Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 06:17 PM EST

PDB ID	:	8SDG
Title	:	Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing antibody CC25.43
Authors	:	Yuan, M.; Wilson, I.A.
Deposited on	:	2023-04-06
Resolution	:	2.71 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

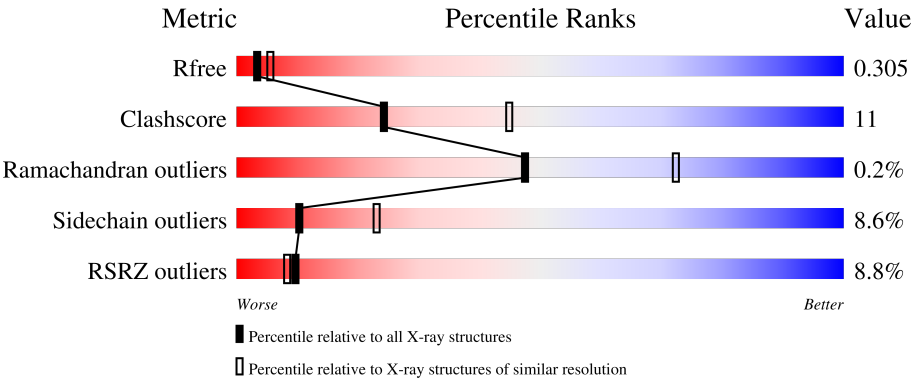
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	226	73% 23%
1	G	226	76% 19%
2	B	215	73% 24%
2	I	215	4% 77% 20%
3	C	205	22% 56% 32% 7%

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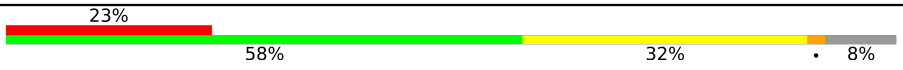
Mol	Chain	Length	Quality of chain
3	D	205	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9536 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 Neutralizing antibody CC25.43 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	219	Total	C	N	O	S	0	0	0
			1635	1032	271	324	8			
1	A	218	Total	C	N	O	S	0	0	0
			1629	1029	270	322	8			

- Molecule 2 is a protein called Neutralizing antibody CC25.43 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	213	Total	C	N	O	S	0	0	0
			1633	1022	273	334	4			
2	B	213	Total	C	N	O	S	0	0	0
			1633	1022	273	334	4			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	190	Total	C	N	O	S	0	0	0
			1501	960	251	282	8			
3	D	189	Total	C	N	O	S	0	0	0
			1491	954	248	281	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	531	GLY	-	expression tag	UNP P0DTC2
C	532	HIS	-	expression tag	UNP P0DTC2
C	533	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
C	536	HIS	-	expression tag	UNP P0DTC2
C	537	HIS	-	expression tag	UNP P0DTC2
D	531	GLY	-	expression tag	UNP P0DTC2

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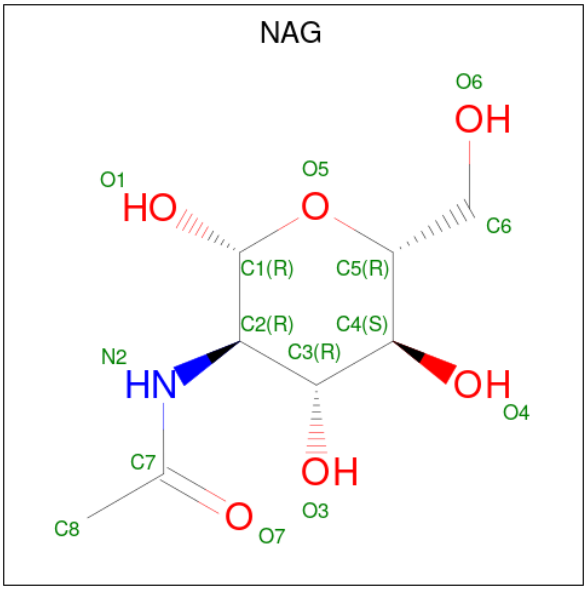
Chain	Residue	Modelled	Actual	Comment	Reference
D	532	HIS	-	expression tag	UNP P0DTC2
D	533	HIS	-	expression tag	UNP P0DTC2
D	534	HIS	-	expression tag	UNP P0DTC2
D	535	HIS	-	expression tag	UNP P0DTC2
D	536	HIS	-	expression tag	UNP P0DTC2
D	537	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



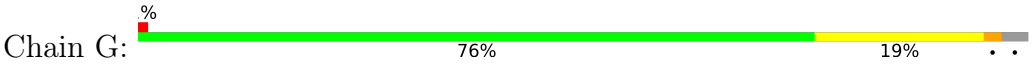
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

