Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:26 AM GMT

PDB ID	:	3IET
Title	:	Crystal Structure of 237mAb with antigen
Authors	:	Brooks, C.L.; Evans, S.V.; Borisova, S.N.
Deposited on	:	2009-07-23
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

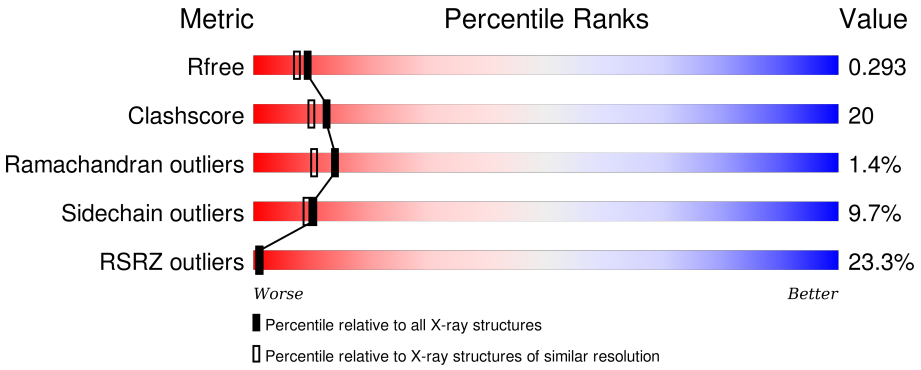
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	217	12% 68% 28%
1	C	217	39% 62% 33% 5%
2	B	218	14% 64% 23% 7%
2	D	218	22% 61% 30% 6%
3	Q	9	67% 22% 33% 11% 33%

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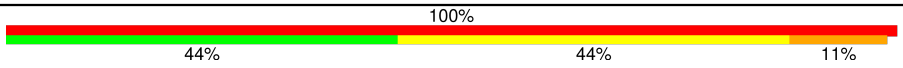
Mol	Chain	Length	Quality of chain
3	X	9	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7204 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 Immunoglobulin light chain (IgG2a).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1660	1037	282	336	5			
1	C	217	Total	C	N	O	S	0	0	0
			1674	1044	284	340	6			

- Molecule 2 is a protein called Immunoglobulin heavy chain (IgG2a).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1598	1004	271	315	8			
2	D	211	Total	C	N	O	S	0	0	0
			1609	1010	275	316	8			

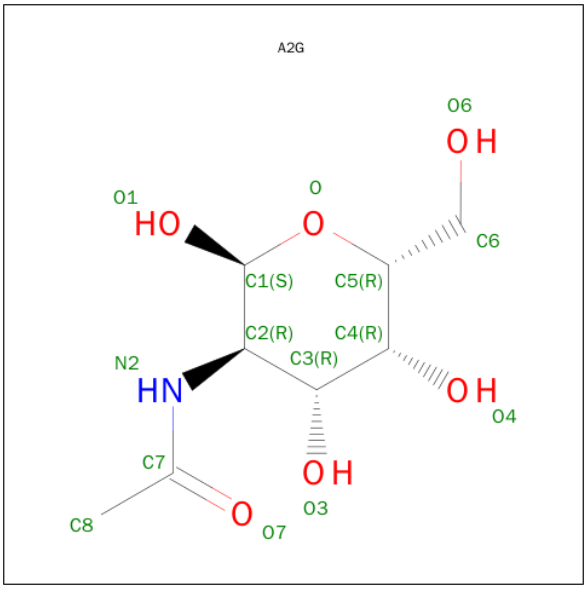
- Molecule 3 is a protein called Podoplanin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	X	9	Total	C	N	O	0	0	0
			68	44	10	14			
3	Q	6	Total	C	N	O	0	0	0
			42	28	7	7			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is SUGAR (N-ACETYL-2-DEOXY-2-AMINO-GALACTOSE) (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	X	1	Total C N O 14 8 1 5	0	0
5	Q	1	Total C N O 14 8 1 5	0	0

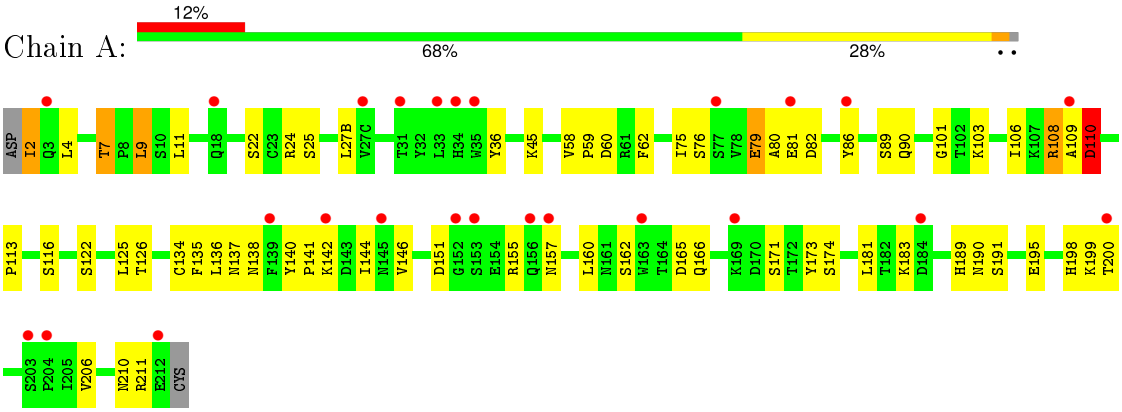
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	160	Total O 160 160	0	0
6	B	116	Total O 116 116	0	0
6	C	111	Total O 111 111	0	0
6	X	7	Total O 7 7	0	0
6	D	120	Total O 120 120	0	0
6	Q	7	Total O 7 7	0	0

