Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:38 PM GMT

PDB ID	:	5DO2
Title	:	Complex structure of MERS-RBD bound with 4C2 antibody
Authors	:	Li, Y.; Wan, Y.; Liu, P.; Zhao, J.; Lu, G.; Qi, J.; Wang, Q.; Lu, X.; Wu, Y.; Liu, W.; Yuen, K.Y.; Perlman, S.; Gao, G.F.; Yan, J.
Deposited on	:	2015-09-10
Resolution	:	2.41 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 ⓘ symbol.

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

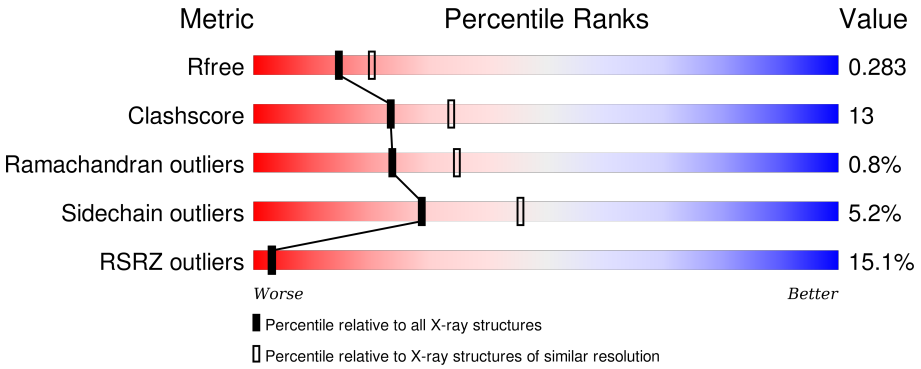
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.41 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	251	3% 62% 18% • 17%
1	B	251	46% 55% 25% • 17%
2	C	219	21% 72% 24% • •
2	H	219	% 80% 16% • •
3	D	214	9% 79% 20%

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Mol	Chain	Length	Quality of chain
3	L	214	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9937 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 S protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1608	1026	256	315	11			
1	B	208	Total	C	N	O	S	0	0	0
			1608	1026	256	315	11			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	ALA	-	expression tag	UNP W5ZZM0
A	363	ASP	-	expression tag	UNP W5ZZM0
A	364	GLY	-	expression tag	UNP W5ZZM0
A	365	ILE	-	expression tag	UNP W5ZZM0
A	366	GLN	-	expression tag	UNP W5ZZM0
A	607	HIS	-	expression tag	UNP W5ZZM0
A	608	HIS	-	expression tag	UNP W5ZZM0
A	609	HIS	-	expression tag	UNP W5ZZM0
A	610	HIS	-	expression tag	UNP W5ZZM0
A	611	HIS	-	expression tag	UNP W5ZZM0
A	612	HIS	-	expression tag	UNP W5ZZM0
B	362	ALA	-	expression tag	UNP W5ZZM0
B	363	ASP	-	expression tag	UNP W5ZZM0
B	364	GLY	-	expression tag	UNP W5ZZM0
B	365	ILE	-	expression tag	UNP W5ZZM0
B	366	GLN	-	expression tag	UNP W5ZZM0
B	607	HIS	-	expression tag	UNP W5ZZM0
B	608	HIS	-	expression tag	UNP W5ZZM0
B	609	HIS	-	expression tag	UNP W5ZZM0
B	610	HIS	-	expression tag	UNP W5ZZM0
B	611	HIS	-	expression tag	UNP W5ZZM0
B	612	HIS	-	expression tag	UNP W5ZZM0

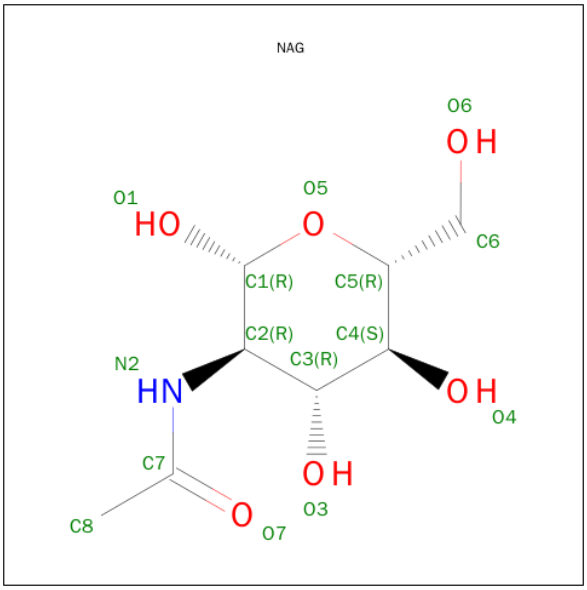
- Molecule 2 is a protein called 4C2 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1621	1021	264	327	9			
2	C	215	Total	C	N	O	S	0	0	0
			1621	1021	264	327	9			

- Molecule 3 is a protein called 4C2 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1663	1026	284	346	7			
3	D	214	Total	C	N	O	S	0	0	0
			1663	1026	284	346	7			