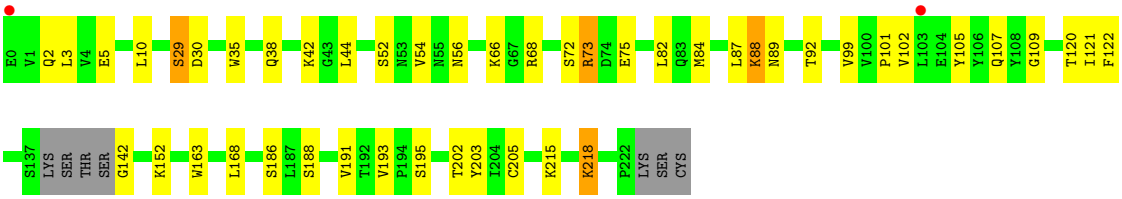
3 Residue-property plots (i)

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: Neutralizing antibody CC25.43 heavy chain

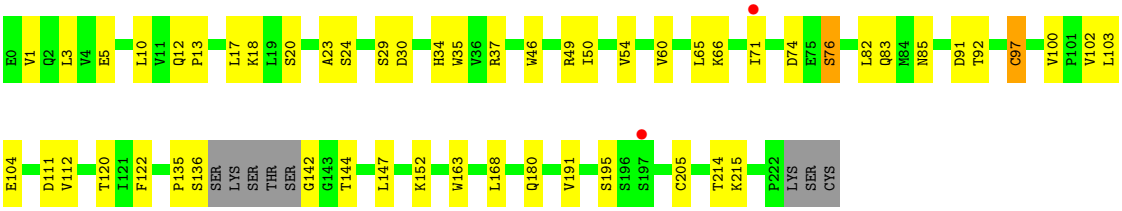
Chain G:





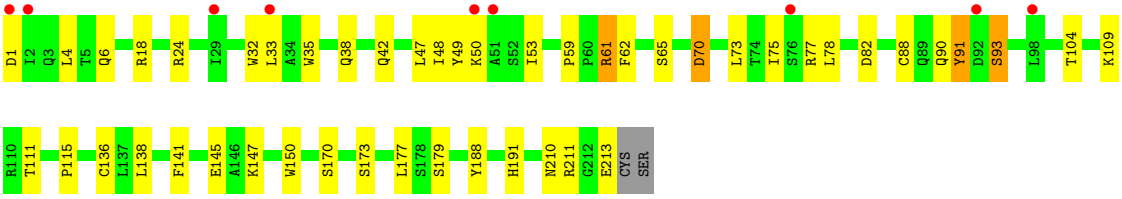
• Molecule 1: Neutralizing antibody CC25.43 heavy chain

Chain A:



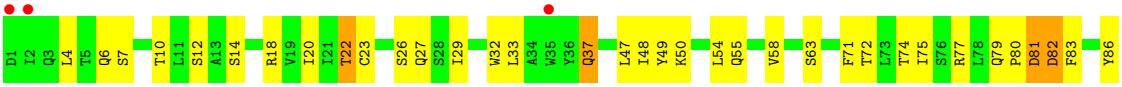
• Molecule 2: Neutralizing antibody CC25.43 light chain

Chain I:



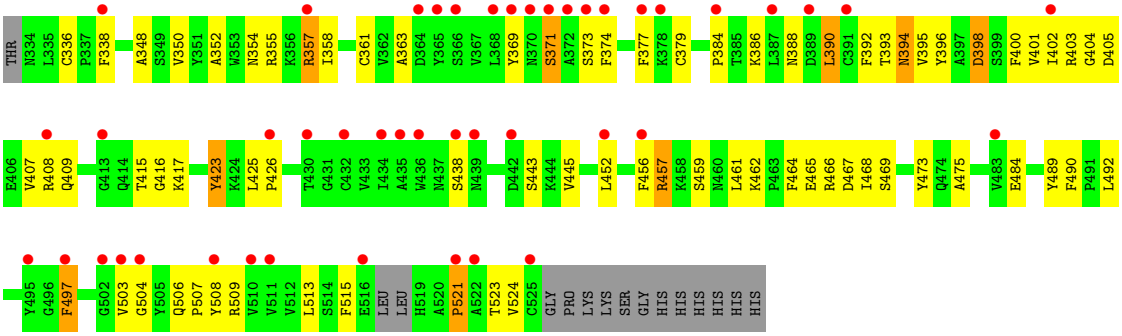
• Molecule 2: Neutralizing antibody CC25.43 light chain

Chain B:



