



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:05 AM UTC

PDB ID : 7BNV / pdb_00007bnv
Title : Crystal Structure of the SARS-CoV-2 Receptor Binding Domain in Complex with Antibody ION-300
Authors : Hall, G.; Cowan, R.; Carr, M.
Deposited on : 2021-01-22
Resolution : 2.35 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

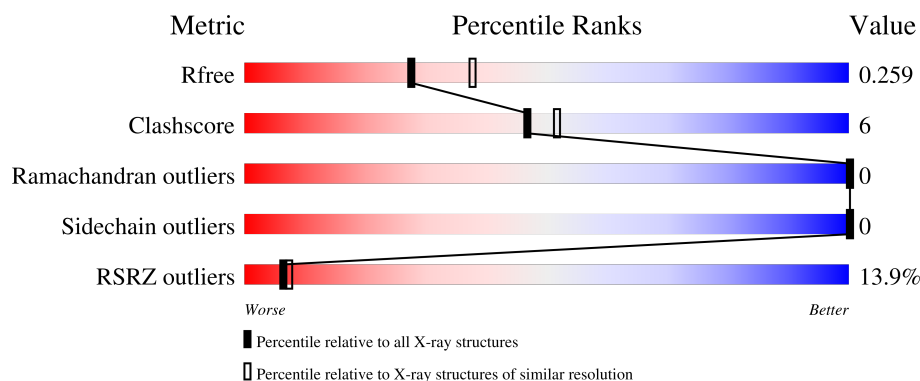
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	234	10% 74% 9% 17%
2	H	230	14% 87% 10% •
3	L	219	15% 82% 16% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4977 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 Surface glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1510	968	252	282	8			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	ALA	-	expression tag	UNP A0A6M5UN06
A	543	ALA	-	expression tag	UNP A0A6M5UN06
A	544	ALA	-	expression tag	UNP A0A6M5UN06
A	545	GLY	-	expression tag	UNP A0A6M5UN06
A	546	SER	-	expression tag	UNP A0A6M5UN06
A	547	HIS	-	expression tag	UNP A0A6M5UN06
A	548	HIS	-	expression tag	UNP A0A6M5UN06
A	549	HIS	-	expression tag	UNP A0A6M5UN06
A	550	HIS	-	expression tag	UNP A0A6M5UN06
A	551	HIS	-	expression tag	UNP A0A6M5UN06
A	552	HIS	-	expression tag	UNP A0A6M5UN06

- Molecule 2 is a protein called Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	223	Total	C	N	O	S	0	0	0
			1658	1058	267	326	7			

- Molecule 3 is a protein called Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	0	0
			1630	1018	271	335	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is water.

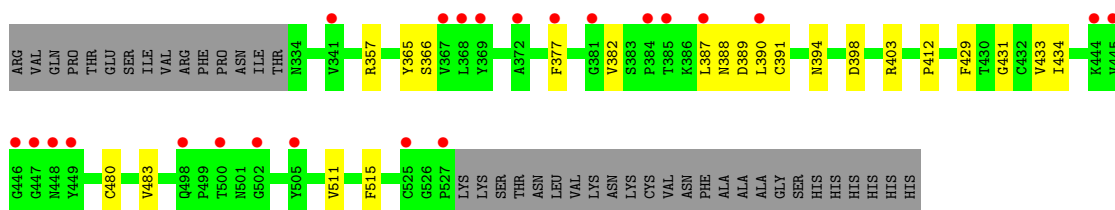
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total	O	0	0
			63	63		
5	H	74	Total	O	0	0
			74	74		
5	L	28	Total	O	0	0
			28	28		

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.

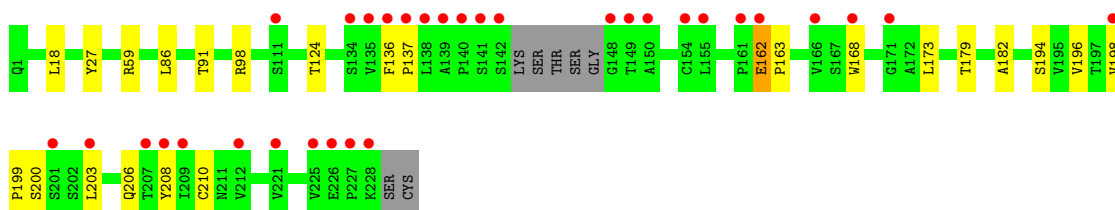
• Molecule 1: Surface glycoprotein

Chain A: 



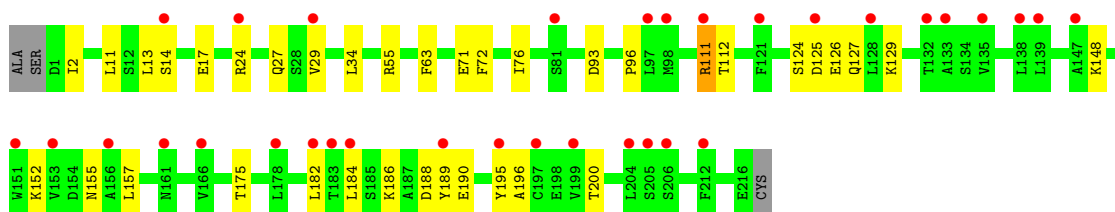
• Molecule 2: Heavy Chain

Chain H: 



