



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 12:51 AM EDT

PDB ID : 7LQ7
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with antibodies CV503 and COVA1-16
Authors : Yuan, M.; Zhu, X.; Wilson, I.A.
Deposited on : 2021-02-13
Resolution : 3.40 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 : 2.35.1
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) : 2.35.1

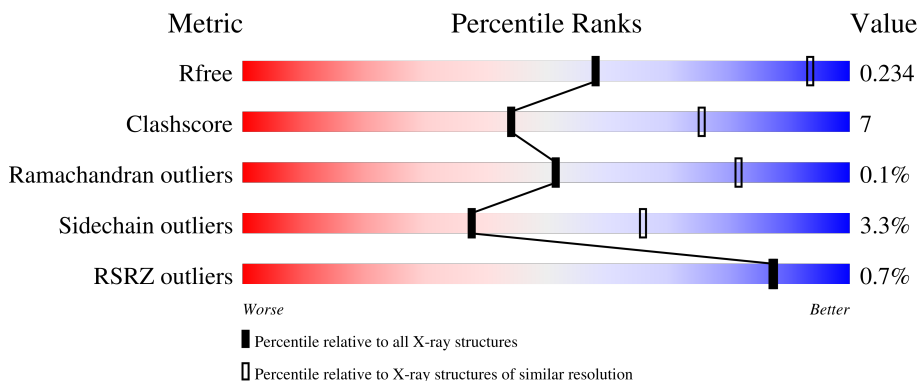
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.









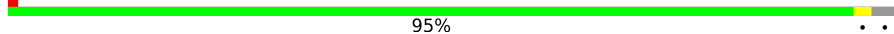


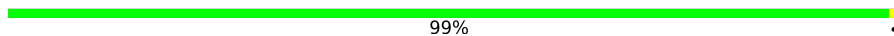
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	205	82% 13% 5%
1	B	205	2% 83% 12% 5%
1	E	205	% 85% 10% 5%
2	C	224	82% 17% .
2	F	224	3% 76% 20% . .

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Mol	Chain	Length	Quality of chain
2	H	224	 76% 23%
3	D	216	 82% 17%
3	G	216	 81% 17%
3	L	216	 81% 16%
4	P	232	 85% 15%
4	T	232	 82% 15%
4	y	232	 95%
5	Q	214	 85% 14%
5	U	214	 87% 12%
5	z	214	 99%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	B	601	-	-	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 24312 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	195	1543	989	257	289	8	0	0	0
1	B	195	1543	989	257	289	8	0	0	0
1	E	195	1543	989	257	289	8	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called CV503 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	224	Total	C	N	O	S	0	0	0
			1651	1038	278	328	7			
2	F	219	Total	C	N	O	S	0	0	0
			1616	1018	271	320	7			
2	H	223	Total	C	N	O	S	0	0	0
			1646	1036	277	327	6			

- Molecule 3 is a protein called CV503 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	214	Total	C	N	O	S	0	0	0
			1544	964	254	320	6			
3	G	215	Total	C	N	O	S	0	0	0
			1584	986	264	328	6			
3	L	213	Total	C	N	O	S	0	0	0
			1564	976	260	323	5			

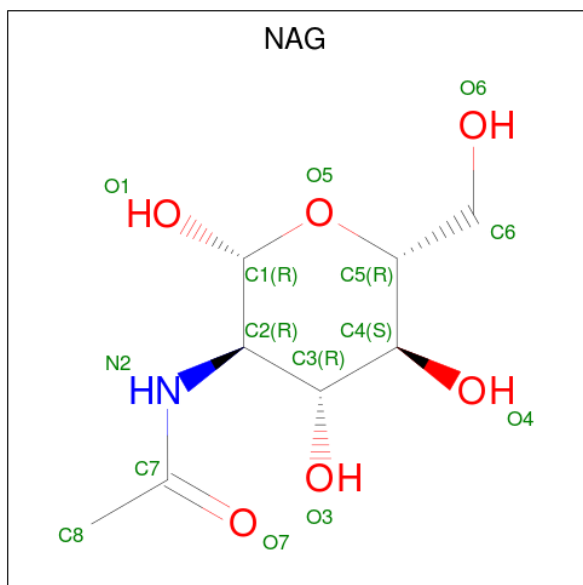
- Molecule 4 is a protein called COVA1-16 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	226	Total	C	N	O	S	0	0	0
			1699	1071	289	330	9			
4	P	232	Total	C	N	O	S	0	0	0
			1737	1092	296	340	9			
4	y	226	Total	C	N	O	S	0	0	0
			1695	1069	288	329	9			

- Molecule 5 is a protein called COVA1-16 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	U	213	Total	C	N	O	S	0	0	0
			1635	1022	272	337	4			
5	Q	213	Total	C	N	O	S	0	0	0
			1635	1022	272	337	4			
5	z	213	Total	C	N	O	S	0	0	0
			1635	1022	272	337	4			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).




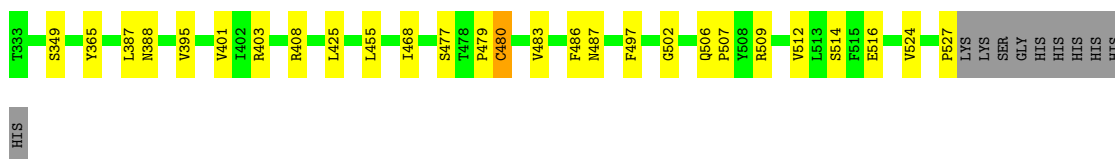
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	Total 14	8	1	5	0	0
6	B	1	Total 14	8	1	5	0	0
6	E	1	Total 14	8	1	5	0	0

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.