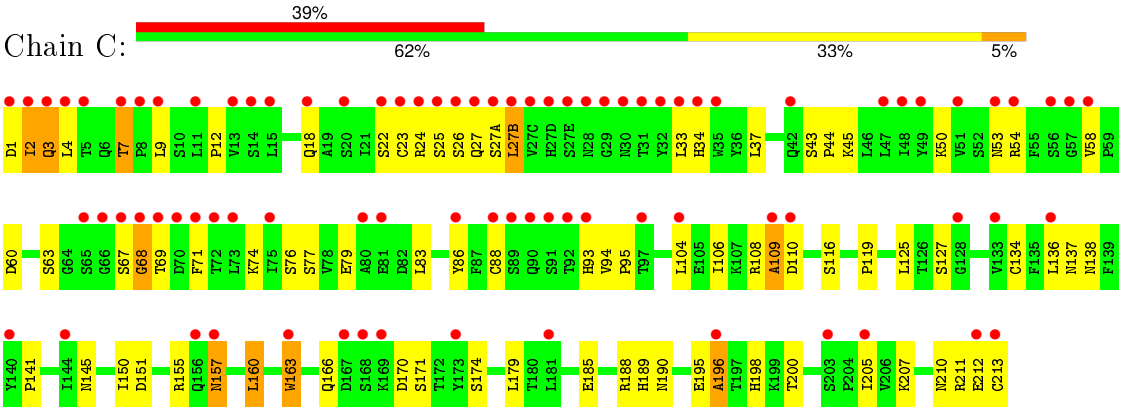
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

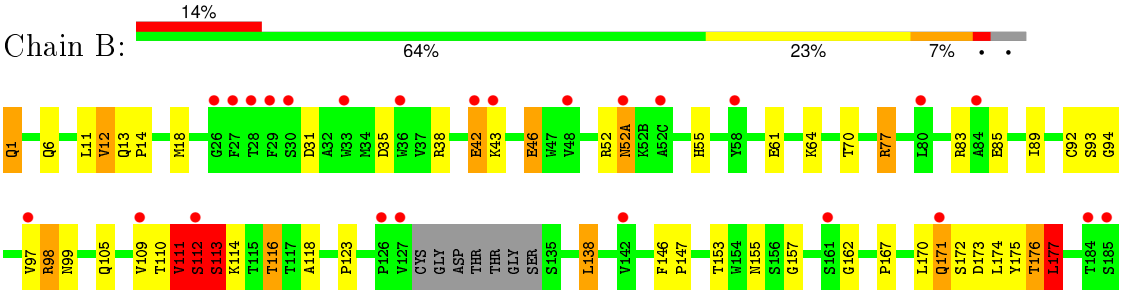
- Molecule 1: Immunoglobulin light chain (IgG2a)



- Molecule 1: Immunoglobulin light chain (IgG2a)

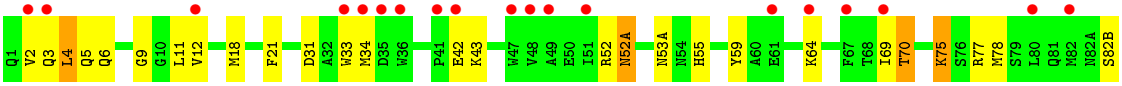


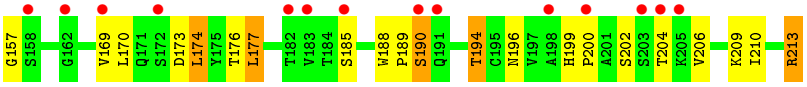
- Molecule 2: Immunoglobulin heavy chain (IgG2a)



• Molecule 2: Immunoglobulin heavy chain (IgG2a)

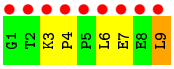
Chain D:





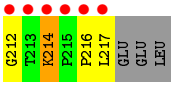
• Molecule 3: Podoplanin

Chain X:



• Molecule 3: Podoplanin

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	277.91Å 38.24Å 95.91Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	19.86 – 2.20 19.86 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.86-2.20) 98.5 (19.86-2.38)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.48 (at 2.38Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_4)	Depositor
R, R_{free}	0.227 , 0.271 0.287 , 0.293	Depositor DCC
R_{free} test set	1938 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.8	EDS
Estimated twinning fraction	0.004 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 38602 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7204	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A2G

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	0.34	0/1698	0.55	0/2305
1	C	0.38	0/1712	0.56	0/2324
2	B	0.36	0/1636	0.65	3/2227 (0.1%)
2	D	0.35	0/1647	0.61	1/2241 (0.0%)
3	Q	0.52	0/43	0.78	0/58
3	X	0.41	0/69	0.71	0/93
All	All	0.36	0/6805	0.60	4/9248 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	112	SER	N-CA-C	7.08	130.12	111.00
2	D	177	LEU	CA-CB-CG	7.05	131.50	115.30
2	B	177	LEU	CA-CB-CG	5.92	128.91	115.30
2	B	77	ARG	NE-CZ-NH1	-5.61	117.50	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	111	VAL	Peptide
2	B	112	SER	Peptide

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	1660	0	1603	51	0
1	C	1674	0	1615	69	0
2	B	1598	0	1557	76	0
2	D	1609	0	1570	59	0
3	Q	42	0	46	5	0
3	X	68	0	72	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	Q	14	0	13	0	0
5	X	14	0	13	0	0
6	A	160	0	0	12	0
6	B	116	0	0	11	2
6	C	111	0	0	17	3
6	D	120	0	0	12	1
6	Q	7	0	0	2	0
6	X	7	0	0	0	0
All	All	7204	0	6489	257	3

