48	0.48
2:F:190:LYS:O	2:F:210:ASN:HA	2.13	0.48
1:H:87:THR:O	1:H:88:ALA:HB2	2.13	0.48
2:D:8:PRO:O	2:D:102:THR:OG1	2.21	0.48
1:H:70:SER:HB3	4:H:403:HOH:O	2.14	0.48
1:C:67:PHE:CD2	1:C:80:LEU:HD21	2.48	0.48
1:C:121:VAL:HG22	1:C:142:VAL:HG22	1.96	0.48
2:L:1:ASP:CG	2:L:95:PRO:HD2	2.32	0.48
1:H:28:ASN:ND2	1:H:30:LYS:HB2	2.29	0.47
2:B:35:TRP:O	2:B:47:LEU:HB2	2.14	0.47
2:F:117:ILE:HG23	2:F:117:ILE:O	2.14	0.47
1:E:34:ILE:O	1:E:50:ARG:HA	2.13	0.47
2:L:159:SER:HA	2:L:178:THR:O	2.14	0.47
1:A:97:GLY:HA3	4:A:305:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:VAL:HG22	2:D:75:ILE:HB	1.97	0.47
2:D:39:LYS:HE2	2:D:81:GLU:O	2.15	0.47
1:C:192:GLN:OE1	1:C:193:THR:N	2.48	0.47
1:H:39:GLN:C	1:H:88:ALA:HB1	2.35	0.47
1:A:92:CYS:N	4:A:301:HOH:O	2.48	0.47
1:C:105:GLN:NE2	1:C:106:GLY:O	2.47	0.47
2:F:145:LYS:HE2	2:F:147:GLN:HE22	1.80	0.47
2:B:166:GLN:HB2	2:B:173:TYR:CE2	2.49	0.46
2:D:142:ARG:HD2	4:D:301:HOH:O	2.15	0.46
2:B:130:ALA:N	2:B:181:LEU:O	2.44	0.46
1:A:29:ILE:O	1:A:52(A):PRO:HG2	2.16	0.46
2:B:145:LYS:HE2	2:B:147:GLN:OE1	2.15	0.46
2:D:170:ASP:HB2	2:D:172:THR:OG1	2.15	0.46
2:L:30:ASN:O	2:L:66:ARG:HD2	2.16	0.46
1:E:156:SER:HA	1:E:197:ASN:OD1	2.15	0.46
2:F:30:ASN:OD1	2:F:31:THR:HG22	2.16	0.46
2:F:89:GLN:NE2	2:F:98:PHE:CZ	2.83	0.46
2:L:158:ASN:O	2:L:179:LEU:HD12	2.16	0.46
2:F:166:GLN:HA	4:F:310:HOH:O	2.15	0.46
1:A:16:GLY:O	1:A:82(C):LEU:HD12	2.16	0.46
2:B:147:GLN:HG2	2:B:154:LEU:HD11	1.96	0.46
1:H:154:TRP:CH2	1:H:196[B]:CYS:HB3	2.50	0.46
1:A:6:GLU:OE1	1:A:104:GLY:HA3	2.16	0.45
4:E:302:HOH:O	2:F:164:THR:HG21	2.16	0.45
2:D:146:VAL:HG13	2:D:194[B]:CYS:SG	2.56	0.45
1:H:121:VAL:HG22	1:H:142:VAL:HG22	1.99	0.45
2:L:148:TRP:CE3	2:L:194[A]:CYS:HB2	2.51	0.45
1:E:178:LEU:C	1:E:178:LEU:HD12	2.37	0.45
1:C:103:TRP:CE3	2:D:44:PRO:HD2	2.52	0.45
2:L:142:ARG:HD3	2:L:173:TYR:CE2	2.51	0.45
1:C:11:LEU:HD11	1:C:112:SER:HB3	1.97	0.45
1:C:112:SER:OG	1:C:114:ALA:HB3	2.17	0.45
2:D:173:TYR:C	2:D:174:SER:HG	2.15	0.45
2:F:37:GLN:HG3	2:F:84:ALA:CB	2.47	0.45
2:D:35:TRP:HB2	2:D:48:ILE:HB	1.97	0.45
2:L:173:TYR:C	4:L:308:HOH:O	2.54	0.45
1:A:80:LEU:HD23	1:A:82:MET:SD	2.57	0.45
1:A:91:TYR:C	4:A:301:HOH:O	2.55	0.45
2:D:89:GLN:HG2	2:D:90:GLN:O	2.17	0.45