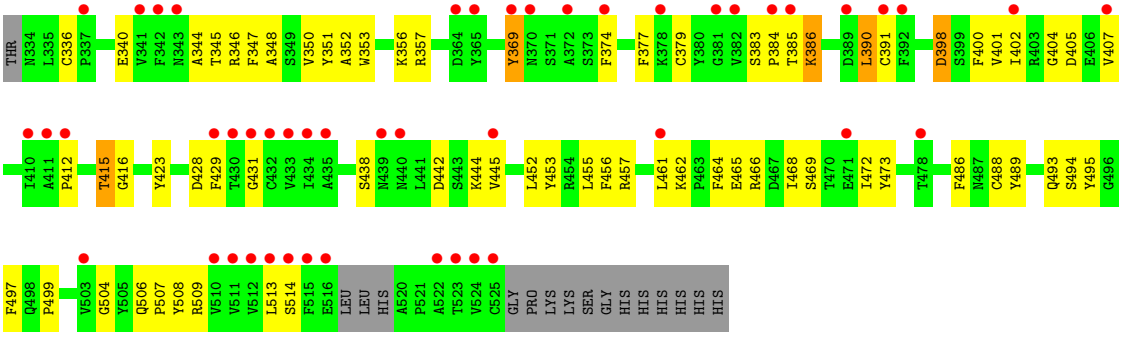
• Molecule 3: Spike protein S1

Chain C:



• Molecule 3: Spike protein S1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	311.95Å 83.79Å 74.15Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	72.84 – 2.71 72.84 – 2.71	Depositor EDS
% Data completeness (in resolution range)	93.2 (72.84-2.71) 93.2 (72.84-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.255 , 0.308 0.253 , 0.305	Depositor DCC
R_{free} test set	2385 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9536	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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, 0.333 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: 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	0/1665	0.50	0/2269
1	G	0.26	0/1671	0.50	0/2277
2	B	0.27	0/1667	0.55	1/2269 (0.0%)
2	I	0.28	0/1667	0.55	0/2269
3	C	0.34	0/1543	0.60	2/2098 (0.1%)
3	D	0.27	0/1532	0.54	1/2083 (0.0%)
All	All	0.28	0/9745	0.54	4/13265 (0.0%)

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	81	ASP	CB-CG-OD1	5.23	123.01	118.30
3	C	390	LEU	CA-CB-CG	5.20	127.26	115.30
3	C	390	LEU	CB-CG-CD2	5.11	119.68	111.00
3	D	455	LEU	CA-CB-CG	5.00	126.81	115.30

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	1629	0	1591	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1635	0	1596	26	0
2	B	1633	0	1577	34	0
2	I	1633	0	1577	29	0
3	C	1501	0	1399	54	0
3	D	1491	0	1393	44	0
4	C	14	0	13	0	0
All	All	9536	0	9146	206	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 11.