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	H	31	Total	O	0	0
			31	31		

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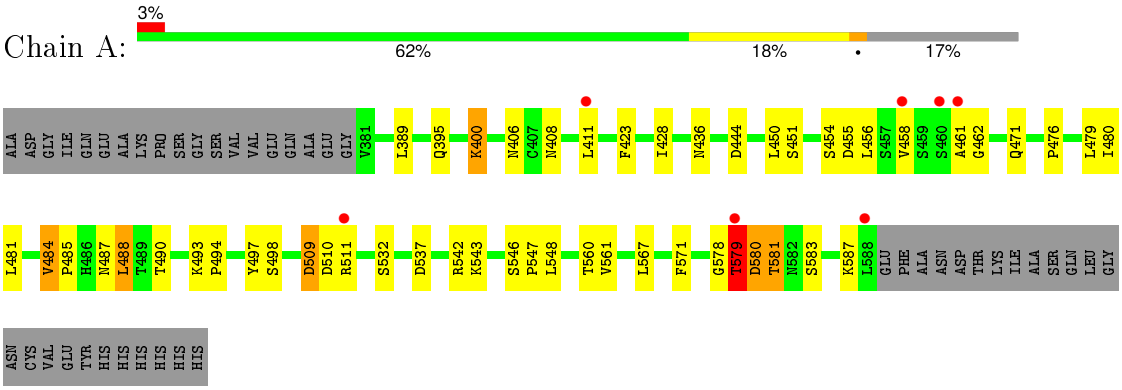
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	29	Total O 29 29	0	0
5	B	23	Total O 23 23	0	0
5	C	11	Total O 11 11	0	0
5	D	21	Total O 21 21	0	0

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.

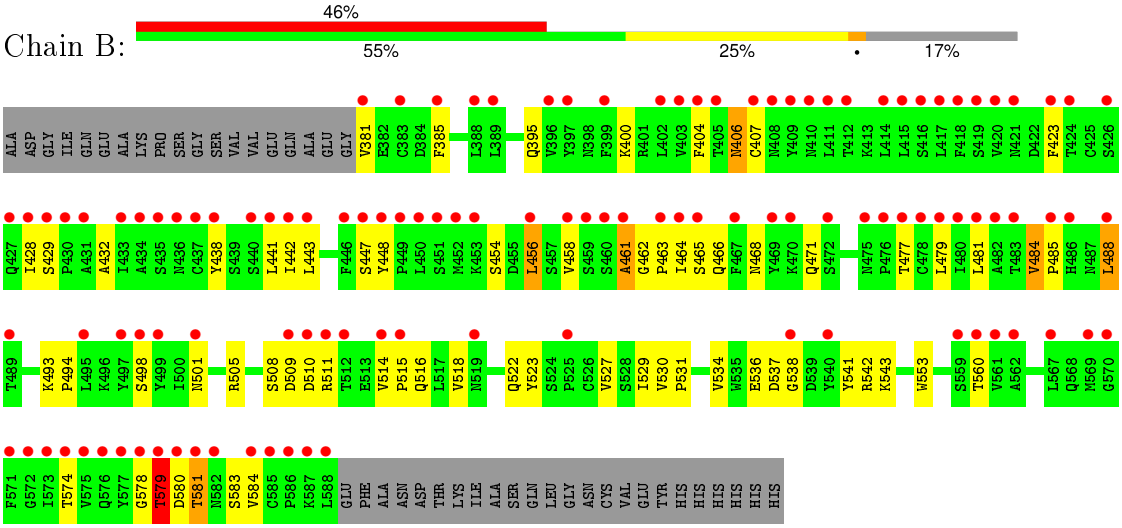
- Molecule 1: S protein

Chain A:



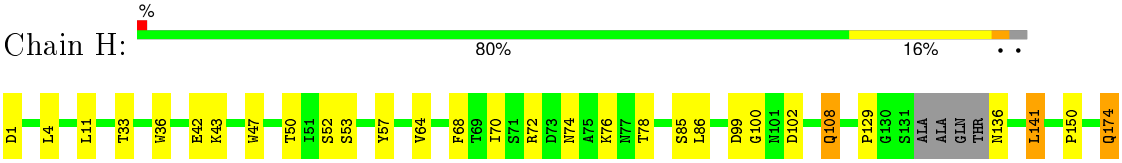
- Molecule 1: S protein

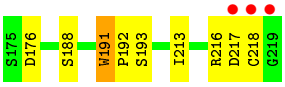
Chain B:



- Molecule 2: 4C2 heavy chain

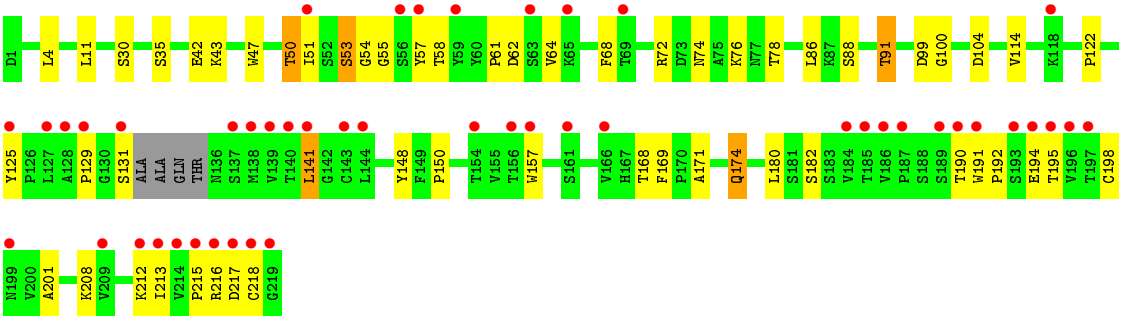
Chain H:





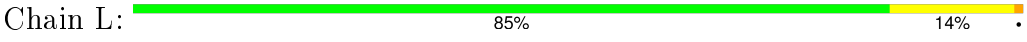
• Molecule 2: 4C2 heavy chain

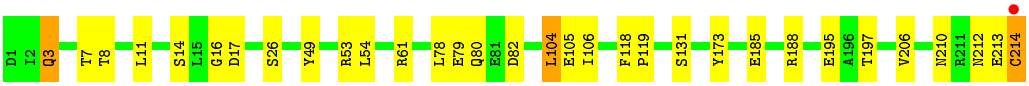
Chain C:



