



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:20 PM UTC

PDB ID : 9B82 / pdb_00009b82
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing antibody COVA2-15
Authors : Yuan, M.; Zhu, X.; Wilson, I.A.
Deposited on : 2024-03-28
Resolution : 3.38 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

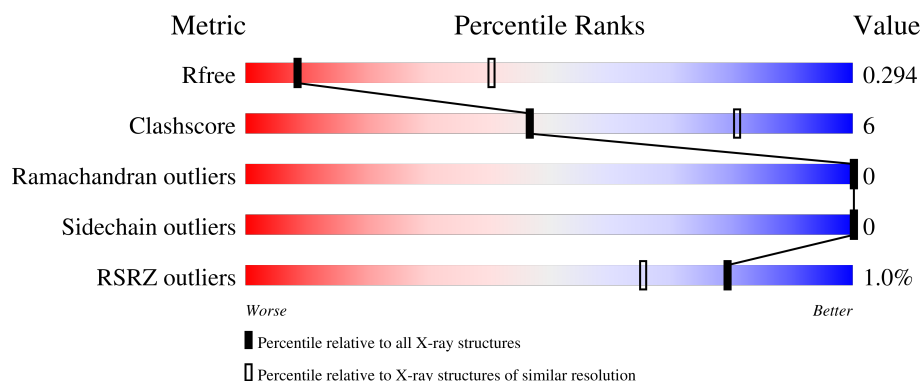
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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.



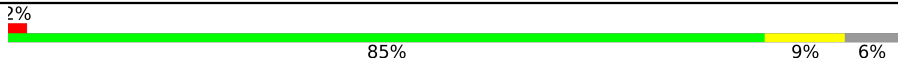
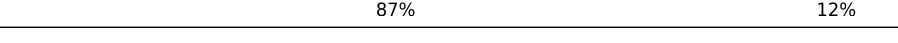
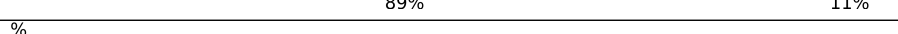
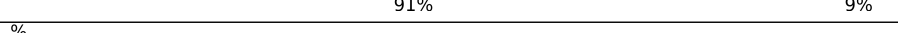
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	81%13%6%
1	B	205	3% 84%7%9%
1	C	205	85%9%6%
1	D	205	% 83%11%6%
1	E	205	83%11%6%

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Mol	Chain	Length	Quality of chain
1	F	205	
2	H	232	
2	I	232	
2	K	232	
2	N	232	
2	P	232	
2	R	232	
3	G	219	
3	J	219	
3	L	219	
3	M	219	
3	O	219	
3	Q	219	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29362 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
1	A	193	Total	C	N	O	S	0	0	0
			1529	980	255	286	8			
1	C	193	Total	C	N	O	S	0	0	0
			1529	980	255	286	8			
1	B	187	Total	C	N	O	S	0	0	0
			1487	952	247	280	8			
1	D	193	Total	C	N	O	S	0	0	0
			1526	977	255	286	8			
1	E	193	Total	C	N	O	S	0	0	0
			1529	980	255	286	8			
1	F	193	Total	C	N	O	S	0	0	0
			1529	980	255	286	8			

There are 42 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
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
B	531	GLY	-	expression tag	UNP P0DTC2
B	532	HIS	-	expression tag	UNP P0DTC2
B	533	HIS	-	expression tag	UNP P0DTC2