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 20.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:PRO:HD2	6:D:517:HOH:O	1.52	1.09
2:B:12:VAL:O	2:B:112:SER:HB2	1.56	1.03
2:D:6:GLN:HE21	2:D:92:CYS:H	0.98	0.92
1:A:2:ILE:HD11	1:A:25:SER:HB2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:6:LEU:HA	3:X:9:LEU:HD22	1.51	0.92
2:B:6:GLN:HE21	2:B:92:CYS:H	1.10	0.91
1:C:2:ILE:HD11	1:C:93:HIS:CD2	2.07	0.89
2:D:75:LYS:HB2	2:D:75:LYS:NZ	1.88	0.87
1:A:106:ILE:H	1:A:166:GLN:HE22	1.21	0.87
2:B:83:ARG:NH2	2:B:85:GLU:HG3	1.90	0.86
1:A:109:ALA:O	1:A:110:ASP:HB2	1.74	0.86
1:C:7:THR:HG22	1:C:22:SER:HB2	1.57	0.86
2:B:194:THR:HB	2:B:209:LYS:HA	1.59	0.85
1:C:83:LEU:HB3	1:C:106:ILE:CD1	2.07	0.83
2:D:149:PRO:O	6:D:517:HOH:O	1.94	0.83
2:B:18:MET:HE1	2:B:109:VAL:HG13	1.62	0.82
1:C:195:GLU:O	1:C:205:ILE:O	2.00	0.80
1:C:54:ARG:NH2	6:C:501:HOH:O	2.16	0.79
1:C:2:ILE:HD11	1:C:93:HIS:CG	2.20	0.77
1:C:138:ASN:ND2	6:D:306:HOH:O	2.14	0.77
2:D:6:GLN:NE2	2:D:92:CYS:H	1.79	0.77
2:B:153:THR:HG23	2:B:196:ASN:OD1	1.85	0.77
2:B:138:LEU:HG	2:B:210:ILE:HG21	1.67	0.76
2:B:14:PRO:HD3	2:B:112:SER:HB3	1.69	0.74
2:B:123:PRO:HG3	2:B:208:LYS:HG3	1.71	0.73
1:C:160:LEU:HD11	2:D:169:VAL:HB	1.70	0.73
1:C:213:CYS:SG	6:C:466:HOH:O	2.46	0.73
1:A:7:THR:HG23	2:D:21:PHE:CZ	2.24	0.72
2:B:147:PRO:O	2:B:199:HIS:HE1	1.73	0.72
2:B:83:ARG:HH21	2:B:85:GLU:HG3	1.55	0.70
2:B:18:MET:CE	2:B:109:VAL:HG13	2.22	0.70
1:C:83:LEU:HB3	1:C:106:ILE:HD13	1.74	0.69
1:C:4:LEU:HD23	1:C:23:CYS:SG	2.32	0.69
2:D:75:LYS:HB2	2:D:75:LYS:HZ2	1.57	0.69
1:A:4:LEU:HD11	1:A:90:GLN:HG3	1.74	0.69
2:B:114:LYS:HD3	2:B:173:ASP:HA	1.74	0.69
1:A:7:THR:HG22	6:A:382:HOH:O	1.92	0.69
2:D:100:ALA:O	6:D:323:HOH:O	2.09	0.69
2:B:153:THR:HG22	2:B:196:ASN:HB2	1.74	0.68
2:B:171:GLN:O	2:B:171:GLN:HG3	1.91	0.68
2:B:11:LEU:HD23	2:B:116:THR:HG22	1.74	0.68
2:D:6:GLN:HE21	2:D:92:CYS:N	1.83	0.68
2:D:96:LYS:HG2	6:D:271:HOH:O	1.93	0.68
2:B:114:LYS:HB2	2:B:146:PHE:CE1	2.30	0.67
1:C:145:ASN:O	1:C:196:ALA:HA	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:SER:OG	2:B:204:THR:HG23	1.96	0.66
2:B:43:LYS:HD3	6:B:224:HOH:O	1.95	0.65
1:C:2:ILE:CD1	1:C:93:HIS:CD2	2.80	0.65
1:A:60:ASP:OD2	6:A:304:HOH:O	2.15	0.65
3:Q:214:LYS:NZ	3:Q:214:LYS:HB2	2.12	0.65
2:B:112:SER:OG	2:B:113:SER:N	2.30	0.65
2:D:153:THR:HG23	2:D:157:GLY:N	2.10	0.65
2:B:97:VAL:O	2:B:98:ARG:HB3	1.96	0.65
2:D:135:SER:HB3	2:D:185:SER:OG	1.97	0.65
2:D:97:VAL:O	2:D:98:ARG:HB3	1.97	0.64
1:C:157:ASN:N	1:C:157:ASN:OD1	2.28	0.63
1:A:122:SER:O	1:A:126:THR:HG23	1.99	0.63
2:B:114:LYS:HD2	2:B:146:PHE:CZ	2.33	0.63
3:Q:212:GLY:N	6:Q:336:HOH:O	2.31	0.63
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.80	0.63
2:D:153:THR:HG22	2:D:196:ASN:OD1	1.99	0.62
2:D:190:SER:HB2	6:D:290:HOH:O	2.00	0.61
2:B:85:GLU:CD	2:B:85:GLU:H	2.03	0.61
1:C:83:LEU:HB3	1:C:106:ILE:HD11	1.83	0.61
1:A:36:TYR:HE1	1:A:89:SER:HB3	1.65	0.61
2:D:138:LEU:HG	2:D:210:ILE:HG21	1.83	0.61
1:A:190:ASN:O	1:A:210:ASN:HA	2.01	0.61
2:B:83:ARG:HD2	2:B:85:GLU:HG2	1.83	0.61
1:A:60:ASP:OD1	6:A:471:HOH:O	2.16	0.61
2:D:114:LYS:HE2	2:D:173:ASP:OD2	2.00	0.60
2:B:85:GLU:OE2	6:B:396:HOH:O	2.16	0.60
1:C:190:ASN:HB3	6:C:316:HOH:O	2.02	0.60
2:D:75:LYS:HB2	2:D:75:LYS:HZ3	1.65	0.60
2:D:96:LYS:HE3	6:D:271:HOH:O	2.01	0.59
2:B:1:GLN:HA	2:B:1:GLN:OE1	2.03	0.59
2:D:105:GLN:C	2:D:105:GLN:HE21	2.04	0.59
1:C:104:LEU:HD23	1:C:104:LEU:C	2.23	0.59
1:A:142:LYS:HD3	1:A:173:TYR:CE2	2.38	0.59
1:A:189:HIS:O	1:A:211:ARG:HD3	2.02	0.59
1:C:150:ILE:HD11	1:C:179:LEU:HD21	1.84	0.59
2:D:31:ASP:HB3	2:D:96:LYS:HD2	1.85	0.58
1:C:190:ASN:ND2	6:C:316:HOH:O	2.36	0.58
1:A:109:ALA:O	1:A:110:ASP:CB	2.49	0.58
1:C:106:ILE:H	1:C:166:GLN:HE22	1.50	0.58
2:B:116:THR:HB	6:B:448:HOH:O	2.03	0.58
1:A:108:ARG:HG3	1:A:171:SER:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:PRO:O	2:D:199:HIS:HE1	1.85	0.58
1:C:198:HIS:CD2	1:C:200:THR:HG23	2.38	0.57
2:D:11:LEU:HB2	2:D:147:PRO:HG3	1.86	0.57