All (206) 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)
3:C:358:ILE:HD13	3:C:395:VAL:HG12	1.55	0.89
3:C:357:ARG:HH22	3:C:394:ASN:ND2	1.74	0.85
3:C:354:ASN:OD1	3:C:355:ARG:N	2.10	0.84
2:B:142:TYR:CD1	2:B:143:PRO:HA	2.15	0.82
1:G:88:LYS:HD3	1:G:89:ASN:H	1.46	0.80
3:C:503:VAL:HA	3:C:506:GLN:HB2	1.65	0.77
3:C:338:PHE:HZ	3:C:363:ALA:HB1	1.50	0.76
1:G:38:GLN:NE2	1:G:42:LYS:O	2.19	0.75
3:D:472:ILE:HD11	3:D:488:CYS:HB3	1.70	0.73
2:B:7:SER:HG	2:B:22:THR:HG1	1.36	0.73
3:D:344:ALA:HB3	3:D:347:PHE:HE1	1.54	0.73
3:D:442:ASP:OD1	3:D:509:ARG:NH2	2.22	0.72
3:C:393:THR:HA	3:C:523:THR:HG21	1.73	0.69
2:B:37:GLN:HB3	2:B:47:LEU:HD21	1.78	0.66
2:I:138:LEU:HD22	2:I:177:LEU:HD22	1.78	0.65
2:B:110:ARG:HG3	2:B:142:TYR:CD2	2.34	0.62
1:A:104:GLU:N	1:A:104:GLU:OE2	2.32	0.62
1:A:100:VAL:HG12	1:A:111:ASP:HA	1.82	0.62
1:A:46:TRP:HH2	1:A:60:VAL:HG23	1.64	0.62
1:G:3:LEU:HD11	1:G:99:VAL:HG23	1.84	0.60
1:G:84:MET:HB3	1:G:87:LEU:HD11	1.83	0.60
1:G:30:ASP:HB2	3:C:468:ILE:HD11	1.84	0.59
2:B:107:GLU:OE1	2:B:175:TYR:OH	2.21	0.58
1:G:101:PRO:HG2	1:G:109:GLY:HA3	1.84	0.58
2:I:4:LEU:HD21	2:I:90:GLN:HG2	1.85	0.58
3:C:521:PRO:O	3:C:523:THR:HG23	2.04	0.58
1:A:92:THR:HG23	1:A:120:THR:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ARG:H	2:B:142:TYR:HE2	1.51	0.57
3:D:401:VAL:HG22	3:D:509:ARG:HG2	1.87	0.57
3:C:523:THR:OG1	3:C:524:VAL:N	2.37	0.56
1:A:168:LEU:HD21	1:A:191:VAL:HG21	1.86	0.56
2:I:115:PRO:HB3	2:I:141:PHE:HB3	1.88	0.56
3:D:438:SER:HB3	3:D:509:ARG:HD2	1.87	0.56
3:C:379:CYS:HB2	3:C:384:PRO:HG3	1.86	0.56
1:A:1:VAL:HG12	1:A:112:VAL:HG21	1.86	0.56
1:A:30:ASP:HB2	3:D:468:ILE:HD11	1.87	0.55
3:D:369:TYR:CE2	3:D:384:PRO:HB2	2.41	0.55
3:D:383:SER:H	3:D:386:LYS:HE3	1.71	0.55
2:I:75:ILE:HG21	2:I:78:LEU:HD12	1.89	0.55
1:A:12:GLN:H	1:A:12:GLN:CD	2.10	0.55
3:C:355:ARG:HH22	3:C:464:PHE:HE2	1.55	0.55
1:G:35:TRP:CD2	1:G:82:LEU:HD12	2.42	0.55
3:D:444:LYS:HE3	3:D:445:VAL:H	1.72	0.55
1:A:37:ARG:NH2	1:A:65:LEU:HD21	2.22	0.55
3:C:403:ARG:HB3	3:C:497:PHE:HE1	1.71	0.54
2:I:38:GLN:NE2	2:I:42:GLN:O	2.36	0.54
3:D:431:GLY:HA3	3:D:514:SER:HA	1.90	0.54
2:B:83:PHE:HD1	2:B:106:LEU:HG	1.73	0.53
1:A:74:ASP:OD1	1:A:76:SER:OG	2.24	0.53
1:A:13:PRO:HD3	1:A:122:PHE:O	2.08	0.53
2:I:62:PHE:CE1	2:I:75:ILE:HD11	2.43	0.53
2:B:82:ASP:N	2:B:82:ASP:OD1	2.43	0.52
1:A:83:GLN:NE2	1:A:85:ASN:OD1	2.41	0.52
3:D:456:PHE:CZ	3:D:489:TYR:HD2	2.27	0.52
1:G:29:SER:HA	1:G:73:ARG:HH12	1.74	0.52
3:D:412:PRO:HG3	3:D:429:PHE:HD2	1.75	0.52
2:I:191:HIS:O	2:I:211:ARG:NH1	2.42	0.52
1:G:105:TYR:OH	2:I:93:SER:N	2.35	0.52
3:D:453:TYR:CE1	3:D:493:GLN:HB3	2.44	0.52
2:B:79:GLN:HG3	2:B:80:PRO:HD2	1.93	0.51
2:I:35:TRP:CE3	2:I:73:LEU:HD12	2.45	0.51
3:D:461:LEU:HD21	3:D:465:GLU:O	2.09	0.51
3:C:409:GLN:NE2	3:C:416:GLY:HA3	2.25	0.51
3:C:404:GLY:HA3	3:C:504:GLY:O	2.11	0.51
1:G:105:TYR:HE1	2:I:91:TYR:HB2	1.75	0.51
3:C:357:ARG:CZ	3:C:396:TYR:HE2	2.24	0.51
2:B:115:PRO:HB3	2:B:141:PHE:HB3	1.92	0.51
3:D:461:LEU:HD23	3:D:462:LYS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:473:TYR:HE2	3:C:475:ALA:HA	1.75	0.50
2:B:6:GLN:NE2	2:B:104:THR:OG1	2.44	0.50
1:G:29:SER:HA	1:G:73:ARG:HH22	1.76	0.50