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

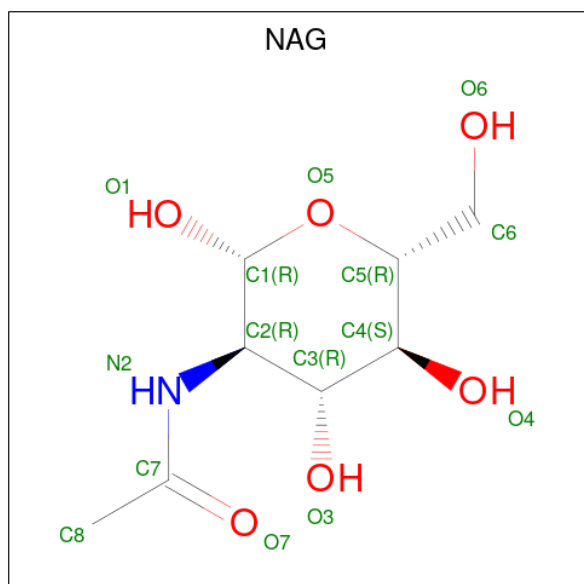
- Molecule 2 is a protein called COVA2-15 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	0	0
			1680	1055	282	335	8			
2	I	224	Total	C	N	O	S	0	0	0
			1659	1043	278	330	8			
2	K	225	Total	C	N	O	S	0	0	0
			1663	1045	279	331	8			
2	N	223	Total	C	N	O	S	0	0	0
			1653	1040	277	328	8			
2	P	224	Total	C	N	O	S	0	0	0
			1659	1043	278	330	8			
2	R	225	Total	C	N	O	S	0	0	0
			1657	1040	278	331	8			

- Molecule 3 is a protein called COVA2-15 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	219	Total	C	N	O	S	0	0	0
			1699	1058	295	339	7			
3	G	219	Total	C	N	O	S	0	0	0
			1699	1058	295	339	7			
3	J	218	Total	C	N	O	S	0	0	0
			1689	1052	293	338	6			
3	M	219	Total	C	N	O	S	0	0	0
			1699	1058	295	339	7			
3	O	219	Total	C	N	O	S	0	0	0
			1699	1058	295	339	7			
3	Q	218	Total	C	N	O	S	0	0	0
			1693	1055	294	338	6			

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

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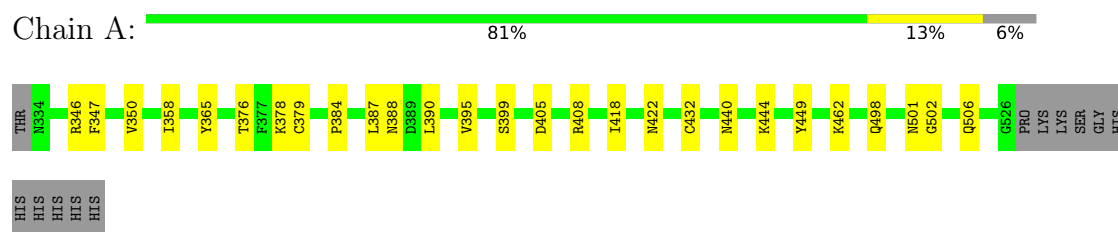
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

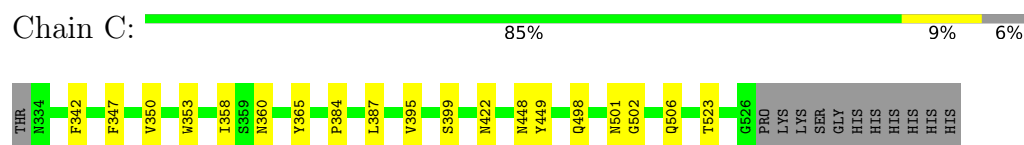
3 Residue-property plots [i](#)

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.