2:D:170:ASP:CB	2:D:172:THR:OG1	2.65	0.45
1:E:152:VAL:HA	1:E:197:ASN:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:PHE:HD1	2:D:104:VAL:O	1.99	0.45
1:A:41:PRO:HD3	1:A:88:ALA:HA	2.00	0.44
1:C:40:ALA:O	1:C:43:LYS:HB2	2.17	0.44
1:A:145:TYR:CE1	1:A:150:VAL:CG2	2.97	0.44
2:L:24:ARG:NH2	2:L:70:ASP:OD2	2.49	0.44
2:B:170:ASP:OD1	2:B:170:ASP:C	2.55	0.44
1:C:14:PRO:C	1:C:16:GLY:H	2.21	0.44
2:L:150:VAL:CG1	2:L:192:TYR:CE2	3.00	0.44
1:H:201:LYS:N	1:H:202:PRO:CD	2.81	0.44
1:H:11:LEU:HD21	1:H:114:ALA:O	2.18	0.44
1:E:159:LEU:HD12	1:E:159:LEU:HA	1.85	0.44
1:H:154:TRP:CZ3	1:H:196[B]:CYS:HB3	2.52	0.44
1:A:191:THR:HG22	1:A:192:GLN:N	2.33	0.44
2:D:115:VAL:HA	2:D:135:LEU:O	2.18	0.44
1:E:192:GLN:OE1	1:E:193:THR:N	2.30	0.44
2:B:39:LYS:HE2	2:B:81:GLU:O	2.18	0.43
1:H:12:VAL:HG11	1:H:82(C):LEU:HD13	1.98	0.43
1:A:100:PHE:CD1	1:A:100:PHE:C	2.91	0.43
1:E:201:LYS:N	1:E:202:PRO:CD	2.81	0.43
2:F:84:ALA:HB3	2:F:86:TYR:CE1	2.54	0.43
2:B:46:LEU:HD11	2:B:48:ILE:O	2.19	0.43
1:C:6:GLU:HA	1:C:21:SER:O	2.18	0.43
2:B:170:ASP:OD1	2:B:172:THR:CB	2.66	0.43
1:H:2:VAL:CG1	1:H:94:ARG:NH1	2.76	0.43
1:E:120:SER:HB3	1:E:122:PHE:CZ	2.54	0.43
1:H:184:VAL:HG11	1:H:194:TYR:CE2	2.53	0.43
1:A:31:ASP:O	1:A:32:THR:CG2	2.61	0.43
1:A:190:GLY:O	1:A:191:THR:C	2.57	0.43
2:B:176:SER:O	2:B:176:SER:OG	2.36	0.43
1:C:71:ALA:HA	1:C:78:ALA:HA	2.00	0.43
1:E:124:LEU:HB3	2:F:118:PHE:CD2	2.54	0.43
2:F:79:GLN:O	2:F:80:PRO:C	2.57	0.42
2:L:151:ASP:OD2	2:L:189:HIS:HB3	2.19	0.42
2:B:193:ALA:HB2	2:B:208:CYS:HB3	2.00	0.42
1:C:22:CYS:O	1:C:22:CYS:SG	2.77	0.42
1:C:149:PRO:O	1:C:149:PRO:CD	2.66	0.42
2:D:161:GLU:HA	2:D:176:SER:O	2.19	0.42
1:H:12:VAL:O	1:H:111:VAL:HA	2.18	0.42
2:D:118:PHE:N	2:D:118:PHE:CD2	2.87	0.42
2:D:152:ASN:HD22	2:D:152:ASN:HA	1.72	0.42
2:L:191:VAL:HG22	2:L:210:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:148:TRP:CZ3	2:F:194[A]:CYS:HB3	2.55	0.42
2:B:124:GLN:HG2	2:B:129:THR:O	2.20	0.42
1:H:11:LEU:CD1	1:H:112:SER:HB3	2.49	0.42
2:L:79:GLN:O	2:L:80:PRO:C	2.58	0.42
2:L:117:ILE:O	2:L:117:ILE:HG23	2.17	0.42
1:C:74:SER:HB2	4:C:401:HOH:O	2.20	0.42
1:C:80:LEU:HD23	1:C:82:MET:SD	2.59	0.42
2:F:198:HIS:O	2:F:201:LEU:HB2	2.20	0.42