• Molecule 3: 4C2 light chain

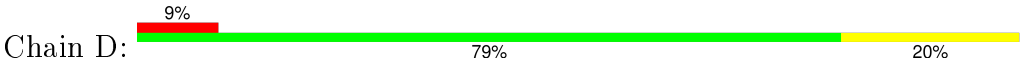
Chain L:

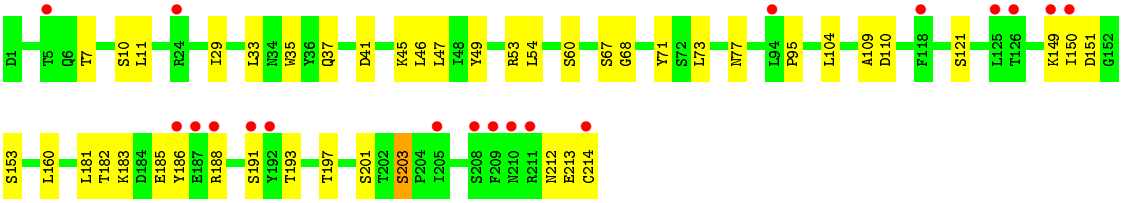




• Molecule 3: 4C2 light chain

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.08Å 110.40Å 172.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.53 – 2.41 46.53 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.53-2.41) 93.7 (46.53-2.41)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.245 , 0.289 0.242 , 0.283	Depositor DCC
R_{free} test set	2641 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 54988 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9937	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: NAG

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	0.26	0/1647	0.48	0/2249
1	B	0.25	0/1647	0.47	0/2249
2	C	0.28	0/1662	0.49	0/2266
2	H	0.34	0/1662	0.50	0/2266
3	D	0.24	0/1696	0.48	0/2299
3	L	0.27	0/1696	0.51	0/2299
All	All	0.28	0/10010	0.49	0/13628

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

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	1608	0	1573	37	0
1	B	1608	0	1574	86	0
2	C	1621	0	1572	44	0
2	H	1621	0	1572	29	0
3	D	1663	0	1587	51	0
3	L	1663	0	1587	20	0
4	A	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	24	0	0	12	0
5	B	23	0	0	56	0
5	C	11	0	0	17	0
5	D	21	0	0	38	0
5	H	31	0	0	12	0
5	L	29	0	0	6	0
All	All	9937	0	9478	257	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 13.