2:D:52(A):ASN:HB3	2:D:53(A):ASN:H	1.69	0.57
2:B:199:HIS:HD2	2:B:202:SER:OG	1.88	0.57
2:B:155:ASN:OD1	6:B:410:HOH:O	2.18	0.57
2:B:194:THR:HG23	6:B:410:HOH:O	2.04	0.56
3:Q:214:LYS:HG3	3:Q:214:LYS:O	2.05	0.56
2:D:153:THR:CG2	2:D:157:GLY:N	2.69	0.56
2:B:114:LYS:HE3	2:B:173:ASP:OD2	2.06	0.56
1:C:2:ILE:HA	1:C:26:SER:OG	2.05	0.56
2:D:119:PRO:HB3	2:D:145:TYR:HB3	1.88	0.56
2:D:199:HIS:HD2	2:D:202:SER:OG	1.89	0.55
2:D:105:GLN:NE2	2:D:106:GLY:O	2.40	0.55
1:C:185:GLU:OE2	1:C:189:HIS:NE2	2.39	0.55
2:D:202:SER:O	2:D:204:THR:HG23	2.06	0.55
1:A:2:ILE:CG2	1:A:90:GLN:NE2	2.70	0.55
2:B:83:ARG:HB2	2:B:85:GLU:OE2	2.08	0.54
2:D:18:MET:HE1	2:D:109:VAL:HG22	1.89	0.54
2:B:194:THR:CG2	6:B:410:HOH:O	2.55	0.54
2:B:94:GLY:HA2	6:B:215:HOH:O	2.08	0.54
2:B:153:THR:CG2	2:B:196:ASN:HB2	2.38	0.54
2:D:125:ALA:O	2:D:213:ARG:NH1	2.41	0.54
2:D:188:TRP:CG	2:D:189:PRO:HA	2.43	0.54
2:B:83:ARG:NH2	2:B:85:GLU:CG	2.68	0.54
1:A:2:ILE:HG21	1:A:90:GLN:NE2	2.22	0.53
2:D:52:ARG:O	2:D:55:HIS:HA	2.08	0.53
2:D:9:GLY:HA2	2:D:18:MET:HE3	1.88	0.53
1:C:190:ASN:HB2	1:C:211:ARG:HB2	1.91	0.53
2:B:209:LYS:HE3	2:B:211:GLU:OE1	2.09	0.53
2:D:18:MET:CE	2:D:109:VAL:HG22	2.39	0.53
2:D:5:GLN:NE2	6:D:430:HOH:O	2.42	0.52
1:C:163:TRP:NE1	6:C:429:HOH:O	2.32	0.52
1:A:137:ASN:HB3	1:A:138:ASN:OD1	2.09	0.52
1:C:157:ASN:O	6:C:414:HOH:O	2.19	0.52
1:C:37:LEU:HD13	1:C:86:TYR:CZ	2.45	0.52
1:C:79:GLU:OE1	6:C:492:HOH:O	2.19	0.52
2:B:162:GLY:N	6:B:343:HOH:O	2.15	0.52
1:A:137:ASN:HD22	1:A:174:SER:HB3	1.75	0.52
1:C:24:ARG:NH1	6:C:399:HOH:O	2.23	0.51
2:B:83:ARG:HD2	2:B:85:GLU:CG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLN:CA	2:B:1:GLN:OE1	2.58	0.51
2:B:187:THR:O	2:B:191:GLN:HB2	2.10	0.51
1:A:151:ASP:HA	1:A:191:SER:HB3	1.93	0.51
1:A:113:PRO:HG3	1:A:144:ILE:HD11	1.92	0.51
2:B:189:PRO:HB3	2:B:212:PRO:HG3	1.93	0.50
2:B:35:ASP:OD2	2:B:98:ARG:HD2	2.11	0.50
2:D:194:THR:HB	2:D:209:LYS:HA	1.94	0.50
1:C:45:LYS:HG3	6:C:260:HOH:O	2.12	0.50
3:X:6:LEU:HD12	3:X:7:GLU:N	2.27	0.50
3:Q:212:GLY:N	6:Q:409:HOH:O	2.44	0.50
1:A:165:ASP:OD1	6:A:287:HOH:O	2.19	0.49
2:B:170:LEU:HB2	2:B:175:TYR:CE2	2.47	0.49
2:B:116:THR:CB	6:B:448:HOH:O	2.61	0.49
2:B:118:ALA:HB1	2:B:204:THR:HG21	1.95	0.49
1:C:155:ARG:NH1	6:C:469:HOH:O	2.41	0.49
1:A:45:LYS:HD3	6:A:482:HOH:O	2.11	0.49
2:D:2:VAL:HG11	2:D:102:TYR:CG	2.48	0.49
2:B:105:GLN:NE2	6:B:305:HOH:O	2.31	0.49
1:C:54:ARG:NH2	6:C:454:HOH:O	2.46	0.48
2:D:153:THR:HG23	2:D:157:GLY:H	1.78	0.48
1:C:195:GLU:O	1:C:196:ALA:HB3	2.13	0.48
1:A:136:LEU:HD12	1:A:136:LEU:N	2.29	0.48
1:A:135:PHE:C	1:A:136:LEU:HD12	2.33	0.48
2:D:105:GLN:HE21	2:D:106:GLY:N	2.12	0.47
2:D:121:VAL:HG21	2:D:206:VAL:HG22	1.95	0.47
1:A:2:ILE:HG21	1:A:90:GLN:CD	2.35	0.47
2:B:64:LYS:HB2	2:B:64:LYS:NZ	2.28	0.47
1:C:74:LYS:NZ	6:C:371:HOH:O	2.32	0.47
1:A:142:LYS:O	1:A:142:LYS:HG3	2.15	0.47
1:C:27:GLN:NE2	6:C:331:HOH:O	2.47	0.47
2:D:33:TRP:CZ3	3:Q:216:PRO:HG3	2.49	0.47
2:B:83:ARG:HH21	2:B:85:GLU:CG	2.24	0.47
1:C:185:GLU:OE1	1:C:188:ARG:NE	2.39	0.47
1:A:9:LEU:HD22	2:D:77:ARG:HD2	1.97	0.47
2:B:31:ASP:C	2:B:52(A):ASN:OD1	2.53	0.47
1:C:141:PRO:O	1:C:198:HIS:HE1	1.98	0.47
2:B:13:GLN:HA	2:B:112:SER:CB	2.45	0.47
2:B:114:LYS:HD2	2:B:146:PHE:CE2	2.49	0.47
2:D:114:LYS:HB2	2:D:146:PHE:CE1	2.49	0.47
1:C:3:GLN:CD	1:C:26:SER:HB3	2.35	0.47
2:D:96:LYS:NZ	6:D:393:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:GLU:HB2	1:C:188:ARG:HH11	1.80	0.47
2:B:85:GLU:N	2:B:85:GLU:CD	2.69	0.46
1:C:151:ASP:OD1	1:C:189:HIS:ND1	2.37	0.46
1:A:198:HIS:HD2	1:A:200:THR:OG1	1.97	0.46
1:C:190:ASN:O	1:C:210:ASN:HA	2.14	0.46
1:C:198:HIS:HD2	1:C:200:THR:OG1	1.99	0.46
1:C:155:ARG:NE	6:C:469:HOH:O	2.20	0.46
1:C:137:ASN:ND2	1:C:174:SER:HB3	2.31	0.46
1:A:116:SER:O	1:A:134:CYS:HA	2.16	0.46
1:A:2:ILE:O	1:A:2:ILE:HG23	2.16	0.45
1:A:140:TYR:CG	1:A:141:PRO:HA	2.51	0.45
2:B:153:THR:OG1	2:B:157:GLY:N	2.49	0.45
2:B:43:LYS:HE2	2:B:46:GLU:CD	2.37	0.45
2:B:38:ARG:HA	2:B:89:ILE:O	2.16	0.45