1:A:54:VAL:HG21	3:D:348:ALA:HB2	1.93	0.50
3:C:386:LYS:NZ	3:C:390:LEU:HD12	2.26	0.50
3:C:396:TYR:O	3:C:513:LEU:HA	2.12	0.50
3:C:402:ILE:HD11	3:C:407:VAL:HG22	1.94	0.50
1:G:102:VAL:HG11	2:I:49:TYR:HB2	1.94	0.49
3:C:392:PHE:CD2	3:C:515:PHE:CD1	3.00	0.49
1:G:38:GLN:HB2	1:G:44:LEU:HD23	1.94	0.49
3:C:401:VAL:HG22	3:C:509:ARG:HG2	1.94	0.49
2:I:6:GLN:NE2	2:I:104:THR:OG1	2.46	0.49
3:C:490:PHE:HE2	3:C:492:LEU:HB2	1.77	0.48
3:D:404:GLY:HA3	3:D:504:GLY:O	2.13	0.48
3:C:357:ARG:NH2	3:C:394:ASN:ND2	2.52	0.48
2:B:55:GLN:O	2:B:58:VAL:HG12	2.13	0.48
2:B:79:GLN:HB3	2:B:82:ASP:OD1	2.14	0.48
3:D:442:ASP:OD2	3:D:509:ARG:NE	2.46	0.48
1:A:35:TRP:CZ3	1:A:97:CYS:HB3	2.48	0.48
3:D:340:GLU:OE1	3:D:356:LYS:NZ	2.47	0.48
3:D:344:ALA:HB3	3:D:347:PHE:CE1	2.42	0.48
2:I:173:SER:O	2:I:173:SER:OG	2.32	0.48
3:D:402:ILE:HD11	3:D:407:VAL:HG22	1.95	0.47
2:B:32:TRP:CZ2	3:D:357:ARG:HD2	2.50	0.47
3:C:357:ARG:NH2	3:C:396:TYR:HE2	2.13	0.47
3:C:456:PHE:CE1	3:C:489:TYR:HD2	2.32	0.47
2:B:142:TYR:HD1	2:B:143:PRO:HA	1.72	0.47
1:G:92:THR:HG23	1:G:120:THR:HA	1.95	0.47
2:I:210:ASN:HB2	2:I:213:GLU:HG3	1.95	0.47
1:A:5:GLU:OE1	1:A:97:CYS:N	2.36	0.47
3:D:499:PRO:HA	3:D:506:GLN:HE22	1.80	0.47
3:D:405:ASP:OD1	3:D:405:ASP:N	2.41	0.47
1:A:50:ILE:HB	1:A:71:ILE:HG21	1.96	0.47
3:D:390:LEU:HD23	3:D:391:CYS:H	1.80	0.47
2:B:47:LEU:C	2:B:48:ILE:HD13	2.35	0.46
2:B:20:ILE:O	2:B:20:ILE:HD12	2.15	0.46
3:C:352:ALA:HA	3:C:466:ARG:HE	1.80	0.46
1:G:87:LEU:HB3	1:G:121:ILE:CD1	2.46	0.46
2:I:35:TRP:CZ3	2:I:88:CYS:HB3	2.50	0.46
2:I:50:LYS:HB3	2:I:53:ILE:CD1	2.46	0.46
1:A:163:TRP:CH2	1:A:205:CYS:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:TRP:CZ3	2:B:50:LYS:HE3	2.51	0.46
3:C:357:ARG:HH12	3:C:394:ASN:ND2	2.14	0.46
3:D:350:VAL:O	3:D:353:TRP:HD1	1.99	0.46
1:G:142:GLY:O	1:G:195:SER:OG	2.27	0.46
3:C:357:ARG:HH12	3:C:394:ASN:CG	2.19	0.46
1:G:87:LEU:HB3	1:G:121:ILE:HD13	1.98	0.45
1:G:105:TYR:HB3	3:C:357:ARG:HG3	1.97	0.45
1:A:102:VAL:HG11	2:B:49:TYR:CG	2.51	0.45
1:G:168:LEU:HD21	1:G:191:VAL:HG21	1.98	0.45
1:G:163:TRP:CH2	1:G:205:CYS:HB3	2.52	0.45
2:I:47:LEU:C	2:I:48:ILE:HD13	2.37	0.45
1:A:35:TRP:CD2	1:A:82:LEU:HD12	2.52	0.45
2:I:136:CYS:HB3	2:I:179:SER:HB3	1.99	0.45
3:C:404:GLY:O	3:C:407:VAL:HG23	2.17	0.45
1:A:34:HIS:CE1	1:A:49:ARG:HG3	2.52	0.45
3:D:415:THR:OG1	3:D:416:GLY:N	2.50	0.44
2:I:109:LYS:HB2	2:I:109:LYS:HE3	1.81	0.44
2:B:37:GLN:HB2	2:B:86:TYR:CE2	2.52	0.44
3:D:386:LYS:H	3:D:386:LYS:HG3	1.70	0.44
2:I:91:TYR:N	2:I:91:TYR:CD1	2.85	0.44
3:C:452:LEU:HD12	3:C:492:LEU:HB3	1.99	0.44
3:C:497:PHE:HE2	3:C:507:PRO:HB3	1.82	0.44
1:G:88:LYS:CD	1:G:89:ASN:H	2.21	0.44
3:C:438:SER:OG	3:C:507:PRO:HB2	2.17	0.44
2:B:110:ARG:HG3	2:B:142:TYR:HD2	1.78	0.44
3:D:497:PHE:CE2	3:D:507:PRO:HB3	2.52	0.44
1:G:88:LYS:HE3	1:G:88:LYS:HA	1.99	0.44
3:C:371:SER:HB3	3:C:374:PHE:CE2	2.53	0.44
2:B:29:ILE:HD11	2:B:71:PHE:CZ	2.53	0.43
3:D:412:PRO:HG3	3:D:429:PHE:HB3	2.00	0.43
3:C:425:LEU:HD22	3:C:426:PRO:HD2	1.99	0.43
3:C:358:ILE:N	3:C:358:ILE:HD12	2.33	0.43
3:C:490:PHE:CE2	3:C:492:LEU:HB2	2.52	0.43
3:C:350:VAL:HG23	3:C:401:VAL:O	2.18	0.43
2:B:12:SER:OG	2:B:108:ILE:O	2.37	0.43