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)
1:B:514:VAL:HG12	5:B:704:HOH:O	1.22	1.26
1:B:432:ALA:HB3	5:B:705:HOH:O	1.07	1.22
5:H:328:HOH:O	3:L:214:CYS:SG	2.01	1.17
3:D:186:TYR:HB3	5:D:304:HOH:O	1.47	1.14
1:B:448:TYR:N	5:B:701:HOH:O	1.80	1.11
1:B:447:SER:C	5:B:701:HOH:O	1.86	1.09
2:H:136:ASN:N	5:H:301:HOH:O	1.84	1.09
3:D:110:ASP:N	5:D:305:HOH:O	1.88	1.04
1:B:471:GLN:HB3	5:B:707:HOH:O	1.59	1.03
3:D:151:ASP:HA	5:D:308:HOH:O	1.60	1.02
1:B:584:VAL:HB	5:B:720:HOH:O	1.60	1.00
1:B:541:TYR:CD2	5:B:712:HOH:O	2.14	1.00
1:B:428:ILE:HG12	5:B:705:HOH:O	1.60	1.00
1:B:511:ARG:HB3	5:B:717:HOH:O	1.60	0.99
2:C:88:SER:HB2	5:C:311:HOH:O	1.62	0.99
1:B:438:TYR:HB2	5:B:720:HOH:O	1.60	0.98
2:C:30:SER:O	5:C:301:HOH:O	1.81	0.98
1:B:447:SER:O	5:B:702:HOH:O	1.80	0.97
3:D:150:ILE:O	5:D:302:HOH:O	1.82	0.97
3:D:197:THR:OG1	5:D:301:HOH:O	1.81	0.97
2:C:53:SER:CB	5:C:301:HOH:O	2.11	0.97
2:C:169:PHE:N	5:C:302:HOH:O	1.98	0.97
1:B:442:ILE:HA	5:B:715:HOH:O	1.63	0.96
3:D:188:ARG:NE	5:D:306:HOH:O	1.97	0.96
1:A:436:ASN:OD1	5:A:801:HOH:O	1.82	0.96
1:B:537:ASP:O	5:B:703:HOH:O	1.83	0.95
1:B:514:VAL:C	5:B:704:HOH:O	2.05	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:VAL:O	5:B:704:HOH:O	1.88	0.92
3:D:67:SER:O	5:D:303:HOH:O	1.85	0.92
3:D:182:THR:O	5:D:304:HOH:O	1.87	0.91
1:B:429:SER:O	5:B:705:HOH:O	1.89	0.91
2:H:176:ASP:OD2	5:H:302:HOH:O	1.88	0.90
2:C:53:SER:CA	5:C:301:HOH:O	2.20	0.89
1:B:458:VAL:HG23	5:B:706:HOH:O	1.73	0.89
2:C:168:THR:HA	5:C:302:HOH:O	1.73	0.89
1:A:546:SER:HB2	5:A:803:HOH:O	1.73	0.88
1:B:580:ASP:OD1	1:B:581:THR:HG23	1.74	0.87
1:A:406:ASN:H	1:A:583:SER:HB2	1.39	0.86
3:D:191:SER:HB2	5:D:308:HOH:O	1.76	0.86
1:B:574:THR:OG1	5:B:707:HOH:O	1.94	0.84
3:D:188:ARG:CZ	5:D:306:HOH:O	2.25	0.84
1:A:458:VAL:HG23	5:A:811:HOH:O	1.78	0.82
1:B:541:TYR:CG	5:B:712:HOH:O	2.27	0.82
3:D:95:PRO:HD2	5:D:312:HOH:O	1.80	0.82
1:A:471:GLN:HB2	5:A:802:HOH:O	1.79	0.82
3:D:183:LYS:CA	5:D:304:HOH:O	2.28	0.81
1:B:542:ARG:O	5:B:708:HOH:O	1.98	0.81
1:B:442:ILE:CA	5:B:709:HOH:O	2.29	0.79
1:B:442:ILE:C	5:B:709:HOH:O	2.19	0.79
1:B:443:LEU:N	5:B:709:HOH:O	2.15	0.79
1:B:505:ARG:NH1	5:B:714:HOH:O	2.15	0.79
2:H:191:TRP:C	5:H:303:HOH:O	2.20	0.79
1:A:455:ASP:O	5:A:804:HOH:O	2.01	0.78
1:A:546:SER:CB	5:A:803:HOH:O	2.30	0.78
3:L:197:THR:OG1	5:L:301:HOH:O	2.02	0.78
1:B:530:VAL:HA	5:B:712:HOH:O	1.82	0.78
3:D:201:SER:C	5:D:307:HOH:O	2.22	0.78
3:D:201:SER:O	5:D:307:HOH:O	2.00	0.77
3:D:183:LYS:HA	5:D:304:HOH:O	1.83	0.77
1:B:538:GLY:HA3	5:B:703:HOH:O	1.82	0.77
2:C:88:SER:O	5:C:304:HOH:O	2.03	0.76
1:B:516:GLN:NE2	5:B:704:HOH:O	2.14	0.76
1:B:441:LEU:O	5:B:709:HOH:O	2.02	0.76
2:C:131:SER:O	5:C:305:HOH:O	2.04	0.76
3:D:183:LYS:C	5:D:304:HOH:O	2.23	0.75
3:D:153:SER:O	5:D:302:HOH:O	2.05	0.75
3:D:109:ALA:C	5:D:305:HOH:O	2.21	0.74
3:L:214:CYS:O	5:L:302:HOH:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:SER:OG	5:B:710:HOH:O	2.05	0.74
3:D:191:SER:O	5:D:308:HOH:O	2.05	0.74
1:B:406:ASN:H	1:B:583:SER:HB2	1.53	0.73
1:B:448:TYR:CB	5:B:701:HOH:O	2.35	0.73
1:B:448:TYR:HB2	5:B:701:HOH:O	1.87	0.73
1:B:441:LEU:HD23	5:B:709:HOH:O	1.87	0.73
3:D:110:ASP:O	5:D:309:HOH:O	2.06	0.71
3:D:191:SER:CB	5:D:308:HOH:O	2.32	0.71
1:B:385:PHE:O	5:B:711:HOH:O	2.08	0.71
2:C:53:SER:HB3	5:C:301:HOH:O	1.82	0.70
2:C:168:THR:CA	5:C:302:HOH:O	2.34	0.70
2:C:174:GLN:OE1	3:D:160:LEU:HD21	1.91	0.70
1:B:395:GLN:HA	5:B:702:HOH:O	1.91	0.70
2:C:11:LEU:HB2	2:C:150:PRO:HG3	1.74	0.70
2:H:136:ASN:N	5:H:307:HOH:O	2.24	0.70
1:B:538:GLY:CA	5:B:703:HOH:O	2.40	0.69
2:H:136:ASN:OD1	5:H:301:HOH:O	2.11	0.68
1:B:442:ILE:HG12	5:B:715:HOH:O	1.92	0.68
3:D:95:PRO:CD	5:D:312:HOH:O	2.41	0.68
1:B:484:VAL:HG23	1:B:488:LEU:HB3	1.76	0.68
1:B:509:ASP:O	1:B:511:ARG:N	2.24	0.68
2:H:85:SER:OG	5:H:305:HOH:O	2.11	0.68
3:D:185:GLU:HA	3:D:188:ARG:HD3	1.75	0.67
1:B:580:ASP:CG	1:B:581:THR:HA	2.14	0.67
1:B:536:GLU:O	5:B:713:HOH:O	2.12	0.67
1:B:529:ILE:O	5:B:712:HOH:O	2.12	0.66
1:A:532:SER:O	5:A:805:HOH:O	2.12	0.66
2:C:104:ASP:O	5:C:307:HOH:O	2.12	0.66
3:D:203:SER:O	5:D:307:HOH:O	2.14	0.65
1:B:515:PRO:O	5:B:704:HOH:O	2.14	0.65
2:H:64:VAL:HG13	2:H:68:PHE:HB2	1.79	0.65
3:D:150:ILE:N	5:D:302:HOH:O	2.25	0.64
2:C:47:TRP:HE1	2:C:50:THR:HG22	1.64	0.63
1:B:471:GLN:CB	5:B:707:HOH:O	2.27	0.63
1:A:484:VAL:HG23	1:A:488:LEU:HB3	1.81	0.63
3:D:150:ILE:CA	5:D:302:HOH:O	2.47	0.62
1:B:441:LEU:C	5:B:709:HOH:O	2.38	0.61
2:C:141:LEU:HG	2:C:213:ILE:HG21	1.82	0.61
1:A:543:LYS:HG2	3:L:49:TYR:CZ	2.36	0.61
3:D:67:SER:N	5:D:303:HOH:O	2.14	0.60
2:C:88:SER:O	2:C:91:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLN:CB	5:A:802:HOH:O	2.39	0.60
1:A:548:LEU:O	3:D:77:ASN:ND2	2.34	0.59
1:A:509:ASP:O	1:A:511:ARG:N	2.29	0.58
1:A:408:ASN:HB3	1:A:587:LYS:HB3	1.86	0.58
2:C:51:ILE:HG13	2:C:58:THR:HG22	1.86	0.58
2:H:11:LEU:HB2	2:H:150:PRO:HG3	1.86	0.57
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.86	0.57
2:C:122:PRO:HB3	2:C:148:TYR:HB3	1.85	0.57
2:H:193:SER:N	5:H:303:HOH:O	2.01	0.56
3:L:195:GLU:HG2	3:L:206:VAL:HG22	1.88	0.56
1:B:541:TYR:CB	5:B:712:HOH:O	2.48	0.56
3:L:188:ARG:NH1	5:L:306:HOH:O	2.23	0.56
2:H:216:ARG:O	2:H:218:CYS:N	2.39	0.55
2:H:99:ASP:OD1	2:H:100:GLY:N	2.35	0.55
2:H:72:ARG:HD3	2:H:74:ASN:OD1	2.06	0.55
2:C:91:THR:HG22	2:C:114:VAL:HB	1.88	0.55
1:B:381:VAL:N	5:B:719:HOH:O	2.39	0.55
3:L:131:SER:O	5:L:304:HOH:O	2.18	0.55
2:H:47:TRP:HZ2	2:H:50:THR:HG22	1.72	0.55
1:B:442:ILE:CG1	5:B:715:HOH:O	2.52	0.55
1:B:536:GLU:HG2	5:B:713:HOH:O	2.08	0.54
1:B:580:ASP:OD2	1:B:581:THR:HA	2.07	0.54
2:H:192:PRO:N	5:H:303:HOH:O	2.41	0.54
2:C:201:ALA:HA	2:C:208:LYS:HG2	1.89	0.54
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.42	0.53
3:D:151:ASP:CA	5:D:308:HOH:O	2.33	0.53
3:D:151:ASP:N	5:D:308:HOH:O	2.42	0.53
1:B:580:ASP:CG	1:B:581:THR:HG23	2.28	0.53