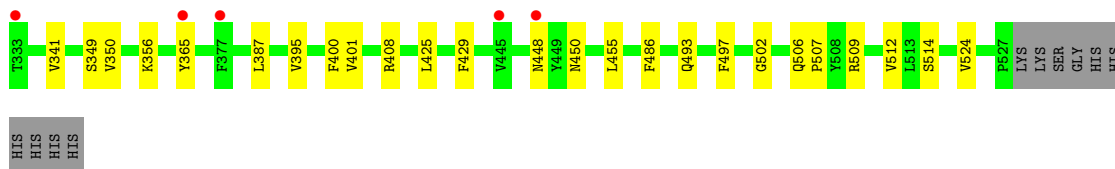
- Molecule 1: Spike protein S1

Chain A: 




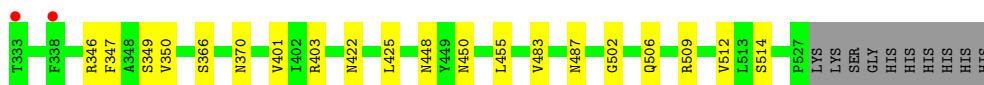
- Molecule 1: Spike protein S1

Chain B: 




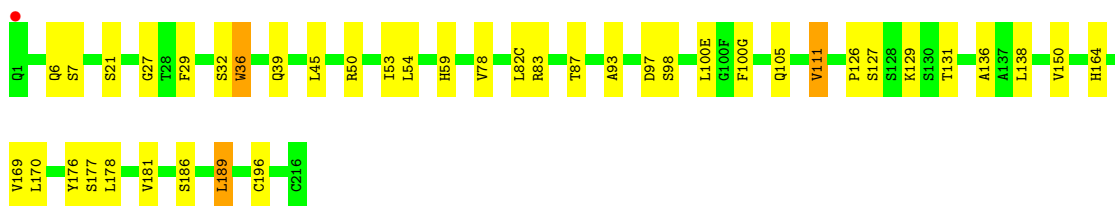
- Molecule 1: Spike protein S1

Chain E: 

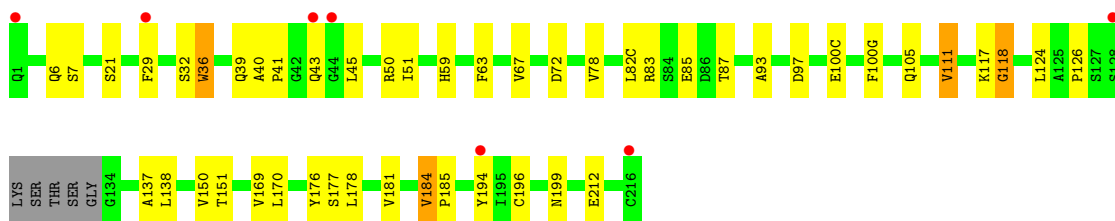
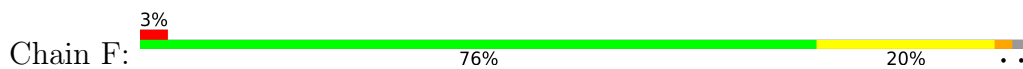


- Molecule 2: CV503 heavy chain

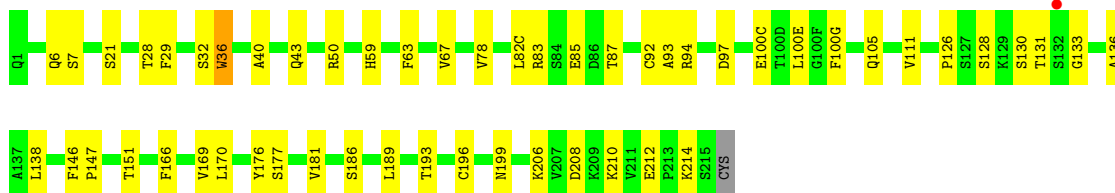
Chain C: 



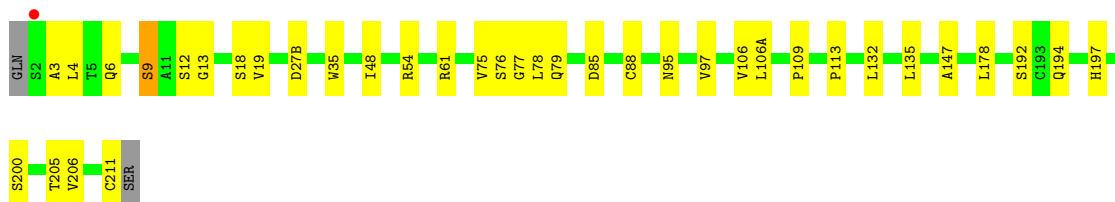
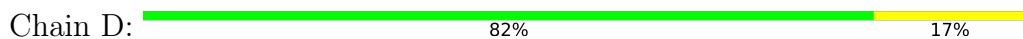
- Molecule 2: CV503 heavy chain



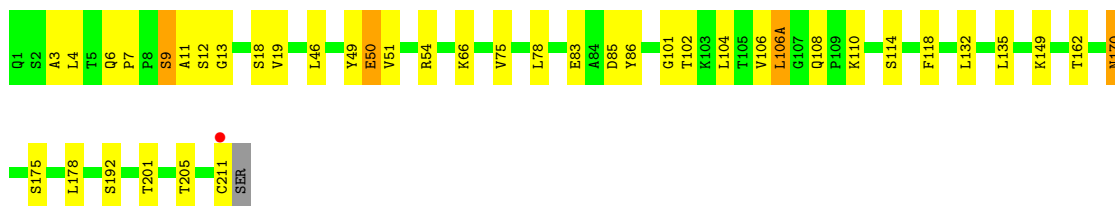
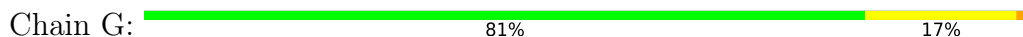
- Molecule 2: CV503 heavy chain



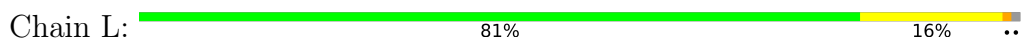
- Molecule 3: CV503 light chain



- Molecule 3: CV503 light chain

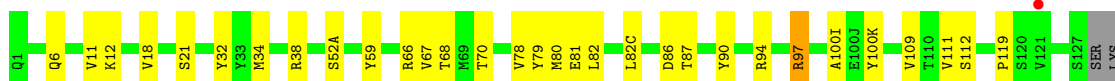
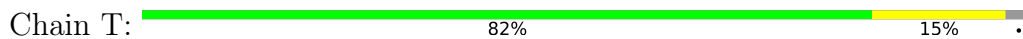