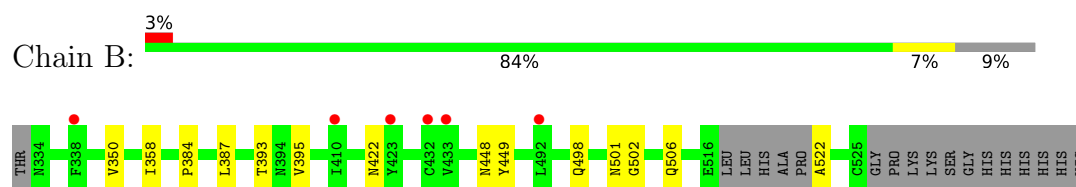
- Molecule 1: Spike protein S1



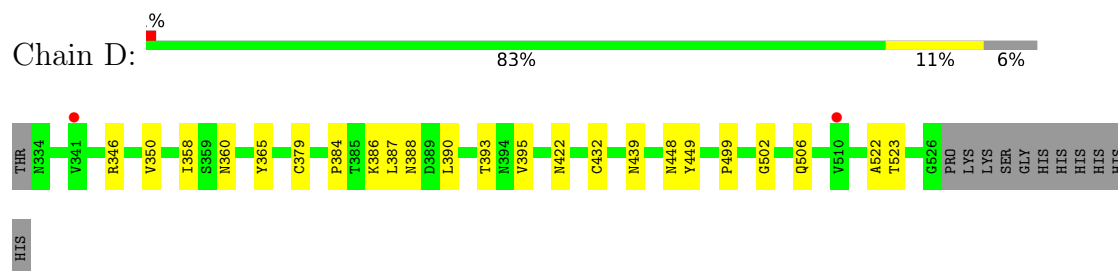
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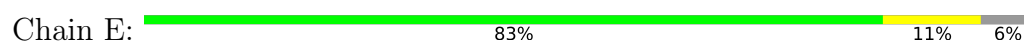
- Molecule 1: Spike protein S1



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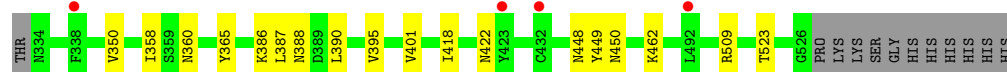
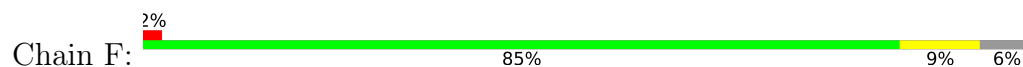


- Molecule 1: Spike protein S1

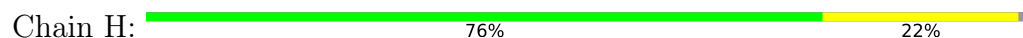




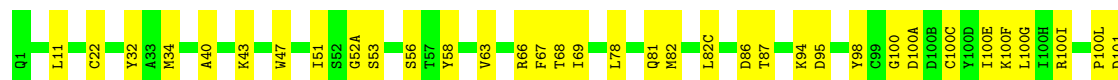
- Molecule 1: Spike protein S1



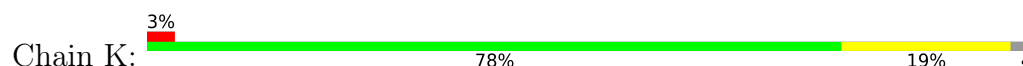
- Molecule 2: COVA2-15 antibody heavy chain



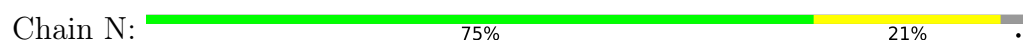
- Molecule 2: COVA2-15 antibody heavy chain



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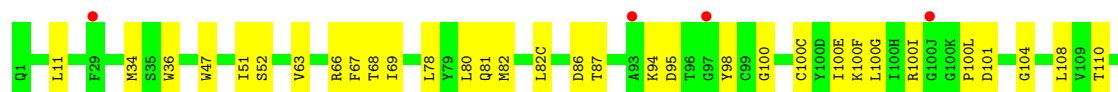
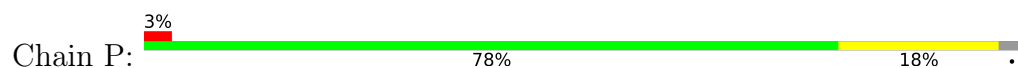