2:B:42:GLU:H	2:B:42:GLU:CD	2.19	0.45
1:C:195:GLU:OE1	6:C:505:HOH:O	2.21	0.45
1:C:76:SER:O	1:C:77:SER:C	2.55	0.45
2:D:64:LYS:HB2	2:D:64:LYS:HE3	1.74	0.45
2:D:199:HIS:CD2	2:D:202:SER:OG	2.69	0.45
2:B:123:PRO:HG3	2:B:208:LYS:CG	2.41	0.44
2:B:205:LYS:O	2:B:206:VAL:HG13	2.17	0.44
2:B:6:GLN:HE21	2:B:92:CYS:N	1.94	0.44
2:D:34:MET:SD	2:D:94:GLY:HA3	2.58	0.44
1:A:76:SER:HB2	6:A:284:HOH:O	2.17	0.44
2:D:4:LEU:HG	2:D:92:CYS:SG	2.58	0.44
1:A:62:PHE:CD1	1:A:75:ILE:HG12	2.53	0.44
2:B:52:ARG:O	2:B:55:HIS:HA	2.18	0.44
2:D:82(B):SER:OG	6:D:347:HOH:O	2.21	0.44
1:C:54:ARG:NH1	1:C:58:VAL:O	2.51	0.44
1:C:170:ASP:O	1:C:171:SER:HB2	2.17	0.44
1:C:33:LEU:HD13	1:C:33:LEU:C	2.38	0.44
2:B:93:SER:OG	2:B:99:ASN:HA	2.17	0.44
2:D:70:THR:O	2:D:78:MET:HB2	2.17	0.44
1:C:106:ILE:N	1:C:106:ILE:HD12	2.33	0.44
1:C:108:ARG:HG2	1:C:109:ALA:N	2.32	0.44
1:C:25:SER:OG	1:C:69:THR:HA	2.17	0.43
1:C:34:HIS:O	1:C:88:CYS:HA	2.18	0.43
1:A:113:PRO:HG3	1:A:144:ILE:CD1	2.48	0.43
1:C:137:ASN:HD22	1:C:174:SER:HB3	1.82	0.43
1:A:79:GLU:O	1:A:82:ASP:HB2	2.18	0.43
2:B:11:LEU:CD2	2:B:116:THR:HG22	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:TRP:CD1	2:D:189:PRO:HA	2.53	0.43
1:C:94:VAL:HA	1:C:95:PRO:HD3	1.85	0.43
2:B:172:SER:O	2:B:173:ASP:HB2	2.19	0.43
3:X:3:LYS:HA	3:X:4:PRO:HD3	1.80	0.43
2:B:114:LYS:HG2	2:B:173:ASP:CG	2.39	0.43
1:C:27(B):LEU:HD22	1:C:71:PHE:CE1	2.53	0.43
1:A:2:ILE:CG2	1:A:2:ILE:O	2.65	0.43
1:C:207:LYS:HE2	6:C:455:HOH:O	2.19	0.43
1:C:119:PRO:HD2	6:D:274:HOH:O	2.19	0.43
2:B:11:LEU:HD11	2:B:112:SER:HA	2.01	0.43
1:A:80:ALA:HA	1:A:106:ILE:HG13	2.00	0.43
2:B:188:TRP:CG	2:B:189:PRO:HA	2.53	0.43
2:B:177:LEU:HD12	2:B:177:LEU:C	2.39	0.43
2:D:126:PRO:HD3	2:D:138:LEU:HD12	2.01	0.42
1:A:162:SER:OG	2:B:167:PRO:HD2	2.19	0.42
1:A:125:LEU:O	1:A:183:LYS:HD3	2.19	0.42
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.80	0.42
2:D:200:PRO:CD	6:D:517:HOH:O	2.33	0.42
1:A:160:LEU:HD11	2:B:171:GLN:HG2	2.01	0.42
2:B:188:TRP:CD1	2:B:189:PRO:HA	2.55	0.42
1:A:2:ILE:N	6:A:272:HOH:O	2.52	0.42
2:B:191:GLN:HB3	2:B:191:GLN:HE21	1.67	0.42
2:D:152:LEU:C	2:D:152:LEU:HD23	2.40	0.42
1:C:50:LYS:HB2	1:C:53:ASN:HD22	1.83	0.42
2:B:77:ARG:NH1	6:B:494:HOH:O	2.15	0.42
1:C:125:LEU:C	1:C:127:SER:H	2.22	0.42
1:C:104:LEU:C	1:C:104:LEU:CD2	2.88	0.42
2:B:83:ARG:HD2	2:B:85:GLU:OE2	2.20	0.42
1:A:137:ASN:HD22	1:A:174:SER:CB	2.32	0.42
1:A:79:GLU:CD	6:A:413:HOH:O	2.58	0.42
1:C:136:LEU:N	1:C:136:LEU:HD12	2.34	0.42
2:D:170:LEU:HD12	2:D:174:LEU:O	2.19	0.42
2:D:59:TYR:OH	2:D:69:ILE:HG22	2.19	0.41
1:C:43:SER:HB2	1:C:44:PRO:HD2	2.02	0.41
1:C:116:SER:O	1:C:134:CYS:HA	2.19	0.41
1:C:198:HIS:CD2	1:C:200:THR:H	2.39	0.41
1:A:136:LEU:HD21	1:A:146:VAL:HG22	2.03	0.41
1:A:79:GLU:OE2	6:A:413:HOH:O	2.21	0.41
1:C:18:GLN:HB2	1:C:18:GLN:HE21	1.67	0.41
1:A:110:ASP:HB2	6:A:254:HOH:O	2.20	0.41
2:D:87:THR:HA	2:D:109:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:HG3	6:A:305:HOH:O	2.21	0.41
1:A:86:TYR:O	1:A:101:GLY:HA2	2.21	0.41
1:C:27:GLN:C	1:C:69:THR:HG22	2.41	0.41
2:B:111:VAL:O	2:B:111:VAL:HG22	2.20	0.40
1:C:54:ARG:NE	6:C:337:HOH:O	2.51	0.40
1:C:27(A):SER:HA	1:C:68:GLY:O	2.21	0.40
6:A:275:HOH:O	2:B:176:THR:HG21	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:431:HOH:O	6:D:420:HOH:O[1_545]	2.17	0.03
6:B:320:HOH:O	6:C:244:HOH:O[1_556]	2.18	0.02
6:B:446:HOH:O	6:C:230:HOH:O[1_556]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	213/217 (98%)	204 (96%)	8 (4%)	1 (0%)	34 35
1	C	215/217 (99%)	200 (93%)	10 (5%)	5 (2%)	8 4
2	B	206/218 (94%)	198 (96%)	5 (2%)	3 (2%)	13 9
2	D	207/218 (95%)	202 (98%)	2 (1%)	3 (1%)	14 10
3	Q	4/9 (44%)	4 (100%)	0	0	100 100
3	X	7/9 (78%)	7 (100%)	0	0	100 100
All	All	852/888 (96%)	815 (96%)	25 (3%)	12 (1%)	14 10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
2	B	52(A)	ASN
2	B	113	SER
1	C	110	ASP
2	D	52(A)	ASN
2	B	112	SER
2	D	43	LYS
1	C	109	ALA
1	C	68	GLY
1	C	196	ALA
1	C	2	ILE
2	D	98	ARG