- Molecule 3: CV503 light chain

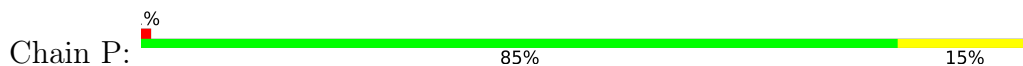




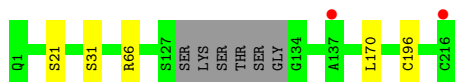
- Molecule 4: COVA1-16 heavy chain



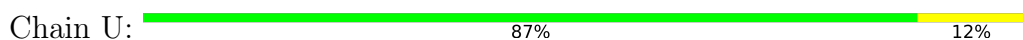
- Molecule 4: COVA1-16 heavy chain



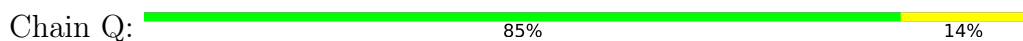
- Molecule 4: COVA1-16 heavy chain



- Molecule 5: COVA1-16 light chain



- Molecule 5: COVA1-16 light chain



- Molecule 5: COVA1-16 light chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	172.22Å 122.74Å 175.46Å 90.00° 118.22° 90.00°	Depositor
Resolution (Å)	41.29 – 3.40 41.25 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (41.29-3.40) 98.5 (41.25-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.197 , 0.233 0.199 , 0.234	Depositor DCC
R_{free} test set	2000 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å ²)	126.4	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.024 for -h-l,k,h 0.024 for l,k,-h-l 0.026 for h,-k,-h-l 0.025 for -h-l,-k,l 0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24312	wwPDB-VP
Average B, all atoms (Å ²)	132.0	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.*

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	0.30	0/1587	0.54	0/2161
1	B	0.30	0/1587	0.53	0/2161
1	E	0.31	0/1587	0.54	0/2161
2	C	0.38	0/1688	0.67	0/2296
2	F	0.37	0/1652	0.68	0/2249
2	H	0.38	0/1683	0.66	0/2290
3	D	0.38	1/1583 (0.1%)	0.61	2/2170 (0.1%)
3	G	0.40	1/1623 (0.1%)	0.63	2/2217 (0.1%)
3	L	0.41	1/1603 (0.1%)	0.63	2/2191 (0.1%)
4	P	0.38	0/1781	0.65	0/2426
4	T	0.38	0/1742	0.68	0/2373
4	y	0.37	0/1738	0.65	0/2368
5	Q	0.32	0/1670	0.56	0/2272
5	U	0.31	0/1670	0.55	0/2272
5	z	0.31	0/1670	0.56	0/2272
All	All	0.36	3/24864 (0.0%)	0.61	6/33879 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
3	G	0	1
3	L	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	9	SER	C-N	8.78	1.54	1.34
3	G	9	SER	C-N	8.33	1.53	1.34
3	D	9	SER	C-N	7.93	1.52	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	9	SER	C-N-CA	-6.70	104.94	121.70
3	D	9	SER	C-N-CA	-5.94	106.86	121.70
3	L	7	PRO	N-CA-C	-5.21	98.55	112.10
3	D	109	PRO	N-CD-CG	-5.19	95.42	103.20
3	L	9	SER	CA-C-N	-5.12	105.93	117.20
3	G	7	PRO	N-CA-C	-5.07	98.92	112.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	9	SER	Mainchain
3	G	9	SER	Mainchain
3	L	9	SER	Mainchain

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	1543	0	1459	12	0
1	B	1543	0	1459	15	0
1	E	1543	0	1459	8	0
2	C	1651	0	1627	30	0
2	F	1616	0	1584	33	1
2	H	1646	0	1625	38	0
3	D	1544	0	1439	27	0
3	G	1584	0	1514	27	0
3	L	1564	0	1490	31	0
4	P	1737	0	1658	20	1
4	T	1699	0	1619	20	0
4	y	1695	0	1613	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Q	1635	0	1572	18	0
5	U	1635	0	1572	19	0
5	z	1635	0	1572	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	E	14	0	13	0	0
All	All	24312	0	23301	271	1

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 7.

