



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:35 PM UTC

PDB ID : 8SDG / pdb_00008sdg
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

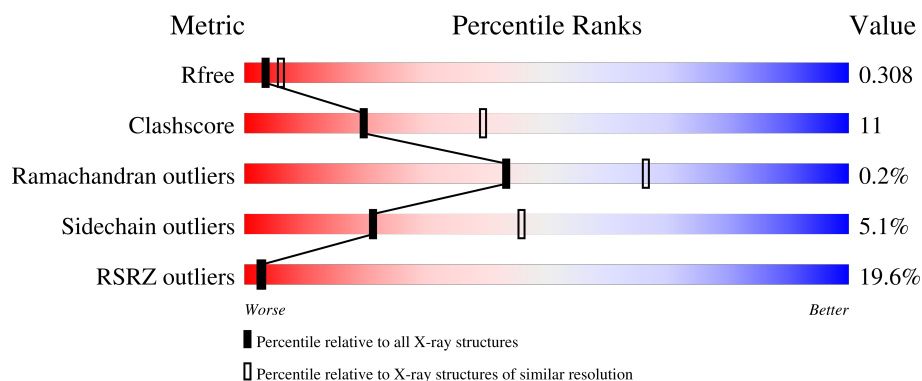
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	226	
1	G	226	
2	B	215	
2	I	215	
3	C	205	

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Mol	Chain	Length	Quality of chain
3	D	205	36% 62% 28% • 8%

2 Entry composition

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:

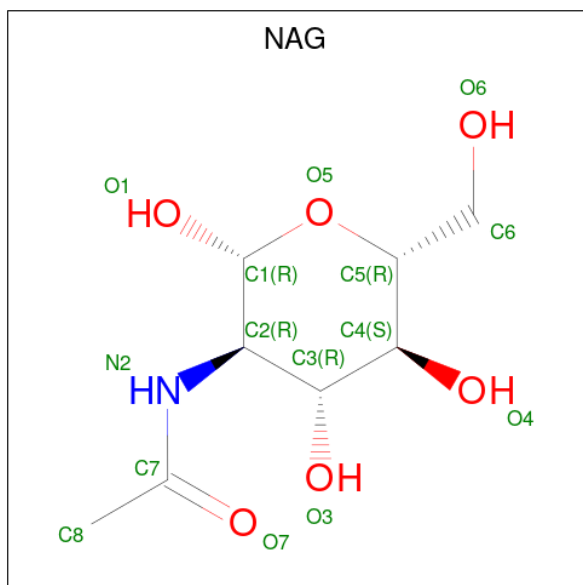
Chain	Residue	Modelled	Actual	Comment	Reference
C	531	GLY	-	expression tag	UNP P0DTC2
C	532	HIS	-	expression tag	UNP P0DTC2
C	533	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
C	536	HIS	-	expression tag	UNP P0DTC2
C	537	HIS	-	expression tag	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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