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	193/195 (99%)	178 (92%)	15 (8%)	16 15
1	C	195/195 (100%)	182 (93%)	13 (7%)	20 21
2	B	180/186 (97%)	159 (88%)	21 (12%)	7 5
2	D	181/186 (97%)	159 (88%)	22 (12%)	6 5
3	Q	5/8 (62%)	3 (60%)	2 (40%)	0 0
3	X	8/8 (100%)	7 (88%)	1 (12%)	6 4
All	All	762/778 (98%)	688 (90%)	74 (10%)	10 9

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	7	THR
1	A	9	LEU
1	A	11	LEU
1	A	22	SER
1	A	24	ARG
1	A	27(B)	LEU

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Mol	Chain	Res	Type
1	A	79	GLU
1	A	103	LYS
1	A	108	ARG
1	A	110	ASP
1	A	155	ARG
1	A	157	ASN
1	A	181	LEU
1	A	199	LYS
2	B	1	GLN
2	B	12	VAL
2	B	42	GLU
2	B	46	GLU
2	B	61	GLU
2	B	70	THR
2	B	98	ARG
2	B	110	THR
2	B	111	VAL
2	B	113	SER
2	B	116	THR
2	B	138	LEU
2	B	171	GLN
2	B	174	LEU
2	B	176	THR
2	B	177	LEU
2	B	194	THR
2	B	196	ASN
2	B	204	THR
2	B	206	VAL
2	B	209	LYS
1	C	1	ASP
1	C	3	GLN
1	C	7	THR
1	C	9	LEU
1	C	12	PRO
1	C	27(B)	LEU
1	C	60	ASP
1	C	63	SER
1	C	67	SER
1	C	157	ASN
1	C	160	LEU
1	C	163	TRP
1	C	212	GLU