All (271) 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:D:3:ALA:O	3:D:4:LEU:HD12	1.22	1.34
3:D:6:GLN:NE2	3:D:88:CYS:SG	2.38	0.96
3:D:3:ALA:O	3:D:4:LEU:CD1	2.16	0.93
3:D:4:LEU:HD13	3:D:97:VAL:CG1	2.00	0.92
3:D:4:LEU:HD13	3:D:97:VAL:HG11	1.51	0.89
3:D:6:GLN:HE22	3:D:88:CYS:H	1.18	0.89
3:L:19:VAL:HG23	3:L:78:LEU:HD11	1.54	0.88
2:C:87:THR:HG22	2:C:111:VAL:H	1.40	0.87
4:T:87:THR:HG22	4:T:111:VAL:H	1.40	0.87
3:D:19:VAL:HG23	3:D:78:LEU:HD11	1.59	0.83
2:H:87:THR:HG22	2:H:111:VAL:H	1.43	0.81
2:C:83:ARG:O	2:C:111:VAL:HG11	1.83	0.78
2:F:87:THR:HG22	2:F:111:VAL:H	1.46	0.78
3:G:19:VAL:HG23	3:G:78:LEU:HD11	1.64	0.78
3:G:6:GLN:HE21	3:G:102:THR:N	1.83	0.76
4:P:87:THR:HG22	4:P:111:VAL:H	1.51	0.75
2:H:83:ARG:O	2:H:111:VAL:HG11	1.86	0.75
2:F:83:ARG:O	2:F:111:VAL:HG11	1.87	0.74
2:C:127:SER:HB2	2:C:129:LYS:HG2	1.69	0.73
4:P:80:MET:HE2	4:P:82:LEU:HB2	1.69	0.73
4:T:80:MET:HE2	4:T:82:LEU:HB2	1.72	0.72
4:P:11:VAL:HB	4:P:147:PRO:HG3	1.73	0.71
4:T:68:THR:HG21	2:H:210:LYS:HD2	1.71	0.71
3:G:6:GLN:NE2	3:G:102:THR:N	2.39	0.70
2:C:7:SER:OG	2:C:21:SER:OG	2.09	0.70
2:H:128:SER:HA	2:H:131:THR:HG22	1.74	0.70
3:G:6:GLN:HE22	3:G:101:GLY:HA2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:6:GLN:HE21	3:L:102:THR:N	1.90	0.69
3:D:6:GLN:NE2	3:D:88:CYS:H	1.89	0.69
2:F:7:SER:OG	2:F:21:SER:OG	2.08	0.69
2:F:117:LYS:O	2:F:118:GLY:O	2.11	0.69
2:H:7:SER:OG	2:H:21:SER:OG	2.10	0.68
3:L:6:GLN:NE2	3:L:102:THR:N	2.42	0.67
5:U:29:ILE:HG22	5:U:92:ASP:HB3	1.77	0.67
3:G:6:GLN:NE2	3:G:86:TYR:O	2.29	0.66
3:L:192:SER:HB3	3:L:205:THR:HG22	1.78	0.66
3:G:6:GLN:NE2	3:G:101:GLY:CA	2.59	0.66
3:L:52:ASN:HD22	3:L:52:ASN:H	1.43	0.65
3:L:132:LEU:HD12	3:L:178:LEU:HD23	1.78	0.65
2:C:129:LYS:HD3	3:D:206:VAL:HG22	1.78	0.65
3:D:132:LEU:HD12	3:D:178:LEU:HD23	1.79	0.65
3:D:192:SER:HB3	3:D:205:THR:HG22	1.78	0.64
3:D:3:ALA:C	3:D:4:LEU:HD12	2.14	0.64
1:B:493:GLN:NE2	2:C:53:ILE:O	2.31	0.64
3:D:6:GLN:HE22	3:D:88:CYS:N	1.91	0.64
4:T:11:VAL:HB	4:T:147:PRO:HG3	1.80	0.64
5:Q:29:ILE:HG22	5:Q:92:ASP:HB3	1.80	0.63
1:B:493:GLN:HE22	2:C:54:LEU:HA	1.63	0.63
3:L:162:THR:HG22	2:H:169:VAL:HB	1.80	0.63
3:D:4:LEU:HD13	3:D:97:VAL:HG12	1.79	0.63
3:G:6:GLN:NE2	3:G:101:GLY:C	2.52	0.63
4:T:32:TYR:O	4:T:52(A):SER:OG	2.15	0.63
3:D:13:GLY:O	3:D:106(A):LEU:HB2	1.99	0.63
3:G:46:LEU:HD21	3:G:49:TYR:HB3	1.80	0.63
4:P:70:THR:HB	4:P:79:TYR:HB2	1.80	0.62
5:U:29:ILE:HG22	5:U:92:ASP:CB	2.29	0.62
3:L:6:GLN:NE2	3:L:101:GLY:C	2.53	0.62
3:G:132:LEU:HD12	3:G:178:LEU:HD23	1.80	0.62
3:G:6:GLN:NE2	3:G:101:GLY:HA2	2.14	0.62
2:C:83:ARG:C	2:C:111:VAL:HG11	2.21	0.61
5:Q:6:GLN:NE2	5:Q:102:THR:OG1	2.32	0.61
3:G:83:GLU:OE2	3:G:170:ASN:ND2	2.28	0.61
3:G:192:SER:HB3	3:G:205:THR:HG22	1.83	0.61
5:Q:29:ILE:HG13	5:Q:29:ILE:O	2.01	0.61
3:L:6:GLN:HE22	3:L:101:GLY:HA2	1.65	0.60
2:H:83:ARG:C	2:H:111:VAL:HG11	2.21	0.60
2:H:93:ALA:HB1	2:H:100(G):PHE:HB3	1.82	0.60
3:L:6:GLN:NE2	3:L:101:GLY:CA	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:PRO:O	1:A:480:CYS:HB2	2.02	0.59
2:C:181:VAL:HG21	3:D:135:LEU:HD13	1.84	0.59
2:F:93:ALA:HB1	2:F:100(G):PHE:HB3	1.85	0.58
4:T:70:THR:HB	4:T:79:TYR:HB2	1.84	0.57
3:G:13:GLY:O	3:G:106(A):LEU:HB2	2.03	0.57
4:P:119:PRO:HB3	4:P:145:TYR:HB3	1.86	0.57
2:F:83:ARG:C	2:F:111:VAL:HG11	2.24	0.57
2:C:131:THR:HG22	2:C:136:ALA:HB2	1.87	0.57
2:F:169:VAL:HB	3:G:162:THR:HG22	1.85	0.57
3:L:80:ALA:O	3:L:170:ASN:ND2	2.37	0.57
3:G:11:ALA:O	3:G:104:LEU:HA	2.05	0.57
3:L:6:GLN:NE2	3:L:86:TYR:O	2.37	0.56
3:G:6:GLN:HG2	3:G:102:THR:OG1	2.06	0.56
3:L:135:LEU:HD13	2:H:181:VAL:HG21	1.88	0.56
4:T:34:MET:HG3	4:T:78:VAL:HG21	1.88	0.56
4:P:34:MET:HG3	4:P:78:VAL:HG21	1.87	0.56
5:U:28:ASP:OD1	5:U:68:GLY:HA2	2.05	0.55
2:F:184:VAL:HG22	2:F:185:PRO:HD2	1.89	0.55
3:L:194:GLN:NE2	3:L:203:GLU:OE1	2.39	0.55
2:C:93:ALA:HB1	2:C:100(G):PHE:HB3	1.87	0.55
3:D:61:ARG:NH2	3:D:77:GLY:O	2.40	0.55
2:H:210:LYS:HE3	2:H:212:GLU:OE2	2.07	0.55
3:D:79:GLN:O	3:D:106:VAL:HG21	2.07	0.54