3:D:452:LEU:HD13	3:D:494:SER:HA	2.00	0.43
3:C:355:ARG:NH2	3:C:464:PHE:HE2	2.15	0.43
2:B:63:SER:OG	2:B:74:THR:OG1	2.36	0.43
3:D:352:ALA:HA	3:D:466:ARG:HD2	1.99	0.43
2:I:24:ARG:NH2	2:I:70:ASP:OD2	2.50	0.43
1:A:37:ARG:HH22	1:A:65:LEU:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:456:PHE:HB3	3:D:473:TYR:CD2	2.54	0.43
3:C:473:TYR:CE2	3:C:475:ALA:HA	2.52	0.43
1:A:102:VAL:HG11	2:B:49:TYR:CD2	2.54	0.42
3:C:409:GLN:HE22	3:C:416:GLY:HA3	1.85	0.42
2:I:32:TRP:CZ2	3:C:357:ARG:CZ	3.02	0.42
3:C:506:GLN:HG3	3:C:507:PRO:HD2	2.00	0.42
1:G:193:VAL:HG11	1:G:203:TYR:CE1	2.55	0.42
1:A:17:LEU:HD12	1:A:18:LYS:H	1.84	0.42
1:A:37:ARG:NH1	1:A:91:ASP:HA	2.35	0.42
3:D:402:ILE:HD12	3:D:508:TYR:HB2	2.00	0.42
1:G:218:LYS:HD3	1:G:218:LYS:HA	1.82	0.42
3:C:461:LEU:HD13	3:C:462:LYS:O	2.20	0.42
2:I:59:PRO:HG2	2:I:61:ARG:NH1	2.34	0.42
3:C:357:ARG:NH2	3:C:396:TYR:CE2	2.88	0.42
2:B:4:LEU:HD12	2:B:23:CYS:SG	2.59	0.42
2:I:188:TYR:CZ	2:I:211:ARG:HG3	2.54	0.42
3:C:405:ASP:HB2	3:C:408:ARG:NH2	2.35	0.42
3:D:398:ASP:OD1	3:D:398:ASP:N	2.52	0.42
3:C:409:GLN:NE2	3:C:415:THR:O	2.52	0.42
1:A:50:ILE:HD12	1:A:50:ILE:HA	1.87	0.42
2:I:61:ARG:NH1	2:I:82:ASP:OD1	2.53	0.41
2:B:48:ILE:HD12	2:B:54:LEU:HD12	2.01	0.41
2:I:47:LEU:HD11	2:I:62:PHE:CE1	2.55	0.41
3:D:379:CYS:HB2	3:D:384:PRO:HG3	2.02	0.41
2:I:35:TRP:CD2	2:I:73:LEU:HD12	2.55	0.41
1:A:100:VAL:HG23	1:A:103:LEU:HG	2.02	0.41
1:A:135:PRO:HG3	1:A:147:LEU:HB3	2.02	0.41
2:B:110:ARG:HD2	2:B:173:SER:HB2	2.03	0.41
1:A:152:LYS:NZ	2:B:126:GLN:HE21	2.18	0.41
2:B:26:SER:OG	2:B:27:GLN:N	2.54	0.41
3:D:345:THR:OG1	3:D:346:ARG:HG3	2.21	0.41
1:G:10:LEU:HB3	1:G:122:PHE:CE1	2.56	0.41
2:B:147:LYS:HB3	2:B:199:THR:HB	2.02	0.41
2:I:18:ARG:HA	2:I:75:ILE:O	2.21	0.41
3:C:357:ARG:NH1	3:C:394:ASN:OD1	2.52	0.41
3:C:398:ASP:OD2	3:C:423:TYR:OH	2.34	0.41
2:B:18:ARG:HA	2:B:75:ILE:O	2.21	0.41
3:D:506:GLN:OE1	3:D:507:PRO:HD2	2.21	0.41
2:I:136:CYS:HB2	2:I:150:TRP:CZ2	2.56	0.41
3:C:392:PHE:O	3:C:523:THR:OG1	2.29	0.41
3:C:457:ARG:NH1	3:C:467:ASP:OD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HB3	1:A:122:PHE:CD2	2.55	0.41
1:A:142:GLY:O	1:A:195:SER:OG	2.29	0.41
3:D:350:VAL:HG23	3:D:400:PHE:CD2	2.56	0.41
3:D:383:SER:HG	3:D:385:THR:HG1	1.66	0.41
1:A:3:LEU:HD23	1:A:23:ALA:HA	2.04	0.40
1:A:180:GLN:HA	2:B:162:GLN:HE22	1.86	0.40
1:A:3:LEU:HD13	1:A:97:CYS:SG	2.61	0.40
2:B:93:SER:CB	2:B:96:GLN:HB2	2.51	0.40
3:D:369:TYR:O	3:D:369:TYR:HD1	2.04	0.40
1:G:54:VAL:HG21	3:C:348:ALA:HB2	2.03	0.40
3:C:403:ARG:O	3:C:403:ARG:HG3	2.21	0.40
3:C:461:LEU:HD11	3:C:465:GLU:O	2.22	0.40
3:D:453:TYR:HE1	3:D:493:GLN:HB3	1.87	0.40
3:D:404:GLY:O	3:D:407:VAL:HG23	2.22	0.40
3:D:428:ASP:N	3:D:428:ASP:OD1	2.55	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	214/226 (95%)	209 (98%)	5 (2%)	0	100	100
1	G	215/226 (95%)	211 (98%)	4 (2%)	0	100	100
2	B	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
2	I	211/215 (98%)	202 (96%)	8 (4%)	1 (0%)	29	53
3	C	186/205 (91%)	175 (94%)	10 (5%)	1 (0%)	29	53
3	D	185/205 (90%)	178 (96%)	7 (4%)	0	100	100
All	All	1222/1292 (95%)	1180 (97%)	40 (3%)	2 (0%)	47	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	93	SER
3	C	521	PRO