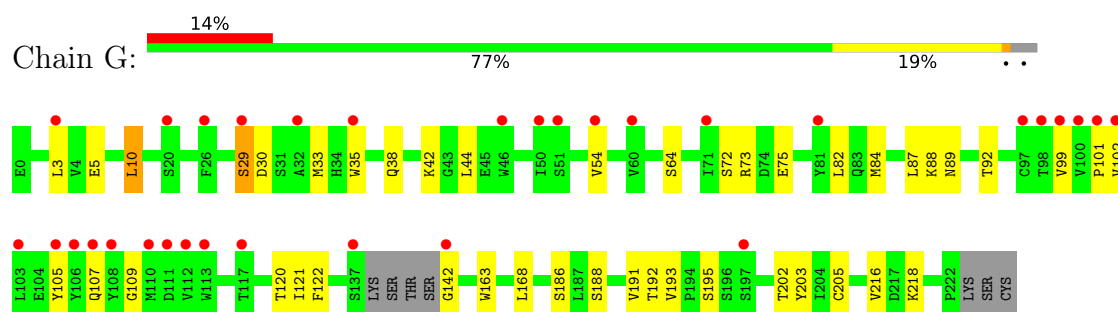


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

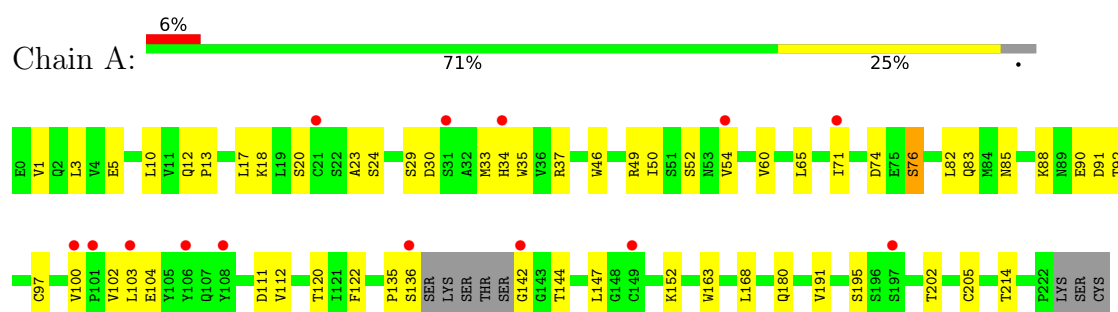
3 Residue-property plots [i](#)

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.

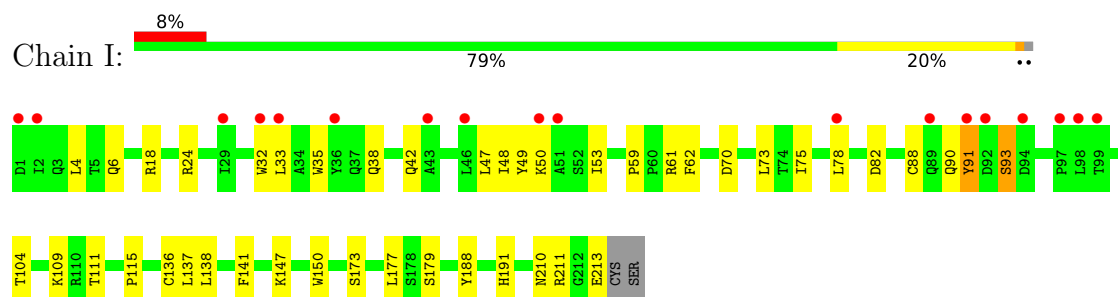
- Molecule 1: Neutralizing antibody CC25.43 heavy chain



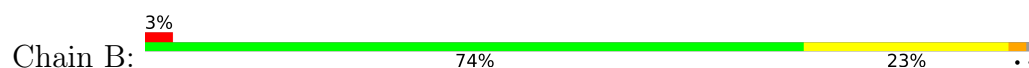
- Molecule 1: Neutralizing antibody CC25.43 heavy chain