- Molecule 2: COVA2-15 antibody heavy chain

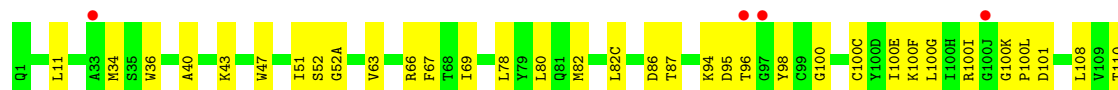
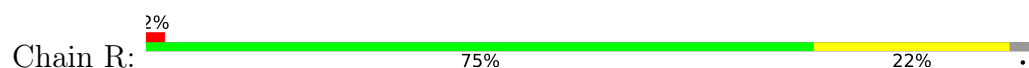




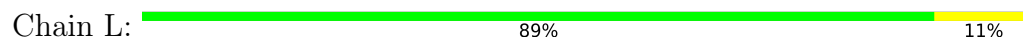
- Molecule 2: COVA2-15 antibody heavy chain



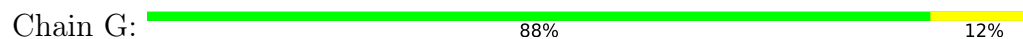
- Molecule 2: COVA2-15 antibody heavy chain



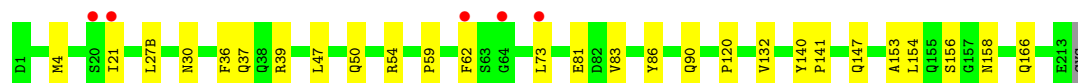
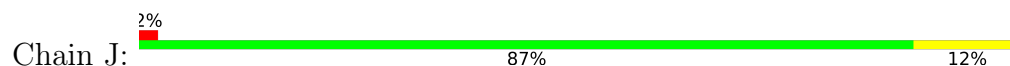
- Molecule 3: COVA2-15 antibody light chain



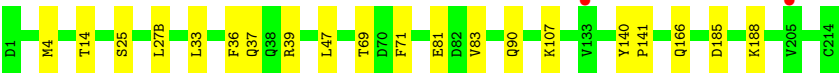
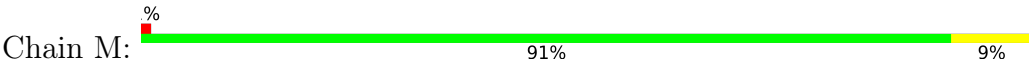
- Molecule 3: COVA2-15 antibody light chain



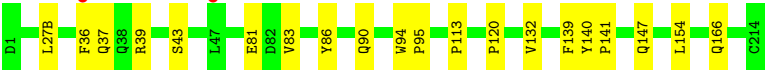
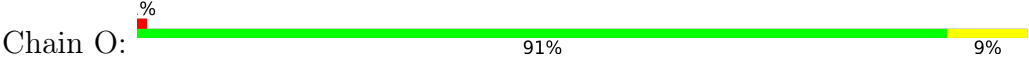
- Molecule 3: COVA2-15 antibody light chain



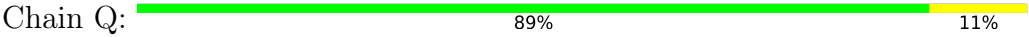
- Molecule 3: COVA2-15 antibody light chain



• Molecule 3: COVA2-15 antibody light chain



• Molecule 3: COVA2-15 antibody 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	101.05Å 218.66Å 122.73Å 90.00° 112.34° 90.00°	Depositor
Resolution (Å)	33.14 – 3.38 33.14 – 3.38	Depositor EDS
% Data completeness (in resolution range)	98.7 (33.14-3.38) 98.6 (33.14-3.38)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.39Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, R_{free}	0.242 , 0.295 0.243 , 0.294	Depositor DCC
R_{free} test set	3278 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	94.0	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	29362	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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	0.09	0/1572	0.25	0/2139
1	B	0.07	0/1527	0.22	0/2075
1	C	0.08	0/1572	0.25	0/2139
1	D	0.08	0/1569	0.22	0/2135
1	E	0.07	0/1572	0.23	0/2139
1	F	0.07	0/1572	0.23	0/2139
2	H	0.12	0/1718	0.31	0/2336
2	I	0.12	0/1697	0.29	0/2309
2	K	0.11	0/1701	0.26	0/2314
2	N	0.09	0/1691	0.26	0/2301
2	P	0.10	0/1697	0.28	0/2309
2	R	0.10	0/1695	0.28	0/2307
3	G	0.09	0/1736	0.27	0/2355
3	J	0.08	0/1726	0.26	0/2343
3	L	0.09	0/1736	0.28	0/2355
3	M	0.07	0/1736	0.25	0/2355
3	O	0.07	0/1736	0.25	0/2355
3	Q	0.08	0/1730	0.25	0/2347
All	All	0.09	0/29983	0.26	0/40752