2:H:188:SER:O	5:H:306:HOH:O	2.18	0.53
1:A:580:ASP:CG	1:A:581:THR:HA	2.28	0.52
2:H:136:ASN:CA	5:H:301:HOH:O	2.44	0.52
3:D:150:ILE:HB	5:D:302:HOH:O	2.09	0.52
2:H:129:PRO:HD3	2:H:141:LEU:HD12	1.91	0.52
1:B:553:TRP:HD1	5:B:721:HOH:O	1.93	0.52
1:B:458:VAL:N	5:B:706:HOH:O	1.90	0.52
1:B:458:VAL:CG2	5:B:706:HOH:O	2.46	0.52
1:A:580:ASP:OD1	1:A:581:THR:HG23	2.10	0.52
1:B:523:TYR:HB3	1:B:527:VAL:HG11	1.90	0.52
3:D:186:TYR:CB	5:D:304:HOH:O	2.26	0.52
2:C:53:SER:HA	5:C:301:HOH:O	1.97	0.52
1:B:442:ILE:CA	5:B:715:HOH:O	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:SER:OG	2:C:50:THR:HB	2.10	0.51
1:B:461:ALA:O	1:B:465:SER:OG	2.28	0.51
1:B:578:GLY:O	1:B:579:THR:C	2.49	0.51
2:C:213:ILE:HA	5:C:306:HOH:O	2.10	0.51
1:A:578:GLY:O	1:A:579:THR:C	2.49	0.51
3:D:68:GLY:O	5:D:310:HOH:O	2.19	0.51
3:L:210:ASN:HB2	3:L:213:GLU:HB3	1.93	0.51
1:B:456:LEU:HG	1:B:481:LEU:HD11	1.93	0.51
2:H:141:LEU:HG	2:H:213:ILE:HG21	1.92	0.51
2:C:182:SER:HA	5:C:302:HOH:O	2.11	0.51
1:A:497:TYR:HB2	1:A:561:VAL:HB	1.93	0.51
1:B:471:GLN:HB3	1:B:477:THR:HG21	1.93	0.50
1:B:458:VAL:CB	5:B:706:HOH:O	2.58	0.50
2:C:125:TYR:HB3	3:D:121:SER:OG	2.11	0.50
1:A:471:GLN:N	5:A:802:HOH:O	1.97	0.50
1:B:471:GLN:CG	5:B:707:HOH:O	2.56	0.50
1:A:389:LEU:O	1:A:490:THR:HG23	2.12	0.49
2:C:191:TRP:CH2	2:C:215:PRO:HG3	2.48	0.49
3:L:212:ASN:OD1	3:L:213:GLU:N	2.46	0.49
3:D:95:PRO:N	5:D:312:HOH:O	2.46	0.49
3:L:11:LEU:HD21	1:B:522:GLN:NE2	2.28	0.49
2:C:216:ARG:O	2:C:218:CYS:N	2.47	0.48
1:A:406:ASN:N	1:A:583:SER:HB2	2.19	0.48
2:H:47:TRP:CZ2	2:H:50:THR:HG22	2.49	0.47
2:C:62:ASP:N	5:C:303:HOH:O	2.46	0.47
1:A:455:ASP:HB3	5:A:804:HOH:O	2.15	0.47
1:B:385:PHE:C	5:B:711:HOH:O	2.48	0.47
1:B:464:ILE:HA	1:B:468:ASN:HB2	1.97	0.47
2:C:129:PRO:HD3	2:C:141:LEU:HD12	1.96	0.47
2:C:54:GLY:N	2:C:55:GLY:HA2	2.30	0.47
1:B:543:LYS:HG2	3:D:49:TYR:CZ	2.49	0.47
3:L:80:GLN:HB3	5:L:319:HOH:O	2.15	0.47
1:B:541:TYR:HB2	5:B:712:HOH:O	2.13	0.46
1:B:442:ILE:HA	5:B:709:HOH:O	2.07	0.46
2:C:47:TRP:NE1	2:C:50:THR:HG22	2.27	0.46
1:A:548:LEU:N	5:A:803:HOH:O	1.98	0.46
2:C:171:ALA:HA	2:C:180:LEU:HB3	1.98	0.46
1:A:580:ASP:CB	1:A:581:THR:HA	2.45	0.46
1:A:428:ILE:HB	1:A:476:PRO:HB3	1.98	0.46
3:L:104:LEU:HD13	3:L:106:ILE:HD11	1.97	0.46
1:A:480:ILE:HB	1:A:571:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:PHE:HB3	1:B:407:CYS:SG	2.56	0.45
1:B:509:ASP:C	1:B:511:ARG:H	2.14	0.45
3:D:29:ILE:HG12	5:D:310:HOH:O	2.15	0.45
2:H:191:TRP:CD1	2:H:192:PRO:HA	2.51	0.45
2:C:53:SER:C	5:C:301:HOH:O	2.48	0.45
1:B:498:SER:HB3	1:B:534:VAL:HG23	1.99	0.45
1:B:485:PRO:HD2	1:B:488:LEU:HB2	1.99	0.45
3:D:183:LYS:O	5:D:304:HOH:O	2.20	0.44
1:A:487:ASN:ND2	4:A:701:NAG:O7	2.50	0.44
2:C:190:THR:HB	2:C:194:GLU:HB2	1.99	0.44
2:H:216:ARG:HD3	5:H:328:HOH:O	2.17	0.44
1:A:485:PRO:HD2	1:A:488:LEU:HB2	1.98	0.44
3:D:35:TRP:CE2	3:D:73:LEU:HB2	2.52	0.44
3:D:41:ASP:N	5:D:313:HOH:O	2.44	0.44
1:A:543:LYS:NZ	2:H:102:ASP:OD2	2.47	0.44
2:C:195:THR:HG23	2:C:212:LYS:HE2	1.98	0.44
1:B:406:ASN:N	1:B:583:SER:HB2	2.27	0.44
3:L:14:SER:O	3:L:17:ASP:HB2	2.18	0.44
1:B:484:VAL:HA	1:B:485:PRO:HD3	1.74	0.43
3:D:186:TYR:N	5:D:304:HOH:O	2.37	0.43
1:B:456:LEU:HD12	1:B:479:LEU:HD21	2.00	0.43
2:C:64:VAL:HG13	2:C:68:PHE:HB2	1.99	0.43
3:D:212:ASN:OD1	3:D:213:GLU:N	2.51	0.43
3:D:203:SER:N	5:D:307:HOH:O	2.50	0.43
1:B:536:GLU:C	5:B:713:HOH:O	2.53	0.43
3:L:118:PHE:HA	3:L:119:PRO:HD3	1.90	0.43
1:B:407:CYS:O	1:B:584:VAL:HA	2.19	0.43
2:H:52:SER:OG	2:H:57:TYR:HB2	2.18	0.43
2:H:33:THR:HG22	2:H:53:SER:N	2.34	0.43
1:B:463:PRO:HB3	1:B:501:ASN:HA	2.01	0.43
2:H:76:LYS:O	2:H:78:THR:HG23	2.19	0.43
2:C:99:ASP:OD1	2:C:100:GLY:N	2.41	0.43
2:H:33:THR:HG22	2:H:53:SER:H	1.83	0.43
2:C:76:LYS:O	2:C:78:THR:HG23	2.19	0.43
3:L:3:GLN:HG2	3:L:26:SER:HB3	2.01	0.42
3:D:197:THR:CB	5:D:301:HOH:O	2.56	0.42
3:L:105:GLU:OE2	3:L:173:TYR:OH	2.26	0.42
2:H:108:GLN:HG3	2:H:108:GLN:H	1.55	0.42
3:L:78:LEU:HA	3:L:78:LEU:HD12	1.83	0.42
1:B:537:ASP:HB2	1:B:560:THR:OG1	2.19	0.42
3:D:33:LEU:HD22	3:D:71:TYR:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:79:GLU:HG2	5:L:319:HOH:O	2.19	0.42
3:L:16:GLY:O	1:B:505:ARG:NH1	2.53	0.42
2:H:36:TRP:HD1	2:H:70:ILE:HD12	1.84	0.42
2:H:174:GLN:HE21	2:H:174:GLN:HB2	1.60	0.42
1:B:538:GLY:C	5:B:703:HOH:O	2.58	0.41
2:C:174:GLN:OE1	3:D:160:LEU:CD2	2.63	0.41
2:C:104:ASP:HA	3:D:46:LEU:HD22	2.02	0.41
2:C:191:TRP:HA	2:C:192:PRO:HA	1.72	0.41
2:C:72:ARG:HD3	2:C:74:ASN:OD1	2.19	0.41
1:A:450:LEU:HD12	1:A:481:LEU:HD23	2.02	0.41
1:A:547:PRO:N	5:A:803:HOH:O	2.53	0.41
2:C:157:TRP:CH2	2:C:198:CYS:HB3	2.55	0.41
1:A:395:GLN:HG3	1:A:498:SER:HB2	2.02	0.41
1:B:466:GLN:O	1:B:518:VAL:HG12	2.20	0.41
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.87	0.41
2:C:61:PRO:HB2	5:C:303:HOH:O	2.21	0.41
1:A:400:LYS:O	1:A:444:ASP:HA	2.22	0.40
1:B:530:VAL:HA	1:B:531:PRO:HD3	1.95	0.40
3:D:10:SER:O	3:D:11:LEU:HD12	2.21	0.40
1:B:456:LEU:HB3	1:B:479:LEU:HD23	2.03	0.40
1:A:493:LYS:HA	1:A:494:PRO:HD3	1.98	0.40
3:D:149:LYS:HB2	3:D:193:THR:HB	2.03	0.40
1:A:537:ASP:HB2	1:A:560:THR:OG1	2.22	0.40
1:A:484:VAL:CG1	1:A:567:LEU:HB3	2.51	0.40
1:B:493:LYS:HA	1:B:494:PRO:HD3	1.88	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	206/251 (82%)	192 (93%)	10 (5%)	4 (2%)	10 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	206/251 (82%)	189 (92%)	13 (6%)	4 (2%)	10 12
2	C	211/219 (96%)	204 (97%)	6 (3%)	1 (0%)	34 48
2	H	211/219 (96%)	205 (97%)	5 (2%)	1 (0%)	34 48
3	D	212/214 (99%)	203 (96%)	9 (4%)	0	100 100
3	L	212/214 (99%)	204 (96%)	8 (4%)	0	100 100
All	All	1258/1368 (92%)	1197 (95%)	51 (4%)	10 (1%)	24 35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	217	ASP
1	B	510	ASP
1	B	579	THR
1	A	462	GLY
1	A	510	ASP
1	B	461	ALA
1	A	461	ALA
1	A	579	THR
1	B	462	GLY
2	C	217	ASP