3:L:76:SER:HB3	4:P:134:GLY:HA2	1.90	0.54
2:F:83:ARG:HH12	3:L:112:ALA:H	1.56	0.54
1:A:487:ASN:OD1	2:H:100(C):GLU:HB2	2.08	0.54
1:B:486:PHE:HD2	2:C:100(E):LEU:HD11	1.72	0.54
3:G:49:TYR:O	3:G:50:GLU:HB2	2.08	0.53
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.90	0.53
4:P:59:TYR:CD1	4:P:67:VAL:HG13	2.44	0.53
4:T:59:TYR:CD1	4:T:67:VAL:HG13	2.44	0.52
5:U:32:TYR:CD1	5:U:32:TYR:N	2.77	0.52
3:L:52:ASN:HD22	3:L:52:ASN:N	2.04	0.52
2:F:181:VAL:HG21	3:G:135:LEU:HD13	1.92	0.52
1:A:425:LEU:HD21	1:A:512:VAL:HG11	1.91	0.52
5:U:50:ASP:OD1	5:U:91:TYR:OH	2.27	0.52
5:Q:50:ASP:OD1	5:Q:91:TYR:OH	2.26	0.52
2:F:82(C):LEU:HB3	2:F:111:VAL:HG21	1.90	0.52
3:G:49:TYR:O	3:G:49:TYR:CD1	2.63	0.52
1:E:401:VAL:HG22	1:E:509:ARG:HG2	1.92	0.52
4:T:119:PRO:HB3	4:T:145:TYR:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:THR:OG1	2:H:136:ALA:HB2	2.10	0.52
3:L:61:ARG:HG2	4:P:134:GLY:HA3	1.92	0.51
5:Q:28:ASP:OD1	5:Q:68:GLY:HA2	2.10	0.51
2:F:170:LEU:HD13	2:F:176:TYR:CE1	2.46	0.51
3:D:147:ALA:HB3	3:D:194:GLN:HG2	1.93	0.51
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.92	0.50
2:H:170:LEU:HD13	2:H:176:TYR:CE1	2.46	0.50
4:T:100(I):ALA:HB1	4:T:100(K):TYR:CE2	2.46	0.50
2:H:82(C):LEU:HB3	2:H:111:VAL:HG21	1.93	0.50
2:C:126:PRO:HD3	2:C:138:LEU:HD23	1.93	0.50
4:T:200:HIS:CD2	4:T:202:PRO:HD2	2.47	0.49
5:U:78:LEU:HD21	5:U:104:LEU:HD21	1.94	0.49
4:P:100(I):ALA:HB1	4:P:100(K):TYR:CE2	2.47	0.49
4:P:18:VAL:HG13	4:P:82(C):LEU:HD11	1.95	0.49
5:Q:78:LEU:HD21	5:Q:104:LEU:HD21	1.94	0.49
2:F:41:PRO:HB2	2:H:133:GLY:HA2	1.94	0.49
3:D:4:LEU:CD1	3:D:97:VAL:HG11	2.34	0.49
3:G:3:ALA:O	3:G:4:LEU:HD23	2.13	0.49
3:G:108:GLN:O	3:G:108:GLN:HG3	2.13	0.49
5:U:32:TYR:N	5:U:32:TYR:HD1	2.10	0.49
3:G:6:GLN:HE21	3:G:101:GLY:C	2.15	0.48
1:E:425:LEU:HD21	1:E:512:VAL:HG11	1.96	0.48
2:H:126:PRO:HD3	2:H:138:LEU:HD23	1.94	0.48
2:C:170:LEU:HD13	2:C:176:TYR:CE1	2.48	0.48
3:G:51:VAL:HG13	3:G:66:LYS:HB2	1.96	0.48
3:L:61:ARG:NH2	3:L:77:GLY:O	2.47	0.48
1:B:486:PHE:HD1	3:D:95:ASN:H	1.61	0.48
3:G:49:TYR:O	3:G:49:TYR:CG	2.67	0.47
2:H:36:TRP:CH2	2:H:78:VAL:HG12	2.49	0.47
2:H:193:THR:HB	2:H:210:LYS:HZ3	1.79	0.47
2:H:87:THR:HG22	2:H:111:VAL:HB	1.96	0.47
5:Q:108:ARG:HG2	5:Q:109:THR:N	2.29	0.47
2:H:199:ASN:HD22	2:H:206:LYS:HG2	1.80	0.47
1:A:408:ARG:HH22	5:Q:56:THR:HB	1.79	0.47
2:F:87:THR:HG22	2:F:111:VAL:HB	1.96	0.47
3:L:120:PRO:HD3	3:L:132:LEU:HD23	1.97	0.47
5:U:113:PRO:HD3	5:U:198:HIS:ND1	2.29	0.47
1:B:486:PHE:CD2	2:C:100(E):LEU:HD11	2.49	0.47
1:B:425:LEU:HD21	1:B:512:VAL:HG11	1.96	0.47
2:C:36:TRP:CH2	2:C:78:VAL:HG12	2.50	0.47
2:F:124:LEU:HB3	3:G:118:PHE:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:149:LYS:HB2	3:G:192:SER:OG	2.15	0.47
5:U:108:ARG:HG2	5:U:109:THR:N	2.30	0.46
4:T:18:VAL:HG11	4:T:109:VAL:HG13	1.96	0.46
2:C:87:THR:HG22	2:C:111:VAL:HB	1.97	0.46
2:C:186:SER:O	2:C:189:LEU:HB2	2.16	0.46
1:B:448:ASN:OD1	1:B:450:ASN:ND2	2.35	0.46
2:H:6:GLN:O	2:H:105:GLN:NE2	2.48	0.46
3:D:18:SER:HA	3:D:75:VAL:O	2.16	0.46
2:C:6:GLN:O	2:C:105:GLN:NE2	2.49	0.46
2:F:36:TRP:CH2	2:F:78:VAL:HG12	2.51	0.46
5:Q:140:TYR:CG	5:Q:141:PRO:HA	2.51	0.46
2:C:131:THR:HG22	2:C:136:ALA:CB	2.46	0.46
2:F:51:ILE:HG21	2:F:78:VAL:HG11	1.98	0.45
2:C:169:VAL:HG12	2:C:177:SER:O	2.15	0.45
2:C:82(C):LEU:HB3	2:C:111:VAL:HG21	1.99	0.45
2:F:40:ALA:HB3	2:F:43:GLN:HB2	1.98	0.45
4:P:38:ARG:NH1	4:P:86:ASP:OD1	2.50	0.45
5:Q:33:LEU:HD22	5:Q:71:PHE:CG	2.52	0.45
3:L:18:SER:HA	3:L:75:VAL:O	2.17	0.45
5:U:140:TYR:CG	5:U:141:PRO:HA	2.52	0.45
2:H:130:SER:O	2:H:136:ALA:HA	2.17	0.45
1:A:486:PHE:HD2	2:H:100(E):LEU:HD11	1.82	0.45
3:L:52:ASN:N	3:L:52:ASN:ND2	2.65	0.45
5:Q:29:ILE:HG22	5:Q:92:ASP:CB	2.45	0.45
3:L:121:SER:HA	2:H:214:LYS:NZ	2.32	0.44
4:T:70:THR:HG23	2:H:208:ASP:O	2.17	0.44
1:A:395:VAL:HG23	1:A:524:VAL:HG21	2.00	0.44
2:C:29:PHE:HB2	2:C:97:ASP:O	2.17	0.44
1:E:502:GLY:O	1:E:506:GLN:HG3	2.17	0.44
3:L:6:GLN:HG2	3:L:102:THR:OG1	2.17	0.44
5:U:92:ASP:O	5:U:93:ASN:ND2	2.44	0.44
2:C:150:VAL:CG1	2:C:178:LEU:HD21	2.48	0.44