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	1529	0	1445	22	0
1	B	1487	0	1400	9	0
1	C	1529	0	1445	12	0
1	D	1526	0	1436	14	0
1	E	1529	0	1445	16	0
1	F	1529	0	1445	13	0
2	H	1680	0	1634	36	0
2	I	1659	0	1611	33	0
2	K	1663	0	1612	31	0
2	N	1653	0	1606	32	0
2	P	1659	0	1611	30	0
2	R	1657	0	1594	38	0
3	G	1699	0	1648	16	0
3	J	1689	0	1632	18	0
3	L	1699	0	1648	15	0
3	M	1699	0	1648	11	0
3	O	1699	0	1648	12	0
3	Q	1693	0	1643	16	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	1	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
All	All	29362	0	28229	330	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 (330) 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)
2:K:82:MET:HB3	2:K:82(C):LEU:HD21	1.63	0.80
2:H:130:SER:HG	2:H:136:GLY:N	1.80	0.80
2:P:82:MET:HB3	2:P:82(C):LEU:HD21	1.63	0.79
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.63	0.79
2:I:82:MET:HB3	2:I:82(C):LEU:HD21	1.65	0.79
2:N:82:MET:HB3	2:N:82(C):LEU:HD21	1.66	0.76
2:R:82:MET:HB3	2:R:82(C):LEU:HD21	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:27:GLN:HG3	3:G:27:GLN:HG3	1.68	0.74
3:G:27(B):LEU:HD21	3:G:90:GLN:HG2	1.71	0.73
2:H:51:ILE:HD11	2:H:69:ILE:HG12	1.72	0.71
2:H:47:TRP:HH2	2:H:100(L):PRO:HG3	1.55	0.70
2:I:51:ILE:HD11	2:I:69:ILE:HG12	1.73	0.70
2:H:100:GLY:N	2:H:100(C):CYS:SG	2.63	0.68
2:N:51:ILE:HD11	2:N:69:ILE:HG12	1.76	0.67
2:N:108:LEU:HD22	2:N:151:PRO:HD3	1.77	0.67
1:C:449:TYR:OH	2:I:100(I):ARG:O	2.08	0.67
3:L:39:ARG:NH1	3:L:81:GLU:O	2.27	0.67
2:R:51:ILE:HD11	2:R:69:ILE:HG12	1.76	0.66
1:A:449:TYR:OH	2:H:100(I):ARG:O	2.10	0.66
2:K:11:LEU:HB2	2:K:149:PRO:HG3	1.76	0.66
1:D:365:TYR:H	1:D:388:ASN:HD21	1.41	0.66
2:P:126:PRO:HG2	2:P:227:PRO:HB3	1.78	0.66
1:E:448:ASN:HA	2:P:98:TYR:HB3	1.78	0.65
2:K:51:ILE:HD11	2:K:69:ILE:HG12	1.78	0.65
2:P:126:PRO:HD3	2:P:140:LEU:HB3	1.78	0.65
1:B:449:TYR:OH	2:K:100(I):ARG:O	2.12	0.65
2:R:66:ARG:NH2	2:R:86:ASP:OD2	2.30	0.65
3:Q:106:ILE:O	3:Q:166:GLN:NE2	2.27	0.65
1:B:448:ASN:HA	2:K:98:TYR:HB3	1.78	0.65
3:L:27(B):LEU:HD21	3:L:90:GLN:HG2	1.79	0.65