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	183/192 (95%)	173 (94%)	10 (6%)	21 44
1	G	184/192 (96%)	166 (90%)	18 (10%)	8 18
2	B	184/189 (97%)	169 (92%)	15 (8%)	11 25
2	I	184/189 (97%)	173 (94%)	11 (6%)	19 40
3	C	161/177 (91%)	140 (87%)	21 (13%)	4 9
3	D	160/177 (90%)	144 (90%)	16 (10%)	7 17
All	All	1056/1116 (95%)	965 (91%)	91 (9%)	10 23

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	2	GLN
1	G	5	GLU
1	G	29	SER
1	G	52	SER
1	G	56	ASN
1	G	66	LYS
1	G	68	ARG
1	G	72	SER
1	G	73	ARG
1	G	75	GLU
1	G	88	LYS
1	G	107	GLN
1	G	152	LYS
1	G	186	SER
1	G	188	SER
1	G	202	THR
1	G	215	LYS

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Mol	Chain	Res	Type
1	G	218	LYS
2	I	1	ASP
2	I	33	LEU
2	I	61	ARG
2	I	65	SER
2	I	70	ASP
2	I	77	ARG
2	I	91	TYR
2	I	111	THR
2	I	145	GLU
2	I	147	LYS
2	I	170	SER
3	C	336	CYS
3	C	357	ARG
3	C	361	CYS
3	C	369	TYR
3	C	371	SER
3	C	373	SER
3	C	377	PHE
3	C	388	ASN
3	C	394	ASN
3	C	398	ASP
3	C	400	PHE
3	C	417	LYS
3	C	423	TYR
3	C	443	SER
3	C	445	VAL
3	C	457	ARG
3	C	459	SER
3	C	469	SER
3	C	484	GLU
3	C	497	PHE
3	C	508	TYR
1	A	20	SER
1	A	24	SER
1	A	29	SER
1	A	66	LYS
1	A	76	SER
1	A	97	CYS
1	A	136	SER
1	A	144	THR
1	A	214	THR

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Mol	Chain	Res	Type
1	A	215	LYS
2	B	10	THR
2	B	14	SER
2	B	22	THR
2	B	33	LEU
2	B	37	GLN
2	B	72	THR
2	B	77	ARG
2	B	81	ASP
2	B	82	ASP
2	B	111	THR
2	B	116	SER
2	B	142	TYR
2	B	168	GLN
2	B	182	THR
2	B	183	LEU
3	D	336	CYS
3	D	351	TYR
3	D	369	TYR
3	D	374	PHE
3	D	377	PHE
3	D	386	LYS
3	D	390	LEU
3	D	398	ASP
3	D	415	THR
3	D	423	TYR
3	D	457	ARG
3	D	464	PHE
3	D	469	SER
3	D	486	PHE
3	D	495	TYR
3	D	513	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	56	ASN
2	I	27	GLN
3	C	394	ASN
3	D	437	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	C	601	3	14,14,15	0.25	0	17,19,21	0.45	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	C	601	3	-	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.