1:H:36:TRP:NE1	1:H:80:LEU:HB2	2.34	0.42
2:L:48:ILE:HG21	2:L:51:ALA:O	2.20	0.42
2:B:87:TYR:CD1	2:B:101:GLY:HA3	2.55	0.42
1:H:6:GLU:OE1	1:H:104:GLY:HA3	2.20	0.42
2:B:58:VAL:HA	2:B:59:PRO:HD3	1.94	0.41
1:E:185:PRO:C	1:E:187:SER:N	2.73	0.41
2:F:46:LEU:HD23	2:F:55:TYR:CD1	2.55	0.41
2:F:130:ALA:N	2:F:181:LEU:O	2.48	0.41
1:A:67:PHE:N	1:A:67:PHE:CD1	2.88	0.41
2:D:150:VAL:O	2:D:153:ALA:N	2.42	0.41
1:H:102:TYR:CD1	1:H:103:TRP:O	2.73	0.41
1:A:6:GLU:CD	1:A:104:GLY:HA3	2.40	0.41
2:B:142:ARG:HH11	2:B:173:TYR:HE2	1.67	0.41
1:C:11:LEU:HD12	1:C:110:THR:O	2.20	0.41
1:C:193:THR:CG2	1:C:210:LYS:HD2	2.50	0.41
2:B:12:SER:HA	2:B:105:GLU:O	2.20	0.41
1:C:14:PRO:C	1:C:16:GLY:N	2.73	0.41
2:B:35:TRP:CH2	2:B:88:CYS:HB3	2.55	0.41
1:C:121:VAL:HA	1:C:141:LEU:O	2.21	0.41
2:F:122:ASP:O	2:F:125:LEU:N	2.54	0.41
2:B:39:LYS:HB3	2:B:40:PRO:HD2	2.03	0.41
2:B:115:VAL:HA	2:B:135:LEU:O	2.21	0.41
1:C:31:ASP:OD1	1:C:31:ASP:N	2.53	0.41
1:C:40:ALA:HB3	1:C:43:LYS:HB2	2.03	0.41
2:D:79:GLN:O	2:D:82:ASP:HB2	2.21	0.41
2:D:120:PRO:HD3	2:D:132:VAL:HG22	2.02	0.41
1:E:166:PHE:CD1	2:F:176:SER:HB3	2.56	0.41
2:F:175:LEU:C	2:F:175:LEU:HD23	2.42	0.41
1:H:119:PRO:HB3	1:H:145:TYR:HB3	2.03	0.41
1:H:40:ALA:O	1:H:41:PRO:C	2.60	0.40
1:H:54:ASN:CG	1:H:56:TYR:CD1	2.94	0.40
1:H:61:ASP:O	1:H:64:LYS:HG2	2.21	0.40
1:H:209:LYS:CA	4:H:401:HOH:O	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HD3	1:A:48:VAL:HG21	2.03	0.40
1:C:60:ALA:O	1:C:61:ASP:C	2.59	0.40
1:C:182:VAL:HG13	1:C:182:VAL:O	2.22	0.40
2:L:203:SER:O	2:L:204:PRO:C	2.59	0.40
2:F:159:SER:HA	2:F:178:THR:O	2.22	0.40
1:H:51:ILE:O	1:H:51:ILE:HG23	2.20	0.40
2:D:138:ASN:N	2:D:138:ASN:OD1	2.54	0.40
2:L:78:LEU:O	2:L:79:GLN:OE1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	220/228 (96%)	190 (86%)	22 (10%)	8 (4%)	3 4
1	C	220/228 (96%)	196 (89%)	18 (8%)	6 (3%)	5 6
1	E	220/228 (96%)	201 (91%)	17 (8%)	2 (1%)	17 26
1	H	220/228 (96%)	188 (86%)	24 (11%)	8 (4%)	3 4
2	B	212/214 (99%)	196 (92%)	14 (7%)	2 (1%)	17 26
2	D	212/214 (99%)	193 (91%)	14 (7%)	5 (2%)	6 7
2	F	212/214 (99%)	193 (91%)	14 (7%)	5 (2%)	6 7
2	L	212/214 (99%)	190 (90%)	18 (8%)	4 (2%)	8 11
All	All	1728/1768 (98%)	1547 (90%)	141 (8%)	40 (2%)	6 8