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	190/224 (85%)	177 (93%)	13 (7%)	20 31
1	B	190/224 (85%)	180 (95%)	10 (5%)	28 44
2	C	187/189 (99%)	177 (95%)	10 (5%)	28 44
2	H	187/189 (99%)	178 (95%)	9 (5%)	31 49
3	D	192/192 (100%)	183 (95%)	9 (5%)	32 50
3	L	192/192 (100%)	184 (96%)	8 (4%)	36 56
All	All	1138/1210 (94%)	1079 (95%)	59 (5%)	29 45

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	LYS
1	A	411	LEU
1	A	423	PHE
1	A	451	SER
1	A	454	SER
1	A	456	LEU
1	A	484	VAL
1	A	488	LEU
1	A	509	ASP
1	A	542	ARG
1	A	579	THR
1	A	580	ASP
1	A	581	THR
2	H	1	ASP
2	H	4	LEU
2	H	42	GLU
2	H	43	LYS
2	H	86	LEU
2	H	108	GLN
2	H	141	LEU
2	H	174	GLN
2	H	191	TRP
3	L	3	GLN
3	L	7	THR
3	L	8	THR
3	L	53	ARG
3	L	54	LEU
3	L	104	LEU
3	L	185	GLU
3	L	214	CYS
1	B	400	LYS
1	B	406	ASN
1	B	423	PHE
1	B	454	SER
1	B	456	LEU
1	B	484	VAL
1	B	488	LEU
1	B	508	SER
1	B	579	THR
1	B	581	THR
2	C	4	LEU
2	C	42	GLU