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	218/226 (96%)	0.21	2 (0%) 84 85	30, 70, 104, 112	0
1	G	219/226 (96%)	0.32	2 (0%) 84 85	29, 68, 104, 134	0
2	B	213/215 (99%)	0.16	3 (1%) 75 77	30, 71, 110, 126	0
2	I	213/215 (99%)	0.45	9 (4%) 36 35	29, 74, 112, 141	0
3	C	190/205 (92%)	1.30	45 (23%) 0 0	84, 131, 162, 177	0
3	D	189/205 (92%)	1.25	48 (25%) 0 0	88, 125, 166, 174	0
All	All	1242/1292 (96%)	0.59	109 (8%) 10 8	29, 86, 153, 177	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	370	ASN	15.6
2	I	1	ASP	9.9
3	C	435	ALA	9.7
3	D	432	CYS	7.0
3	C	366	SER	6.8
3	C	365	TYR	6.6
3	C	384	PRO	5.7
3	D	515	PHE	5.5
3	D	392	PHE	5.4
3	C	516	GLU	5.3
3	D	516	GLU	5.2
2	I	2	ILE	5.1
3	D	385	THR	4.6
3	D	384	PRO	4.5
3	C	368	LEU	4.4
3	C	483	VAL	4.3
2	B	1	ASP	4.3
3	D	513	LEU	4.2
3	D	514	SER	4.2

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Mol	Chain	Res	Type	RSRZ
3	D	503	VAL	4.2
3	C	502	GLY	4.0
3	D	372	ALA	3.9
3	C	369	TYR	3.9
3	D	430	THR	3.9
3	C	521	PRO	3.9
3	D	389	ASP	3.8
3	C	525	CYS	3.8
3	C	373	SER	3.7
3	D	525	CYS	3.7
3	D	337	PRO	3.6
3	D	341	VAL	3.5
3	D	434	ILE	3.4
3	C	372	ALA	3.4
2	I	98	LEU	3.3
3	D	370	ASN	3.3
3	D	433	VAL	3.3
3	D	342	PHE	3.3
3	C	432	CYS	3.2
3	D	407	VAL	3.2
2	B	2	ILE	3.2
3	D	364	ASP	3.2
3	D	374	PHE	3.2
3	D	445	VAL	3.1
1	G	0	GLU	3.1
3	D	522	ALA	3.1
3	C	436	TRP	3.1
2	I	50	LYS	3.1
3	D	411	ALA	3.1
3	D	435	ALA	3.1
2	I	29	ILE	3.1
3	C	438	SER	3.1
3	C	508	TYR	3.1
3	D	381	GLY	3.0
3	D	478	THR	3.0
3	C	389	ASP	3.0
3	C	495	TYR	3.0
3	C	434	ILE	3.0
3	C	442	ASP	2.9
3	D	431	GLY	2.9
2	I	33	LEU	2.9
3	D	382	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	408	ARG	2.8
3	C	387	LEU	2.8
3	C	402	ILE	2.8
3	C	391	CYS	2.8
3	D	524	VAL	2.7
3	C	338	PHE	2.7
2	I	76	SER	2.7
2	I	92	ASP	2.7
3	C	374	PHE	2.7
3	C	377	PHE	2.7
3	C	378	LYS	2.6
3	D	378	LYS	2.6
3	D	343	ASN	2.5
3	C	504	GLY	2.5
3	C	371	SER	2.5
3	C	497	PHE	2.5
3	D	461	LEU	2.4
3	D	471	GLU	2.4
3	D	410	ILE	2.4
3	C	364	ASP	2.4
3	C	510	VAL	2.3
3	D	412	PRO	2.3
3	D	429	PHE	2.3
3	D	523	THR	2.3
3	C	456	PHE	2.3
2	B	35	TRP	2.3
3	C	430	THR	2.3
3	C	522	ALA	2.3
1	A	71	ILE	2.3
3	C	452	LEU	2.2
3	D	369	TYR	2.2
3	C	503	VAL	2.2
3	D	391	CYS	2.2
3	D	402	ILE	2.1
3	C	426	PRO	2.1
3	C	357	ARG	2.1
1	G	103	LEU	2.1
1	A	197	SER	2.1
3	D	512	VAL	2.1
3	D	440	ASN	2.1
3	D	365	TYR	2.1
3	D	511	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	413	GLY	2.1
2	I	51	ALA	2.1
3	D	510	VAL	2.1
3	D	439	ASN	2.0
3	C	439	ASN	2.0
3	C	511	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
4	NAG	C	601	14/15	0.50	0.34	128,138,150,151	0

6.5 Other polymers (i)

There are no such residues in this entry.