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	186	SER
1	H	156	SER

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Mol	Chain	Res	Type
1	A	96	GLY
1	A	173	SER
1	A	191	THR
2	B	55	TYR
1	C	15	GLY
1	C	131	THR
2	D	29	VAL
1	E	96	GLY
2	F	81	GLU
1	H	44	GLY
1	H	61	ASP
2	L	211	ARG
1	A	131	THR
1	A	133	GLY
1	C	61	ASP
1	C	114	ALA
1	C	197	ASN
2	F	9	SER
2	F	211	ARG
1	H	62	SER
1	H	144	ASP
2	D	126	LYS
2	D	204	PRO
2	D	211	ARG
1	A	202	PRO
1	C	14	PRO
2	D	151	ASP
2	F	51	ALA
1	H	133	GLY
1	H	182	VAL
2	L	29	VAL
2	L	30	ASN
1	H	41	PRO
1	A	185	PRO
2	F	40	PRO
2	L	204	PRO
1	A	41	PRO
2	B	41	GLY

5.3.2 Protein sidechains (i)

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	183/189 (97%)	158 (86%)	25 (14%)	3 4
1	C	183/189 (97%)	165 (90%)	18 (10%)	8 11
1	E	183/189 (97%)	161 (88%)	22 (12%)	5 7
1	H	183/189 (97%)	164 (90%)	19 (10%)	7 10
2	B	189/189 (100%)	175 (93%)	14 (7%)	13 21
2	D	189/189 (100%)	170 (90%)	19 (10%)	7 10
2	F	189/189 (100%)	172 (91%)	17 (9%)	9 14
2	L	189/189 (100%)	165 (87%)	24 (13%)	4 6
All	All	1488/1512 (98%)	1330 (89%)	158 (11%)	6 10

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	SER
1	A	13	GLN
1	A	21	SER
1	A	64	LYS
1	A	67	PHE
1	A	74	SER
1	A	86	ASP
1	A	92	CYS
1	A	94	ARG
1	A	100	PHE
1	A	107	THR
1	A	113	SER
1	A	115	SER
1	A	117	LYS
1	A	151	THR
1	A	153	SER
1	A	161	SER
1	A	169	VAL

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Mol	Chain	Res	Type
1	A	183	THR
1	A	186	SER
1	A	191	THR
1	A	193	THR
1	A	206	LYS
1	A	209	LYS
2	B	3	GLN
2	B	7	SER
2	B	19	VAL
2	B	23	CYS
2	B	30	ASN
2	B	50	SER
2	B	72	THR
2	B	100	GLN
2	B	123	GLU
2	B	147	GLN
2	B	149	LYS
2	B	152	ASN
2	B	154	LEU
2	B	183	LYS
1	C	3	GLN
1	C	31	ASP
1	C	43	LYS
1	C	74	SER
1	C	83	ARG
1	C	93	SER
1	C	107	THR
1	C	110	THR
1	C	115	SER
1	C	117	LYS
1	C	135	THR
1	C	149	PRO
1	C	177	SER
1	C	179	SER
1	C	183	THR
1	C	192	GLN
1	C	197	ASN
1	C	209	LYS
2	D	1	ASP
2	D	3	GLN
2	D	11	LEU
2	D	14	SER