• Molecule 3: Light Chain

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	74.86Å 74.86Å 143.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.23 – 2.35 40.23 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.23-2.35) 99.1 (40.23-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.34Å)	Xtriage
Refinement program	REFMAC v1, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.224 , 0.265 (Not available) , 0.259	Depositor DCC
R_{free} test set	3294 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4977	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/1553	0.39	0/2118
2	H	0.19	0/1707	0.47	4/2332 (0.2%)
3	L	0.20	0/1667	0.45	1/2271 (0.0%)
All	All	0.17	0/4927	0.44	5/6721 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	162	GLU	CA-C-N	6.18	141.83	127.00
2	H	162	GLU	C-N-CA	6.18	141.83	127.00
3	L	111	ARG	CB-CG-CD	5.74	124.50	111.30
2	H	162	GLU	C-N-CD	-5.54	108.42	120.60
2	H	162	GLU	N-CA-C	-5.00	104.38	110.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1510	0	1409	14	0
2	H	1658	0	1576	15	0
3	L	1630	0	1534	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	13	0	0
5	A	63	0	0	1	0
5	H	74	0	0	0	0
5	L	28	0	0	0	0
All	All	4977	0	4532	53	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 6.

All (53) 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:L:24:ARG:HE	3:L:71:GLU:HG3	1.48	0.78
3:L:24:ARG:HE	3:L:71:GLU:CG	2.00	0.73
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.34	0.62
3:L:11:LEU:HD22	3:L:13:LEU:HG	1.81	0.61
3:L:148:LYS:HB3	3:L:200:THR:HB	1.82	0.61
1:A:403:ARG:NH1	5:A:702:HOH:O	2.36	0.59
3:L:182:LEU:HD22	3:L:184:LEU:HG	1.84	0.59
3:L:14:SER:N	3:L:17:GLU:OE1	2.34	0.59
2:H:162:GLU:HG2	2:H:163:PRO:HA	1.86	0.56
3:L:29:VAL:HG13	3:L:93:ASP:HB2	1.90	0.54
2:H:91:THR:HG23	2:H:124:THR:HA	1.89	0.54
1:A:357:ARG:NH1	1:A:394:ASN:OD1	2.42	0.53
3:L:111:ARG:NH1	3:L:175:THR:HG23	2.24	0.53
1:A:382:VAL:HG21	1:A:387:LEU:HD13	1.92	0.52
2:H:18:LEU:HB2	2:H:86:LEU:HD11	1.91	0.52
3:L:111:ARG:NH1	3:L:175:THR:CG2	2.73	0.52
1:A:431:GLY:HA2	1:A:515:PHE:CD1	2.45	0.51
1:A:366:SER:H	1:A:388:ASN:HD21	1.58	0.51
2:H:59:ARG:NH2	3:L:96:PRO:HG2	2.27	0.50
3:L:152:LYS:HB2	3:L:196:ALA:HB3	1.94	0.49
2:H:198:VAL:HG22	2:H:199:PRO:HD2	1.94	0.48
1:A:389:ASP:OD1	1:A:389:ASP:N	2.46	0.48
2:H:206:GLN:HG3	2:H:208:TYR:CE1	2.48	0.48
3:L:152:LYS:HZ1	3:L:157:LEU:HD23	1.78	0.48
3:L:184:LEU:HD13	3:L:188:ASP:OD1	2.14	0.48
2:H:162:GLU:OE2	2:H:182:ALA:HB3	2.14	0.47
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.97	0.47
2:H:179:THR:HG23	2:H:194:SER:HB2	1.97	0.47
3:L:24:ARG:NE	3:L:71:GLU:HG3	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:HA	1:A:433:VAL:O	2.15	0.45
2:H:173:LEU:CD2	2:H:196:VAL:HG21	2.46	0.45
3:L:124:SER:O	3:L:126:GLU:N	2.43	0.45
3:L:189:TYR:O	3:L:195:TYR:OH	2.34	0.44
3:L:186:LYS:O	3:L:190:GLU:HG3	2.17	0.44
3:L:34:LEU:HD13	3:L:72:PHE:CD1	2.52	0.44
3:L:55:ARG:HD3	3:L:63:PHE:O	2.18	0.44
3:L:63:PHE:CD2	3:L:76:ILE:HG12	2.53	0.44
2:H:136:PHE:CE1	3:L:127:GLN:HG3	2.53	0.44
3:L:125:ASP:O	3:L:129:LYS:HG3	2.19	0.42
2:H:27:TYR:CZ	2:H:98:ARG:HD2	2.54	0.42
2:H:173:LEU:HD21	2:H:196:VAL:HG21	2.01	0.42
3:L:111:ARG:HH11	3:L:175:THR:HG23	1.83	0.42
1:A:398:ASP:O	1:A:511:VAL:HA	2.20	0.42
1:A:365:TYR:CD2	1:A:387:LEU:HG	2.55	0.42
1:A:366:SER:OG	1:A:388:ASN:ND2	2.53	0.42
1:A:390:LEU:HD12	1:A:391:CYS:H	1.85	0.41
2:H:137:PRO:HD2	3:L:124:SER:CB	2.50	0.41
2:H:200:SER:HA	2:H:203:LEU:HD13	2.02	0.41
3:L:2:ILE:HG12	3:L:27:GLN:HB2	2.01	0.41
3:L:111:ARG:CG	3:L:112:THR:N	2.83	0.41
2:H:168:TRP:CH2	2:H:210:CYS:HB3	2.56	0.41
1:A:480:CYS:O	1:A:483:VAL:HG12	2.22	0.40
3:L:152:LYS:HB3	3:L:155:ASN:HA	2.02	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	192/234 (82%)	180 (94%)	12 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	219/230 (95%)	211 (96%)	8 (4%)	0	100	100
3	L	214/219 (98%)	204 (95%)	10 (5%)	0	100	100
All	All	625/683 (92%)	595 (95%)	30 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	161/203 (79%)	161 (100%)	0	100	100
2	H	182/194 (94%)	182 (100%)	0	100	100
3	L	179/188 (95%)	179 (100%)	0	100	100
All	All	522/585 (89%)	522 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	185	GLN
3	L	127	GLN
3	L	155	ASN