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Mol	Chain	Res	Type
2	D	3	GLN
2	D	4	LEU
2	D	12	VAL
2	D	42	GLU
2	D	70	THR
2	D	75	LYS
2	D	85	GLU
2	D	98	ARG
2	D	105	GLN
2	D	108	THR
2	D	110	THR
2	D	116	THR
2	D	127	VAL
2	D	136	VAL
2	D	138	LEU
2	D	153	THR
2	D	174	LEU
2	D	176	THR
2	D	177	LEU
2	D	190	SER
2	D	194	THR
2	D	213	ARG
3	X	9	LEU
3	Q	214	LYS
3	Q	217	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	161	ASN
1	A	166	GLN
1	A	198	HIS
2	B	3	GLN
2	B	99	ASN
2	B	171	GLN
2	B	191	GLN
2	B	199	HIS
1	C	18	GLN
1	C	42	GLN
1	C	53	ASN
1	C	93	HIS

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Mol	Chain	Res	Type
1	C	137	ASN
1	C	161	ASN
1	C	166	GLN
1	C	198	HIS
2	D	3	GLN
2	D	6	GLN
2	D	13	GLN
2	D	99	ASN
2	D	105	GLN
2	D	199	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	A2G	Q	800	3	14,14,15	0.59	0	15,19,21	1.07	2 (13%)
5	A2G	X	800	3	14,14,15	0.62	0	15,19,21	1.44	1 (6%)

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
5	A2G	Q	800	3	-	0/6/23/26	0/1/1/1
5	A2G	X	800	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	X	800	A2G	C2-N2-C7	-4.30	117.52	123.04
5	Q	800	A2G	C6-C5-C4	-2.32	107.28	113.02
5	Q	800	A2G	C4-C3-C2	-2.31	107.64	111.23