5:U:40:PRO:CG	5:U:165:GLU:HG2	2.48	0.44
2:F:29:PHE:HB2	2:F:97:ASP:O	2.18	0.44
5:Q:40:PRO:CG	5:Q:165:GLU:HG2	2.48	0.44
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.99	0.44
5:U:33:LEU:HD22	5:U:71:PHE:CG	2.52	0.43
4:P:6:GLN:HA	4:P:21:SER:O	2.18	0.43
2:F:63:PHE:HB3	2:F:67:VAL:HG23	2.01	0.43
2:F:126:PRO:HD3	2:F:138:LEU:HD23	2.00	0.43
3:L:35:TRP:HB2	3:L:48:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:38:ARG:NH1	4:T:86:ASP:OD1	2.50	0.43
5:Q:83:ILE:HD12	5:Q:166:GLN:HB3	2.00	0.43
5:Q:108:ARG:HG2	5:Q:109:THR:H	1.83	0.43
4:T:18:VAL:HG13	4:T:82(C):LEU:HD11	1.99	0.43
4:P:24:ALA:HB1	4:P:27:TYR:CE1	2.53	0.43
2:F:117:LYS:O	2:F:117:LYS:HG3	2.19	0.43
2:F:150:VAL:CG1	2:F:178:LEU:HD21	2.49	0.43
3:L:61:ARG:HB3	3:L:77:GLY:H	1.82	0.43
5:U:40:PRO:HG2	5:U:165:GLU:HG2	2.00	0.43
1:A:502:GLY:O	1:A:506:GLN:HG3	2.19	0.43
1:B:497:PHE:CE2	1:B:507:PRO:HB3	2.54	0.43
3:D:113:PRO:HD3	3:D:197:HIS:CD2	2.54	0.43
1:E:347:PHE:CE2	1:E:509:ARG:HD3	2.53	0.43
1:E:448:ASN:OD1	1:E:450:ASN:ND2	2.34	0.43
2:F:169:VAL:HG12	2:F:177:SER:O	2.19	0.42
4:T:6:GLN:NE2	4:T:90:TYR:O	2.42	0.42
2:H:29:PHE:HB2	2:H:97:ASP:O	2.19	0.42
1:B:502:GLY:O	1:B:506:GLN:HG3	2.18	0.42
2:F:83:ARG:HG3	2:F:85:GLU:HG2	2.01	0.42
2:H:63:PHE:HB3	2:H:67:VAL:HG23	2.01	0.42
5:Q:136:LEU:HB2	5:Q:175:LEU:HB3	2.02	0.42
1:A:388:ASN:HB3	1:A:527:PRO:HD2	2.01	0.42
2:C:111:VAL:HG12	2:C:111:VAL:O	2.19	0.42
4:T:12:LYS:HG3	4:T:18:VAL:HG12	2.01	0.42
3:L:120:PRO:O	2:H:214:LYS:NZ	2.53	0.42
1:B:395:VAL:HG23	1:B:524:VAL:HG21	2.01	0.42
4:P:18:VAL:HG11	4:P:109:VAL:HG13	2.02	0.42
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.54	0.42
2:C:36:TRP:HH2	2:C:78:VAL:HG12	1.85	0.42
2:C:39:GLN:HB2	2:C:45:LEU:HD23	2.01	0.42
2:C:181:VAL:CG2	3:D:135:LEU:HD13	2.49	0.42
2:H:111:VAL:HG12	2:H:111:VAL:O	2.20	0.42
2:H:169:VAL:HG12	2:H:177:SER:O	2.18	0.42
1:B:350:VAL:HA	1:B:400:PHE:HB2	2.02	0.42
4:P:62:LYS:HE2	4:P:62:LYS:HB3	1.85	0.42
1:E:487:ASN:OD1	2:F:100(C):GLU:HB2	2.20	0.42
4:P:12:LYS:HG3	4:P:18:VAL:HG12	2.01	0.42
4:P:32:TYR:CG	4:P:94:ARG:HD2	2.54	0.42
2:F:6:GLN:O	2:F:105:GLN:NE2	2.53	0.41
2:F:151:THR:OG1	2:F:199:ASN:HB3	2.20	0.41
5:U:7:SER:HA	5:U:8:PRO:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:87:THR:HA	4:P:109:VAL:O	2.21	0.41
2:H:146:PHE:HA	2:H:147:PRO:HA	1.87	0.41
5:Q:12:SER:HB3	5:Q:107:LYS:HG3	2.02	0.41
2:C:189:LEU:HD23	2:C:189:LEU:HA	1.89	0.41
2:H:83:ARG:HG3	2:H:85:GLU:HG2	2.02	0.41
3:G:18:SER:HA	3:G:75:VAL:O	2.21	0.41
2:H:28:THR:HG23	2:H:94:ARG:HG3	2.02	0.41
2:H:151:THR:OG1	2:H:199:ASN:HB3	2.20	0.41
1:A:365:TYR:CD2	1:A:387:LEU:HB3	2.56	0.41
3:D:61:ARG:HB3	3:D:77:GLY:H	1.85	0.41
3:L:6:GLN:HE21	3:L:101:GLY:C	2.19	0.41
5:U:29:ILE:O	5:U:29:ILE:CG1	2.68	0.41
2:F:111:VAL:HG12	2:F:111:VAL:O	2.20	0.41
3:L:52:ASN:H	3:L:52:ASN:ND2	2.12	0.41
2:H:87:THR:HG22	2:H:111:VAL:N	2.24	0.41
1:A:516:GLU:O	1:A:516:GLU:HG3	2.19	0.41
1:B:429:PHE:O	4:T:97:ARG:NH1	2.51	0.41
2:C:27:GLY:HA3	2:C:98:SER:HB3	2.02	0.41
1:E:366:SER:OG	1:E:370:ASN:OD1	2.38	0.41
2:H:186:SER:O	2:H:189:LEU:HB2	2.21	0.41
2:F:184:VAL:HG21	2:F:194:TYR:CE1	2.56	0.41
3:D:6:GLN:NE2	3:D:88:CYS:N	2.60	0.41
3:L:149:LYS:HB2	3:L:192:SER:OG	2.21	0.41
5:U:83:ILE:HD12	5:U:166:GLN:HB3	2.03	0.41
5:U:136:LEU:HB2	5:U:175:LEU:HB3	2.03	0.41
4:P:6:GLN:NE2	4:P:90:TYR:O	2.39	0.41
5:Q:145:LYS:HB3	5:Q:197:THR:OG1	2.21	0.40
1:B:341:VAL:HG22	1:B:356:LYS:HD3	2.03	0.40
1:E:350:VAL:HG22	1:E:422:ASN:HB3	2.03	0.40
2:F:39:GLN:HB2	2:F:45:LEU:HD23	2.03	0.40
2:F:72:ASP:OD1	2:F:72:ASP:N	2.55	0.40
3:L:135:LEU:HD22	2:H:166:PHE:CD1	2.56	0.40
4:T:119:PRO:HD3	4:T:200:HIS:ND1	2.36	0.40
5:Q:40:PRO:HG3	5:Q:165:GLU:HG2	2.04	0.40
1:B:365:TYR:CD2	1:B:387:LEU:HB3	2.57	0.40
3:D:35:TRP:HB2	3:D:48:ILE:HB	2.02	0.40
2:F:126:PRO:HB3	2:F:137:ALA:O	2.21	0.40
5:U:29:ILE:O	5:U:29:ILE:HG13	2.21	0.40
4:T:18:VAL:O	4:T:81:GLU:HA	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:212:GLU:OE2	4:P:81:GLU:OE2[2_444]	2.09	0.11