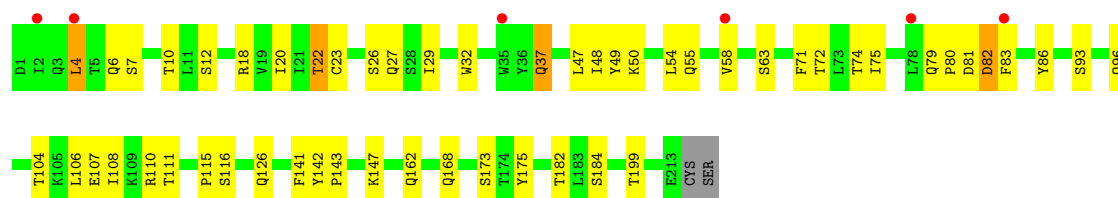


- Molecule 2: Neutralizing antibody CC25.43 light chain

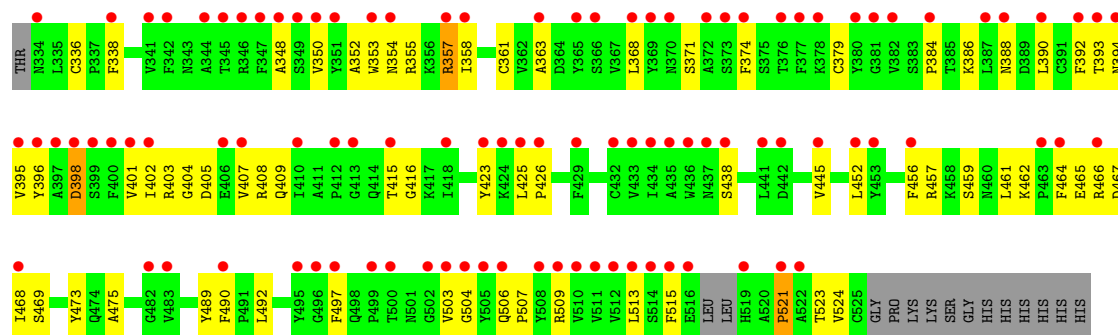


- Molecule 2: Neutralizing antibody CC25.43 light chain

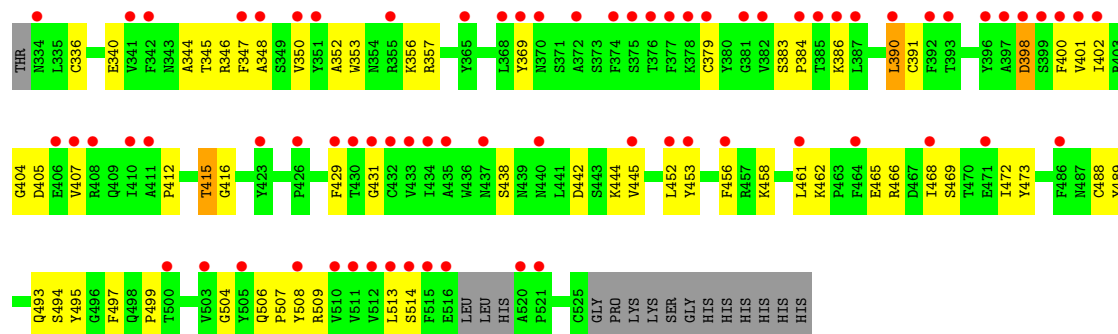




• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.255 , 0.308 0.254 , 0.308	Depositor DCC
R_{free} test set	2390 reflections (4.68%)	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)	0.28 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h-2*1,-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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.12	0/1665	0.30	0/2269
1	G	0.13	0/1671	0.32	0/2277
2	B	0.14	0/1667	0.38	0/2269
2	I	0.16	0/1667	0.39	0/2269
3	C	0.22	0/1543	0.48	0/2098
3	D	0.16	0/1532	0.38	0/2083
All	All	0.16	0/9745	0.38	0/13265