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	215/217 (99%)	1.04	25 (11%)	6 6	22, 34, 47, 56	0
1	C	217/217 (100%)	1.97	84 (38%)	0 0	25, 40, 53, 61	0
2	B	210/218 (96%)	1.11	31 (14%)	3 3	20, 33, 52, 62	0
2	D	211/218 (96%)	1.33	47 (22%)	1 1	24, 35, 50, 59	0
3	Q	6/9 (66%)	9.41	6 (100%)	0 0	45, 47, 49, 52	0
3	X	9/9 (100%)	9.70	9 (100%)	0 0	29, 34, 48, 48	0
All	All	868/888 (97%)	1.51	202 (23%)	1 1	20, 36, 52, 62	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	217	LEU	13.3
3	X	1	GLY	12.5
3	X	4	PRO	12.0
3	X	2	THR	11.2
3	Q	215	PRO	11.0
3	Q	216	PRO	10.9
3	X	9	LEU	10.7
3	X	5	PRO	10.5
1	C	27(C)	VAL	9.1
3	Q	213	THR	9.1
3	X	3	LYS	8.9
3	X	7	GLU	8.1
3	X	6	LEU	7.6
1	C	29	GLY	7.5
1	C	93	HIS	7.1
1	C	27(E)	SER	6.6
1	C	4	LEU	6.5
3	Q	212	GLY	6.5
1	C	71	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	33	LEU	5.9
1	C	32	TYR	5.7
3	Q	214	LYS	5.7
3	X	8	GLU	5.6
1	C	34	HIS	5.5
1	C	2	ILE	5.5
1	C	65	SER	5.4
1	C	27	GLN	5.3
1	C	27(B)	LEU	5.2
1	C	70	ASP	5.2
1	C	67	SER	4.9
1	C	92	THR	4.7
1	C	26	SER	4.4
1	C	51	VAL	4.2
1	A	109	ALA	4.1
1	C	69	THR	4.1
2	D	203	SER	4.1
1	C	128	GLY	4.0
1	A	169	LYS	4.0
1	C	91	SER	4.0
1	C	24	ARG	4.0
1	C	7	THR	4.0
1	C	49	TYR	4.0
2	D	41	PRO	3.9
1	C	89	SER	3.9
1	A	153	SER	3.8
1	A	33	LEU	3.8
1	C	25	SER	3.7
1	C	109	ALA	3.7
2	D	47	TRP	3.6
2	D	33	TRP	3.6
1	C	35	TRP	3.6
1	C	163	TRP	3.6
1	C	5	THR	3.5
1	C	169	LYS	3.5
1	C	66	GLY	3.5
1	C	31	THR	3.4
1	C	3	GLN	3.4
1	C	27(A)	SER	3.3
2	D	97	VAL	3.3
2	D	34	MET	3.2
2	B	52(C)	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	133	VAL	3.2
1	A	163	TRP	3.1
1	C	68	GLY	3.1
2	B	26	GLY	3.1
2	B	97	VAL	3.1
1	A	203	SER	3.1
1	A	34	HIS	3.1
1	C	140	TYR	3.0
2	B	33	TRP	3.0
1	A	157	ASN	3.0
2	D	191	GLN	3.0
1	C	53	ASN	3.0
1	C	15	LEU	3.0
1	C	23	CYS	2.9
1	C	20	SER	2.9
1	C	168	SER	2.9
1	C	196	ALA	2.9
1	C	86	TYR	2.9
2	D	169	VAL	2.9
1	C	156	GLN	2.9
2	D	115	THR	2.8
1	C	81	GLU	2.8
2	B	42	GLU	2.8
1	C	27(D)	HIS	2.8
2	B	43	LYS	2.8
1	A	156	GLN	2.8
1	A	27(C)	VAL	2.8
2	D	190	SER	2.8
2	B	112	SER	2.8
2	B	190	SER	2.8
1	C	136	LEU	2.8
2	D	200	PRO	2.8
2	D	12	VAL	2.7
1	C	73	LEU	2.7
1	C	11	LEU	2.7
2	D	64	LYS	2.7
1	C	203	SER	2.7
2	D	172	SER	2.7
1	C	88	CYS	2.7
1	A	3	GLN	2.7
1	C	58	VAL	2.7
2	D	90	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	30	ASN	2.6
2	B	52(A)	ASN	2.6
2	D	127	VAL	2.6
2	B	80	LEU	2.6
1	C	54	ARG	2.6
1	C	22	SER	2.6
1	C	57	GLY	2.6
2	D	49	ALA	2.6
2	B	184	THR	2.6
2	B	27	PHE	2.6
1	C	42	GLN	2.6
1	C	157	ASN	2.5
1	C	144	ILE	2.5
1	C	8	PRO	2.5
2	D	149	PRO	2.5
2	D	102	TYR	2.5
2	B	185	SER	2.5
1	C	28	ASN	2.5
1	A	18	GLN	2.5
2	B	171	GLN	2.5
1	C	48	ILE	2.5
2	B	189	PRO	2.4
2	D	80	LEU	2.4
1	C	167	ASP	2.4
2	D	183	VAL	2.4
2	D	69	ILE	2.4
1	A	145	ASN	2.4
1	C	97	THR	2.4
2	D	36	TRP	2.4
2	D	67	PHE	2.4
1	C	80	ALA	2.4
2	D	110	THR	2.4
1	C	9	LEU	2.4
1	C	212	GLU	2.4
2	B	142	VAL	2.4
2	D	2	VAL	2.4
1	A	31	THR	2.4
1	C	72	THR	2.4
2	B	28	THR	2.4
2	D	42	GLU	2.4
2	D	152	LEU	2.4
1	C	18	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	142	VAL	2.4
1	A	35	TRP	2.4
2	D	198	ALA	2.4
2	D	204	THR	2.4
1	C	104	LEU	2.3
1	A	184	ASP	2.3
2	B	48	VAL	2.3
2	D	108	THR	2.3
2	B	36	TRP	2.3
1	A	142	LYS	2.3
2	D	61	GLU	2.3
2	B	126	PRO	2.3
1	A	152	GLY	2.3
2	D	158	SER	2.3
1	C	47	LEU	2.3
1	C	110	ASP	2.3
2	D	35	ASP	2.3
2	B	206	VAL	2.3
2	D	51	ILE	2.3
1	A	86	TYR	2.3
2	B	84	ALA	2.3
2	D	182	THR	2.3
1	A	77	SER	2.3
2	D	93	SER	2.3
2	B	161	SER	2.2
1	C	75	ILE	2.2
1	C	13	VAL	2.2
1	C	90	GLN	2.2
2	B	109	VAL	2.2
2	B	212	PRO	2.2
1	A	200	THR	2.2
2	B	192	SER	2.2
2	D	205	LYS	2.2
2	D	3	GLN	2.2
2	D	48	VAL	2.1
1	C	56	SER	2.1
2	D	156	SER	2.1
2	D	185	SER	2.1
2	B	127	VAL	2.1
2	B	58	TYR	2.1
1	A	81	GLU	2.1
2	D	87	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	162	GLY	2.1
1	C	213	CYS	2.1
2	B	191	GLN	2.1
2	D	82	MET	2.1
2	D	114	LYS	2.1
1	C	14	SER	2.1
1	C	1	ASP	2.1
2	B	29	PHE	2.0
1	C	205	ILE	2.0
1	C	181	LEU	2.0
1	C	173	TYR	2.0
1	A	204	PRO	2.0
1	A	212	GLU	2.0
1	A	139	PHE	2.0
2	B	30	SER	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
5	A2G	X	800	14/15	0.77	0.32	-0.05	20,25,30,32	0
5	A2G	Q	800	14/15	0.70	0.26	-0.77	39,41,46,46	0
4	ZN	C	218	1/1	0.97	0.10	-	33,33,33,33	1
4	ZN	B	216	1/1	0.97	0.04	-	31,31,31,31	0
4	ZN	D	214	1/1	0.98	0.08	-	40,40,40,40	0
4	ZN	A	215	1/1	0.95	0.05	-	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.