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Mol	Chain	Res	Type
2	C	43	LYS
2	C	50	THR
2	C	53	SER
2	C	57	TYR
2	C	86	LEU
2	C	91	THR
2	C	141	LEU
2	C	174	GLN
3	D	7	THR
3	D	45	LYS
3	D	53	ARG
3	D	54	LEU
3	D	60	SER
3	D	104	LEU
3	D	181	LEU
3	D	203	SER
3	D	214	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	174	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	NAG	A	701	1	14,14,15	0.44	0	15,19,21	0.23	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	NAG	A	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	208/251 (82%)	-0.01	7 (3%) 49 49	36, 55, 103, 127	0
1	B	208/251 (82%)	3.18	116 (55%) 0 0	44, 131, 191, 230	0
2	C	215/219 (98%)	0.89	47 (21%) 1 1	42, 78, 147, 206	0
2	H	215/219 (98%)	-0.27	3 (1%) 78 77	26, 40, 65, 179	0
3	D	214/214 (100%)	0.73	19 (8%) 12 12	38, 76, 130, 220	0
3	L	214/214 (100%)	-0.05	1 (0%) 91 91	28, 42, 62, 168	0
All	All	1274/1368 (93%)	0.74	193 (15%) 3 3	26, 60, 154, 230	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	577	TYR	20.4
2	H	219	GLY	12.2
1	B	479	LEU	11.7
1	B	414	LEU	11.4
1	B	383	CYS	10.7
1	B	438	TYR	10.5
1	B	575	VAL	10.4
1	B	437	CYS	10.1
1	B	571	PHE	10.0
1	B	434	ALA	9.7
1	B	476	PRO	9.4
1	B	433	ILE	9.2
1	B	572	GLY	9.0
1	B	478	CYS	8.8
1	B	409	TYR	8.7
1	B	584	VAL	8.7
1	B	573	ILE	8.5
1	B	431	ALA	8.0
2	C	137	SER	8.0