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 oligosaccharides 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	601	1	14,14,15	0.31	0	17,19,21	0.37	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	601	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	A	601	NAG	C8-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2

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	194/234 (82%)	0.78	23 (11%) 9 10	42, 60, 104, 158	0
2	H	223/230 (96%)	0.73	32 (14%) 6 7	41, 59, 102, 141	0
3	L	216/219 (98%)	1.06	33 (15%) 5 6	47, 73, 117, 135	0
All	All	633/683 (92%)	0.86	88 (13%) 6 7	41, 66, 112, 158	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	VAL	4.8
2	H	228	LYS	4.4
2	H	135	VAL	4.4
3	L	204	LEU	4.0
1	A	444	LYS	3.8
3	L	197	CYS	3.8
2	H	161	PRO	3.6
3	L	195	TYR	3.4
3	L	183	THR	3.3
1	A	500	THR	3.3
3	L	182	LEU	3.2
2	H	136	PHE	3.1
1	A	341	VAL	3.0
1	A	377	PHE	3.0
2	H	150	ALA	3.0
3	L	128	LEU	3.0
2	H	140	PRO	3.0
2	H	142	SER	2.9
3	L	97	LEU	2.9
1	A	449	TYR	2.8
1	A	368	LEU	2.8
1	A	527	PRO	2.8
2	H	137	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	390	LEU	2.8
3	L	184	LEU	2.8
3	L	156	ALA	2.8
3	L	166	VAL	2.8
3	L	212	PHE	2.7
2	H	227	PRO	2.7
3	L	138	LEU	2.7
2	H	225	VAL	2.7
2	H	201	SER	2.7
2	H	148	GLY	2.6
3	L	189	TYR	2.6
3	L	153	VAL	2.6
2	H	154	CYS	2.6
1	A	369	TYR	2.6
3	L	178	LEU	2.6
2	H	138	LEU	2.5
1	A	502	GLY	2.5
2	H	207	THR	2.5
3	L	29	VAL	2.5
1	A	525	CYS	2.4
3	L	135	VAL	2.4
1	A	498	GLN	2.4
1	A	505	TYR	2.4
1	A	447	GLY	2.4
3	L	132	THR	2.4
2	H	162	GLU	2.4
3	L	14	SER	2.4
3	L	205	SER	2.4
2	H	203	LEU	2.4
2	H	168	TRP	2.4
3	L	133	ALA	2.3
2	H	166	VAL	2.3
3	L	161	ASN	2.3
3	L	139	LEU	2.3
3	L	98	MET	2.3
1	A	367	VAL	2.3
2	H	134	SER	2.3
2	H	141	SER	2.3
1	A	448	ASN	2.2
1	A	446	GLY	2.2
2	H	221	VAL	2.2
2	H	226	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	387	LEU	2.2
3	L	24	ARG	2.2
3	L	125	ASP	2.1
2	H	171	GLY	2.1
2	H	111	SER	2.1
2	H	209	ILE	2.1
2	H	198	VAL	2.1
3	L	111	ARG	2.1
2	H	149	THR	2.1
3	L	206	SER	2.1
2	H	139	ALA	2.1
3	L	147	ALA	2.1
2	H	212	VAL	2.1
3	L	151	TRP	2.1
1	A	385	THR	2.0
1	A	384	PRO	2.0
2	H	208	TYR	2.0
3	L	199	VAL	2.0
1	A	381	GLY	2.0
3	L	121	PHE	2.0
3	L	81	SER	2.0
1	A	372	ALA	2.0
2	H	155	LEU	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	601	14/15	0.60	0.17	93,103,111,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.