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Mol	Chain	Res	Type
2	D	22	THR
2	D	31	THR
2	D	56	SER
2	D	60	SER
2	D	63	SER
2	D	65	SER
2	D	67	SER
2	D	77	SER
2	D	100	GLN
2	D	114	SER
2	D	147	GLN
2	D	152	ASN
2	D	176	SER
2	D	177	SER
2	D	185	ASP
1	E	13	GLN
1	E	21	SER
1	E	22	CYS
1	E	25	SER
1	E	31	ASP
1	E	57	THR
1	E	61	ASP
1	E	68	THR
1	E	70	SER
1	E	72	ASP
1	E	83	ARG
1	E	85[A]	GLU
1	E	92	CYS
1	E	94	ARG
1	E	100	PHE
1	E	102	TYR
1	E	116	THR
1	E	161	SER
1	E	183	THR
1	E	184	VAL
1	E	191	THR
1	E	192	GLN
2	F	9	SER
2	F	11	LEU
2	F	19	VAL
2	F	22	THR
2	F	26	SER

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Mol	Chain	Res	Type
2	F	47	LEU
2	F	52	SER
2	F	61	ARG
2	F	72	THR
2	F	75	ILE
2	F	108	ARG
2	F	123	GLU
2	F	147	GLN
2	F	152	ASN
2	F	154	LEU
2	F	203	SER
2	F	208	CYS
1	H	7	SER
1	H	25	SER
1	H	41	PRO
1	H	50	ARG
1	H	82(B)	SER
1	H	85[A]	GLU
1	H	100	PHE
1	H	101	ASP
1	H	105	GLN
1	H	115	SER
1	H	117	LYS
1	H	153	SER
1	H	161	SER
1	H	169	VAL
1	H	177	SER
1	H	179	SER
1	H	183	THR
1	H	192	GLN
1	H	214	LYS
2	L	5	THR
2	L	7	SER
2	L	9	SER
2	L	11	LEU
2	L	14	SER
2	L	19	VAL
2	L	22	THR
2	L	31	THR
2	L	39	LYS
2	L	63	SER
2	L	65	SER

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Mol	Chain	Res	Type
2	L	77	SER
2	L	107	LYS
2	L	114	SER
2	L	134	CYS
2	L	138	ASN
2	L	142	ARG
2	L	152	ASN
2	L	154	LEU
2	L	170	ASP
2	L	176	SER
2	L	194[A]	CYS
2	L	194[B]	CYS
2	L	203	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	171	GLN
2	B	30	ASN
2	B	152	ASN
1	C	199	ASN
2	D	152	ASN
1	E	164	HIS
1	E	171	GLN
2	F	147	GLN
2	F	152	ASN
1	H	28	ASN
2	L	189	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	PO4	C	301	-	4,4,4	1.06	1 (25%)	6,6,6	0.39	0
3	PO4	H	301	-	4,4,4	1.30	1 (25%)	6,6,6	0.44	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	PO4	P-O1	2.33	1.56	1.50
3	C	301	PO4	P-O1	2.05	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	220/228 (96%)	-0.42	3 (1%)	75	73	39, 65, 104, 127	0
1	C	220/228 (96%)	-0.51	1 (0%)	91	91	49, 72, 103, 121	0
1	E	220/228 (96%)	-0.48	2 (0%)	84	83	47, 71, 102, 127	0
1	H	220/228 (96%)	-0.44	2 (0%)	84	83	48, 73, 114, 137	0
2	B	212/214 (99%)	-0.64	0	100	100	43, 63, 81, 91	0
2	D	212/214 (99%)	-0.59	0	100	100	39, 61, 81, 93	0
2	F	212/214 (99%)	-0.57	0	100	100	43, 68, 93, 104	0
2	L	212/214 (99%)	-0.61	0	100	100	42, 64, 82, 104	0
All	All	1728/1768 (97%)	-0.53	8 (0%)	91	91	39, 67, 98, 137	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	96	GLY	3.3
1	A	132	SER	3.1
1	A	97	GLY	2.4
1	E	98	ASP	2.3
1	C	97	GLY	2.3
1	A	100(A)	TYR	2.1
1	E	100(A)	TYR	2.1
1	H	132	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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(Å^2)	Q<0.9
3	PO4	H	301	5/5	0.97	0.10	51,55,57,64	0
3	PO4	C	301	5/5	0.98	0.07	50,50,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.