2:R:47:TRP:HH2	2:R:100(L):PRO:HG3	1.62	0.64
2:I:66:ARG:NH2	2:I:86:ASP:OD2	2.31	0.63
1:D:449:TYR:OH	2:N:100(I):ARG:O	2.08	0.63
2:R:11:LEU:HB2	2:R:149:PRO:HG3	1.79	0.63
2:N:47:TRP:HH2	2:N:100(L):PRO:HG3	1.63	0.63
3:J:83:VAL:HG21	3:J:166:GLN:HB3	1.81	0.63
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.32	0.63
2:K:47:TRP:HH2	2:K:100(L):PRO:HG3	1.64	0.63
2:P:51:ILE:HD11	2:P:69:ILE:HG12	1.80	0.62
2:I:47:TRP:HH2	2:I:100(L):PRO:HG3	1.64	0.62
2:N:66:ARG:NH2	2:N:86:ASP:OD2	2.32	0.62
1:C:358:ILE:HB	1:C:395:VAL:HB	1.81	0.62
3:G:120:PRO:HD3	3:G:132:VAL:HG22	1.81	0.61
1:D:448:ASN:HA	2:N:98:TYR:HB3	1.81	0.61
2:P:47:TRP:HH2	2:P:100(L):PRO:HG3	1.63	0.61
2:H:108:LEU:HD21	2:H:110:THR:HG23	1.81	0.61
2:P:95:ASP:HA	2:P:100(L):PRO:HA	1.80	0.61
1:B:358:ILE:HB	1:B:395:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:94:LYS:O	2:P:101:ASP:N	2.34	0.61
2:H:11:LEU:HB2	2:H:149:PRO:HG3	1.83	0.60
3:O:83:VAL:HG21	3:O:166:GLN:HB3	1.82	0.60
2:I:108:LEU:HD21	2:I:110:THR:HG23	1.82	0.60
2:N:94:LYS:O	2:N:101:ASP:N	2.34	0.60
1:F:365:TYR:H	1:F:388:ASN:HD21	1.47	0.60
3:J:39:ARG:NH1	3:J:81:GLU:O	2.35	0.60
3:Q:120:PRO:HD3	3:Q:132:VAL:HG22	1.84	0.60
3:J:54:ARG:NH1	3:J:59:PRO:O	2.35	0.60
3:Q:27(B):LEU:HD21	3:Q:90:GLN:HG2	1.84	0.59
2:R:94:LYS:O	2:R:101:ASP:N	2.36	0.59
1:E:365:TYR:H	1:E:388:ASN:HD21	1.49	0.59
3:G:54:ARG:NH1	3:G:62:PHE:O	2.36	0.59
1:F:358:ILE:HB	1:F:395:VAL:HB	1.85	0.59
2:I:11:LEU:HB2	2:I:149:PRO:HG3	1.83	0.59
2:K:66:ARG:NH2	2:K:86:ASP:OD2	2.36	0.58
2:R:34:MET:HB3	2:R:78:LEU:HD22	1.84	0.58
2:K:34:MET:HB3	2:K:78:LEU:HD22	1.86	0.58
2:P:11:LEU:HB2	2:P:149:PRO:HG3	1.86	0.58
3:J:147:GLN:HB3	3:J:154:LEU:HD11	1.85	0.58
2:P:66:ARG:NH2	2:P:86:ASP:OD2	2.36	0.58
2:N:11:LEU:HD22	2:N:149:PRO:HD3	1.86	0.57
1:E:350:VAL:HG22	1:E:422:ASN:HB3	1.86	0.57
2:H:130:SER:O	2:H:136:GLY:N	2.37	0.57
3:L:77:ARG:HH12	2:N:195:SER:HB3	1.70	0.57
3:M:83:VAL:HG21	3:M:166:GLN:HB3	1.87	0.57
2:P:34:MET:HB3	2:P:78:LEU:HD22	1.86	0.57
3:J:27(B):LEU:HD21	3:J:90:GLN:HG2	1.86	0.57
2:N:126:PRO:HD3	2:N:140:LEU:HB3	1.86	0.57