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	1629	0	1591	37	0
1	G	1635	0	1596	27	0
2	B	1633	0	1577	36	0
2	I	1633	0	1577	29	0
3	C	1501	0	1399	56	0
3	D	1491	0	1393	43	0
4	C	14	0	13	0	0
All	All	9536	0	9146	214	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 (214) 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:A:12:GLN:CD	1:A:12:GLN:H	2.10	0.59
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OD1	2:B:82:ASP:N	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
2:B:47:LEU:C	2:B:48:ILE:HD13	2.35	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:C:357:ARG:HH12	3:C:394:ASN:CG	2.19	0.50
3:D:461:LEU:HD23	3:D:462:LYS:O	2.11	0.50
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
2:I:47:LEU:C	2:I:48:ILE:HD13	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:142:GLY:O	1:A:195:SER:OG	2.29	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:20:ILE:HD12	2:B:20:ILE:O	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:G:33:MET:HE3	1:G:33:MET:HB3	1.73	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
2:B:63:SER:OG	2:B:74:THR:OG1	2.36	0.44
3:C:438:SER:OG	3:C:507:PRO:HB2	2.17	0.44
1:A:88:LYS:HG3	1:A:90:GLU:CD	2.42	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:HD12	3:C:358:ILE:N	2.33	0.43
3:C:490:PHE:CE2	3:C:492:LEU:HB2	2.52	0.43
2:B:81:ASP:OD1	2:B:81:ASP:C	2.61	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
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
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
3:D:353:TRP:H	3:D:353:TRP:CD1	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:506:GLN:HG3	3:C:507:PRO:HD2	2.00	0.42
1:A:33:MET:HE1	1:A:35:TRP:CD1	2.54	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:404:GLY:HA3	3:C:504:GLY:C	2.44	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
3:C:353:TRP:CD1	3:C:353:TRP:H	2.36	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
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
1:A:33:MET:HE3	1:A:33:MET:HB3	1.79	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
1:A:10:LEU:HB3	1:A:122:PHE:CD2	2.55	0.41
2:B:29:ILE:C	2:B:29:ILE:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:350:VAL:HG23	3:D:400:PHE:CD2	2.56	0.41
1:A:3:LEU:HD23	1:A:23:ALA:HA	2.04	0.40
1:A:104:GLU:N	1:A:104:GLU:CD	2.79	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:HD1	3:D:369:TYR:O	2.04	0.40
2:B:26:SER:OG	2:B:27:GLN:N	2.54	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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	24	46
3	C	186/205 (91%)	175 (94%)	10 (5%)	1 (0%)	24	46
3	D	185/205 (90%)	178 (96%)	7 (4%)	0	100	100
All	All	1222/1292 (95%)	1180 (97%)	40 (3%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/192 (95%)	174 (95%)	9 (5%)	22	47
1	G	184/192 (96%)	172 (94%)	12 (6%)	15	35
2	B	184/189 (97%)	173 (94%)	11 (6%)	17	39
2	I	184/189 (97%)	179 (97%)	5 (3%)	39	68
3	C	161/177 (91%)	152 (94%)	9 (6%)	19	42
3	D	160/177 (90%)	152 (95%)	8 (5%)	22	46
All	All	1056/1116 (95%)	1002 (95%)	54 (5%)	21	46

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	5	GLU
1	G	10	LEU
1	G	29	SER
1	G	64	SER
1	G	72	SER
1	G	75	GLU
1	G	107	GLN
1	G	186	SER
1	G	188	SER
1	G	192	THR
1	G	202	THR
1	G	216	VAL
2	I	33	LEU
2	I	91	TYR
2	I	111	THR
2	I	137	LEU
2	I	147	LYS

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Mol	Chain	Res	Type
3	C	336	CYS
3	C	357	ARG
3	C	361	CYS
3	C	368	LEU
3	C	388	ASN
3	C	398	ASP
3	C	445	VAL
3	C	459	SER
3	C	469	SER
1	A	20	SER
1	A	24	SER
1	A	29	SER
1	A	52	SER
1	A	76	SER
1	A	136	SER
1	A	144	THR
1	A	202	THR
1	A	214	THR
2	B	4	LEU
2	B	10	THR
2	B	22	THR
2	B	37	GLN
2	B	72	THR
2	B	82	ASP
2	B	111	THR
2	B	116	SER
2	B	168	GLN
2	B	182	THR
2	B	184	SER
3	D	336	CYS
3	D	390	LEU
3	D	398	ASP
3	D	415	THR
3	D	458	LYS
3	D	469	SER
3	D	495	TYR
3	D	513	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	56	ASN

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Mol	Chain	Res	Type
2	I	27	GLN
3	C	394	ASN
3	C	448	ASN
3	C	474	GLN
3	C	493	GLN
1	A	56	ASN
3	D	481	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 oligosaccharides 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	0.26	0	17,19,21	0.47	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/226 (96%)	0.70	14 (6%) 25 23	30, 70, 104, 112	0
1	G	219/226 (96%)	0.88	32 (14%) 6 5	29, 68, 104, 134	0
2	B	213/215 (99%)	0.62	6 (2%) 55 52	30, 71, 110, 126	0
2	I	213/215 (99%)	0.62	18 (8%) 16 14	29, 74, 112, 141	0
3	C	190/205 (92%)	2.26	100 (52%) 0 0	84, 131, 162, 177	0
3	D	189/205 (92%)	1.88	73 (38%) 1 0	88, 125, 166, 174	0
All	All	1242/1292 (96%)	1.12	243 (19%) 3 3	29, 86, 153, 177	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	433	VAL	7.1
3	D	432	CYS	6.7
3	C	435	ALA	6.0
3	D	503	VAL	6.0
3	D	434	ILE	5.6
3	C	366	SER	5.4
3	C	434	ILE	5.4
3	C	502	GLY	5.4
3	D	435	ALA	5.3
3	C	511	VAL	5.3
3	C	433	VAL	5.2
3	D	511	VAL	5.2
3	D	407	VAL	4.9
2	I	98	LEU	4.9
3	C	400	PHE	4.8
3	C	510	VAL	4.8
3	C	365	TYR	4.7
3	D	378	LYS	4.6
3	C	399	SER	4.6