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	193/205 (94%)	182 (94%)	10 (5%)	1 (0%)	29	61
1	B	193/205 (94%)	184 (95%)	9 (5%)	0	100	100
1	E	193/205 (94%)	180 (93%)	13 (7%)	0	100	100
2	C	222/224 (99%)	212 (96%)	10 (4%)	0	100	100
2	F	215/224 (96%)	205 (95%)	9 (4%)	1 (0%)	29	61
2	H	221/224 (99%)	211 (96%)	10 (4%)	0	100	100
3	D	212/216 (98%)	199 (94%)	13 (6%)	0	100	100
3	G	213/216 (99%)	204 (96%)	8 (4%)	1 (0%)	29	61
3	L	211/216 (98%)	201 (95%)	10 (5%)	0	100	100
4	P	230/232 (99%)	218 (95%)	12 (5%)	0	100	100
4	T	222/232 (96%)	212 (96%)	10 (4%)	0	100	100
4	y	222/232 (96%)	211 (95%)	11 (5%)	0	100	100
5	Q	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
5	U	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
5	z	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
All	All	3180/3273 (97%)	3028 (95%)	149 (5%)	3 (0%)	51	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	118	GLY
3	G	50	GLU
1	A	480	CYS

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	168/177 (95%)	161 (96%)	7 (4%)	30	59
1	B	168/177 (95%)	164 (98%)	4 (2%)	49	74
1	E	168/177 (95%)	162 (96%)	6 (4%)	35	63
2	C	185/186 (100%)	177 (96%)	8 (4%)	29	59
2	F	180/186 (97%)	173 (96%)	7 (4%)	32	61
2	H	184/186 (99%)	178 (97%)	6 (3%)	38	66
3	D	167/180 (93%)	160 (96%)	7 (4%)	30	59
3	G	177/180 (98%)	166 (94%)	11 (6%)	18	48
3	L	173/180 (96%)	164 (95%)	9 (5%)	23	53
4	P	189/198 (96%)	185 (98%)	4 (2%)	53	76
4	T	184/198 (93%)	178 (97%)	6 (3%)	38	66
4	y	183/198 (92%)	178 (97%)	5 (3%)	44	70
5	Q	186/189 (98%)	182 (98%)	4 (2%)	52	75
5	U	186/189 (98%)	184 (99%)	2 (1%)	73	86
5	z	186/189 (98%)	184 (99%)	2 (1%)	73	86
All	All	2684/2790 (96%)	2596 (97%)	88 (3%)	38	66