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Mol	Chain	Res	Type	RSRZ
1	B	477	THR	7.9
1	B	441	LEU	7.7
1	B	415	LEU	7.6
1	B	570	GLY	7.4
1	B	482	ALA	7.2
1	B	407	CYS	7.2
1	B	579	THR	6.8
1	B	448	TYR	6.7
1	B	588	LEU	6.7
1	B	480	ILE	6.3
1	B	497	TYR	6.2
3	D	186	TYR	6.2
1	B	576	GLN	6.0
3	D	209	PHE	6.0
1	B	511	ARG	5.9
1	B	442	ILE	5.8
1	B	436	ASN	5.8
1	B	574	THR	5.7
1	B	481	LEU	5.7
2	C	190	THR	5.6
1	B	389	LEU	5.5
1	B	585	CYS	5.5
1	B	562	ALA	5.5
1	B	411	LEU	5.4
1	B	424	THR	5.2
2	C	196	VAL	5.1
3	D	214	CYS	5.1
1	B	396	VAL	5.1
1	B	427	GLN	5.1
2	H	218	CYS	5.0
1	B	402	LEU	4.9
2	C	186	VAL	4.9
1	B	443	LEU	4.9
1	B	582	ASN	4.9
2	C	131	SER	4.8
1	B	450	LEU	4.8
2	H	217	ASP	4.8
1	B	485	PRO	4.7
1	B	410	ASN	4.7
1	B	421	ASN	4.6
1	B	452	MET	4.6
2	C	129	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	419	SER	4.5
1	B	426	SER	4.5
1	A	460	SER	4.4
1	B	463	PRO	4.4
1	B	515	PRO	4.4
2	C	218	CYS	4.4
1	B	416	SER	4.3
1	B	403	VAL	4.3
1	B	561	VAL	4.3
1	B	412	THR	4.3
3	L	214	CYS	4.3
2	C	219	GLY	4.2
3	D	192	TYR	4.2
1	B	456	LEU	4.2
2	C	217	ASP	4.1
1	B	509	ASP	4.1
1	B	560	THR	4.1
3	D	126	THR	4.1
1	B	488	LEU	4.1
1	B	430	PRO	4.0
1	B	408	ASN	4.0
1	B	446	PHE	3.9
1	B	404	PHE	3.9
2	C	193	SER	3.9
3	D	211	ARG	3.9
1	B	486	HIS	3.9
2	C	128	ALA	3.8
1	B	489	THR	3.8
2	C	197	THR	3.8
1	B	435	SER	3.7
2	C	59	TYR	3.7
2	C	214	VAL	3.7
2	C	57	TYR	3.7
3	D	150	ILE	3.6
2	C	215	PRO	3.6
2	C	194	GLU	3.6
1	B	580	ASP	3.6
2	C	213	ILE	3.5
1	B	447	SER	3.5
2	C	138	MET	3.5
1	B	498	SER	3.5
2	C	125	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	459	SER	3.4
1	B	499	TYR	3.4
3	D	191	SER	3.4
1	B	581	THR	3.3
2	C	189	SER	3.3
1	B	469	TYR	3.2
1	B	423	PHE	3.2
2	C	139	VAL	3.2
2	C	195	THR	3.2
2	C	157	TRP	3.2
1	B	510	ASP	3.2
1	B	440	SER	3.1
1	B	559	SER	3.1
3	D	24	ARG	3.1
1	B	418	PHE	3.1
1	B	578	GLY	3.1
1	B	420	VAL	3.1
2	C	166	VAL	3.1
1	B	453	LYS	3.0
1	B	470	LYS	3.0
1	B	483	THR	3.0
1	B	512	THR	3.0
2	C	199	ASN	3.0
1	B	461	ALA	2.9
1	B	399	PHE	2.9
2	C	141	LEU	2.9
1	A	579	THR	2.9
1	B	405	THR	2.8
1	B	475	ASN	2.8
1	B	449	PRO	2.8
1	B	569	MET	2.8
1	B	495	LEU	2.8
1	B	428	ILE	2.8
1	B	460	SER	2.8
2	C	216	ARG	2.8
2	C	56	SER	2.7
3	D	205	ILE	2.7
1	B	464	ILE	2.7
1	B	587	LYS	2.7
2	C	212	LYS	2.6
1	B	567	LEU	2.6
2	C	209	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	143	CYS	2.6
1	B	472	SER	2.6
1	B	381	VAL	2.6
3	D	188	ARG	2.6
3	D	94	LEU	2.6
3	D	118	PHE	2.6
2	C	184	VAL	2.6
1	B	540	TYR	2.6
1	B	514	VAL	2.5
1	B	586	PRO	2.5
1	B	458	VAL	2.5
2	C	161	SER	2.5
2	C	69	THR	2.5
3	D	208	SER	2.5
1	A	511	ARG	2.5
2	C	156	THR	2.5
1	A	458	VAL	2.4
1	B	385	PHE	2.4
1	B	501	ASN	2.4
1	B	451	SER	2.4
1	B	538	GLY	2.4
1	B	429	SER	2.4
1	B	417	LEU	2.3
2	C	51	ILE	2.3
2	C	191	TRP	2.3
2	C	65	LYS	2.3
1	B	519	ASN	2.3
1	B	388	LEU	2.3
1	B	467	PHE	2.3
1	A	588	LEU	2.3
2	C	144	LEU	2.3
2	C	140	THR	2.2
3	D	5	THR	2.2
2	C	185	THR	2.2
2	C	187	PRO	2.2
2	C	63	SER	2.2
1	B	525	PRO	2.2
2	C	127	LEU	2.2
3	D	210	ASN	2.1
3	D	125	LEU	2.1
3	D	149	LYS	2.1
1	A	461	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	154	THR	2.0
2	C	118	LYS	2.0
1	B	465	SER	2.0
1	B	397	TYR	2.0
1	A	411	LEU	2.0
3	D	187	GLU	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
4	NAG	A	701	14/15	0.65	0.28	-	81,81,81,81	0

6.5 Other polymers (i)

There are no such residues in this entry.