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Mol	Chain	Res	Type	RSRZ
3	C	382	VAL	4.6
3	C	387	LEU	4.5
3	C	370	ASN	4.5
3	C	368	LEU	4.5
3	D	513	LEU	4.3
3	C	442	ASP	4.3
1	A	136	SER	4.3
3	D	411	ALA	4.3
3	C	504	GLY	4.2
3	D	515	PHE	4.2
3	C	516	GLU	4.2
3	C	512	VAL	4.2
3	D	514	SER	4.2
3	D	376	THR	4.1
1	G	142	GLY	4.1
3	C	432	CYS	4.1
3	C	464	PHE	4.0
3	D	464	PHE	4.0
3	C	334	ASN	4.0
3	C	338	PHE	4.0
2	I	91	TYR	4.0
1	G	111	ASP	3.9
1	G	137	SER	3.9
3	D	512	VAL	3.9
3	C	357	ARG	3.8
3	C	347	PHE	3.8
1	G	81	TYR	3.8
1	A	142	GLY	3.7
3	D	508	TYR	3.7
3	D	341	VAL	3.7
3	D	334	ASN	3.7
3	D	387	LEU	3.6
3	C	374	PHE	3.6
3	C	341	VAL	3.6
3	C	377	PHE	3.5
3	C	436	TRP	3.5
3	D	342	PHE	3.5
3	D	510	VAL	3.5
3	D	452	LEU	3.4
2	I	92	ASP	3.4
3	C	456	PHE	3.4
3	C	508	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	503	VAL	3.4
3	C	384	PRO	3.4
3	C	393	THR	3.3
3	D	520	ALA	3.3
1	A	21	CYS	3.3
3	D	382	VAL	3.3
3	D	516	GLU	3.3
3	C	395	VAL	3.3
1	G	98	THR	3.3
3	C	376	THR	3.3
3	C	344	ALA	3.3
3	D	377	PHE	3.3
3	D	396	TYR	3.2
1	G	101	PRO	3.2
3	C	407	VAL	3.2
2	I	50	LYS	3.1
3	C	378	LYS	3.1
3	C	398	ASP	3.1
3	C	373	SER	3.1
3	C	351	TYR	3.1
1	A	71	ILE	3.1
3	C	348	ALA	3.1
3	C	418	ILE	3.1
3	C	495	TYR	3.1
2	I	33	LEU	3.1
2	B	83	PHE	3.1
3	C	353	TRP	3.1
1	G	197	SER	3.1
3	C	499	PRO	3.0
3	D	400	PHE	3.0
3	C	468	ILE	3.0
3	D	410	ILE	3.0
3	D	486	PHE	3.0
3	D	369	TYR	3.0
2	I	2	ILE	3.0
1	G	108	TYR	2.9
3	D	392	PHE	2.9
3	D	374	PHE	2.9
3	D	426	PRO	2.9
2	I	89	GLN	2.9
3	C	346	ARG	2.9
3	D	372	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	I	97	PRO	2.9
2	B	35	TRP	2.9
3	C	358	ILE	2.9
2	I	1	ASP	2.9
2	I	51	ALA	2.9
3	C	410	ILE	2.8
3	C	396	TYR	2.8
3	C	505	TYR	2.8
1	G	103	LEU	2.8
2	B	4	LEU	2.8
3	D	390	LEU	2.8
3	D	384	PRO	2.8
3	C	452	LEU	2.8
3	C	426	PRO	2.8
1	G	46	TRP	2.8
3	C	350	VAL	2.8
3	C	423	TYR	2.8
3	C	438	SER	2.7
1	G	60	VAL	2.7
1	G	99	VAL	2.7
3	D	355	ARG	2.7
2	I	36	TYR	2.7
3	D	437	ASN	2.7
3	C	509	ARG	2.7
3	D	397	ALA	2.7
3	C	412	PRO	2.7
1	G	113	TRP	2.7
1	G	54	VAL	2.7
3	D	393	THR	2.7
3	C	402	ILE	2.6
3	C	397	ALA	2.6