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	349	SER
1	A	403	ARG
1	A	455	LEU
1	A	468	ILE
1	A	477	SER
1	A	483	VAL
1	A	514	SER
1	B	349	SER
1	B	408	ARG
1	B	455	LEU

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Mol	Chain	Res	Type
1	B	514	SER
2	C	32	SER
2	C	36	TRP
2	C	50	ARG
2	C	59	HIS
2	C	111	VAL
2	C	164	HIS
2	C	189	LEU
2	C	196	CYS
3	D	12	SER
3	D	27(B)	ASP
3	D	54	ARG
3	D	76	SER
3	D	85	ASP
3	D	200	SER
3	D	211	CYS
1	E	346	ARG
1	E	349	SER
1	E	403	ARG
1	E	455	LEU
1	E	483	VAL
1	E	514	SER
2	F	32	SER
2	F	36	TRP
2	F	50	ARG
2	F	59	HIS
2	F	111	VAL
2	F	184	VAL
2	F	196	CYS
3	G	12	SER
3	G	54	ARG
3	G	85	ASP
3	G	106	VAL
3	G	106(A)	LEU
3	G	110	LYS
3	G	114	SER
3	G	170	ASN
3	G	175	SER
3	G	201	THR
3	G	211	CYS
3	L	12	SER
3	L	52	ASN

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Mol	Chain	Res	Type
3	L	60	ASP
3	L	76	SER
3	L	85	ASP
3	L	110	LYS
3	L	114	SER
3	L	175	SER
3	L	201	THR
4	T	21	SER
4	T	66	ARG
4	T	94	ARG
4	T	97	ARG
4	T	112	SER
4	T	196	CYS
5	U	93	ASN
5	U	176	SER
4	P	21	SER
4	P	66	ARG
4	P	138	LEU
4	P	196	CYS
4	y	21	SER
4	y	31	SER
4	y	66	ARG
4	y	170	LEU
4	y	196	CYS
2	H	32	SER
2	H	36	TRP
2	H	50	ARG
2	H	59	HIS
2	H	92	CYS
2	H	196	CYS
5	Q	67	SER
5	Q	127	SER
5	Q	176	SER
5	Q	190	LYS
5	z	18	ARG
5	z	67	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	498	GLN
1	B	493	GLN

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Mol	Chain	Res	Type
2	F	199	ASN
3	G	6	GLN
3	L	6	GLN
3	L	52	ASN
4	T	39	GLN
5	U	38	GLN
2	H	199	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are 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	$\# Z > 2$
6	NAG	E	601	1	14,14,15	0.68	0	17,19,21	1.28	2 (11%)
6	NAG	B	601	1	14,14,15	0.87	0	17,19,21	1.51	2 (11%)
6	NAG	A	601	1	14,14,15	0.74	0	17,19,21	1.30	2 (11%)

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
6	NAG	E	601	1	-	2/6/23/26	0/1/1/1
6	NAG	B	601	1	-	2/6/23/26	0/1/1/1
6	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	A	601	NAG	C1-O5-C5	3.82	117.36	112.19
6	E	601	NAG	O5-C5-C6	3.29	112.36	107.20
6	B	601	NAG	O5-C5-C6	3.19	112.20	107.20
6	E	601	NAG	C1-O5-C5	3.11	116.40	112.19
6	B	601	NAG	C1-O5-C5	3.09	116.38	112.19
6	A	601	NAG	O5-C5-C6	2.60	111.28	107.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	601	NAG	C4-C5-C6-O6
6	B	601	NAG	C8-C7-N2-C2
6	E	601	NAG	O5-C5-C6-O6
6	B	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	195/205 (95%)	-0.15	0 100 100	81, 123, 177, 217	0
1	B	195/205 (95%)	0.01	5 (2%) 56 54	106, 142, 200, 250	0
1	E	195/205 (95%)	-0.04	2 (1%) 82 81	96, 139, 193, 246	0
2	C	224/224 (100%)	-0.04	1 (0%) 92 92	96, 134, 183, 232	0
2	F	219/224 (97%)	0.02	7 (3%) 47 46	88, 122, 173, 241	0
2	H	223/224 (99%)	-0.11	1 (0%) 92 92	86, 118, 165, 253	0
3	D	214/216 (99%)	-0.30	1 (0%) 91 90	105, 141, 176, 214	0
3	G	215/216 (99%)	-0.13	1 (0%) 91 90	97, 142, 185, 227	0
3	L	213/216 (98%)	-0.25	1 (0%) 91 90	92, 124, 155, 194	0
4	P	232/232 (100%)	-0.22	2 (0%) 84 83	82, 119, 168, 244	0
4	T	226/232 (97%)	-0.27	1 (0%) 92 92	89, 125, 174, 226	0
4	y	226/232 (97%)	-0.13	2 (0%) 84 83	91, 129, 173, 235	0
5	Q	213/214 (99%)	-0.19	0 100 100	91, 116, 151, 164	0
5	U	213/214 (99%)	-0.10	0 100 100	102, 139, 167, 182	0
5	z	213/214 (99%)	-0.13	0 100 100	100, 134, 166, 176	0
All	All	3216/3273 (98%)	-0.14	24 (0%) 87 87	81, 130, 178, 253	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1	GLN	6.7
2	F	216	CYS	5.1
3	L	2	SER	4.5
2	F	1	GLN	3.8
2	F	128	SER	3.7
2	H	132	SER	3.2
1	B	333	THR	3.2

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Mol	Chain	Res	Type	RSRZ
3	G	211	CYS	3.0
1	E	333	THR	3.0
4	P	216	CYS	3.0
2	F	44	GLY	2.7
3	D	2	SER	2.7
4	P	215	SER	2.6
4	y	216	CYS	2.4
1	B	445	VAL	2.3
4	y	137	ALA	2.3
1	B	448	ASN	2.3
1	E	338	PHE	2.2
2	F	29	PHE	2.1
2	F	194	TYR	2.1
4	T	121	VAL	2.1
2	F	43	GLN	2.1
1	B	365	TYR	2.1
1	B	377	PHE	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, 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
6	NAG	B	601	14/15	0.34	0.42	147,210,245,263	0
6	NAG	A	601	14/15	0.74	0.23	149,177,184,195	0
6	NAG	E	601	14/15	0.77	0.16	139,192,224,230	0

6.5 Other polymers [i](#)

There are no such residues in this entry.