3	D	456	PHE	2.6
3	C	513	LEU	2.6
3	C	381	GLY	2.6
1	G	102	VAL	2.6
3	C	372	ALA	2.6
3	D	445	VAL	2.6
3	C	500	THR	2.6
1	G	105	TYR	2.6
3	D	453	TYR	2.6
1	G	32	ALA	2.6
3	C	401	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	522	ALA	2.6
3	D	429	PHE	2.6
3	D	398	ASP	2.6
2	I	46	LEU	2.6
3	D	423	TYR	2.6
3	C	496	GLY	2.6
2	I	43	ALA	2.6
3	C	515	PHE	2.6
3	D	399	SER	2.5
3	D	368	LEU	2.5
3	C	482	GLY	2.5
3	C	415	THR	2.5
1	G	51	SER	2.5
1	A	103	LEU	2.5
3	C	453	TYR	2.5
3	D	347	PHE	2.5
3	D	408	ARG	2.5
3	D	461	LEU	2.5
3	C	437	ASN	2.5
1	G	20	SER	2.5
3	D	406	GLU	2.5
3	C	369	TYR	2.5
3	C	380	TYR	2.5
2	B	2	ILE	2.4
3	D	500	THR	2.4
3	D	370	ASN	2.4
3	C	445	VAL	2.4
3	D	351	TYR	2.4
3	D	365	TYR	2.4
3	D	430	THR	2.4
3	C	406	GLU	2.4
3	C	521	PRO	2.4
1	A	106	TYR	2.4
3	C	514	SER	2.4
3	C	429	PHE	2.4
3	C	345	THR	2.3
2	I	94	ASP	2.3
1	A	149	CYS	2.3
3	D	521	PRO	2.3
1	A	54	VAL	2.3
1	A	100	VAL	2.3
2	I	29	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	58	VAL	2.3
3	C	342	PHE	2.3
3	D	385	THR	2.3
1	G	29	SER	2.3
1	G	71	ILE	2.3
3	D	402	ILE	2.3
1	G	110	MET	2.3
3	D	440	ASN	2.3
2	B	78	LEU	2.3
3	D	350	VAL	2.3
3	D	401	VAL	2.3
1	G	117	THR	2.2
2	I	99	THR	2.2
1	G	106	TYR	2.2
3	C	466	ARG	2.2
3	C	463	PRO	2.2
1	A	197	SER	2.2
3	D	431	GLY	2.2
3	C	390	LEU	2.2
3	D	386	LYS	2.2
3	D	505	TYR	2.2
3	C	354	ASN	2.2
3	C	506	GLN	2.2
3	C	349	SER	2.2
2	I	78	LEU	2.2
3	C	490	PHE	2.2
3	C	497	PHE	2.2
1	A	31	SER	2.2
3	C	424	LYS	2.2
1	G	100	VAL	2.2
3	C	392	PHE	2.2
1	A	101	PRO	2.2
3	C	413	GLY	2.2
1	G	26	PHE	2.2
3	C	394	ASN	2.1
1	A	108	TYR	2.1
1	G	3	LEU	2.1
3	D	381	GLY	2.1
3	C	519	HIS	2.1
3	C	363	ALA	2.1
3	C	441	LEU	2.1
3	D	375	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	34	HIS	2.1
3	D	471	GLU	2.1
1	G	35	TRP	2.1
2	I	32	TRP	2.1
1	G	50	ILE	2.1
3	D	468	ILE	2.1
1	G	112	VAL	2.1
3	C	425	LEU	2.0
3	C	388	ASN	2.0
1	G	97	CYS	2.0
3	C	483	VAL	2.0
3	D	379	CYS	2.0
3	D	348	ALA	2.0
1	G	107	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	601	14/15	0.53	0.18	128,138,150,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.