3:J:120:PRO:HD3	3:J:132:VAL:HG22	1.86	0.57
1:D:358:ILE:HB	1:D:395:VAL:HB	1.86	0.57
3:M:27(B):LEU:HD21	3:M:90:GLN:HG2	1.86	0.56
2:N:95:ASP:HA	2:N:100(L):PRO:HA	1.86	0.56
1:E:358:ILE:HB	1:E:395:VAL:HB	1.88	0.56
2:R:108:LEU:HD21	2:R:110:THR:HG23	1.88	0.56
2:I:95:ASP:HA	2:I:100(L):PRO:HA	1.87	0.56
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.87	0.55
3:L:25:SER:O	3:L:69:THR:OG1	2.19	0.55
2:R:176:ALA:HB2	2:R:187:LEU:HD23	1.88	0.55
3:Q:25:SER:O	3:Q:69:THR:OG1	2.18	0.55
2:P:108:LEU:HD21	2:P:110:THR:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:87:THR:HG23	2:P:110:THR:HA	1.89	0.55
1:C:448:ASN:HA	2:I:98:TYR:HB3	1.88	0.54
2:N:108:LEU:HD21	2:N:110:THR:HG23	1.90	0.54
3:J:158:ASN:HB3	1:E:468:ILE:HD11	1.88	0.54
1:A:444:LYS:HD2	2:H:98:TYR:HD2	1.71	0.54
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.89	0.54
2:P:100:GLY:N	2:P:100(C):CYS:SG	2.67	0.54
2:K:87:THR:HG23	2:K:110:THR:HA	1.89	0.54
1:A:405:ASP:O	1:A:408:ARG:NH2	2.41	0.54
2:H:94:LYS:O	2:H:101:ASP:N	2.41	0.54
3:G:13:VAL:HG23	3:G:17:GLN:HE21	1.72	0.54
2:R:126:PRO:HD3	2:R:140:LEU:HB3	1.88	0.54
2:I:100:GLY:N	2:I:100(C):CYS:SG	2.71	0.54
1:A:408:ARG:NH1	2:K:196:SER:O	2.42	0.53
2:P:198:LEU:HB3	2:P:227:PRO:HG3	1.90	0.53
2:R:119:PRO:HB3	2:R:147:TYR:HB3	1.89	0.53
1:E:376:THR:HG23	1:E:378:LYS:HE2	1.89	0.53
2:I:100(L):PRO:HD2	3:G:36:PHE:HZ	1.74	0.53
2:R:87:THR:HG23	2:R:110:THR:HA	1.91	0.53
1:A:358:ILE:HB	1:A:395:VAL:HB	1.91	0.53
2:K:93:ALA:HB1	2:K:100(L):PRO:HB3	1.91	0.53
1:A:408:ARG:NH1	2:K:198:LEU:O	2.34	0.52
2:K:108:LEU:HD21	2:K:110:THR:HG23	1.90	0.52
2:R:108:LEU:HD22	2:R:151:PRO:HD3	1.89	0.52
3:O:27(B):LEU:HD21	3:O:90:GLN:HG2	1.91	0.52
2:K:100(L):PRO:HD2	3:J:36:PHE:HZ	1.75	0.52
3:O:39:ARG:NH1	3:O:81:GLU:O	2.41	0.52
3:M:39:ARG:NH1	3:M:81:GLU:O	2.42	0.52
2:P:94:LYS:NZ	2:P:101:ASP:OD2	2.43	0.52
2:K:94:LYS:O	2:K:101:ASP:N	2.43	0.51
1:D:393:THR:HA	1:D:522:ALA:HA	1.92	0.51
2:N:34:MET:HB3	2:N:78:LEU:HD22	1.90	0.51
2:I:34:MET:HB3	2:I:78:LEU:HD22	1.92	0.51
3:O:120:PRO:HD3	3:O:132:VAL:HG22	1.91	0.51
2:P:119:PRO:HB3	2:P:147:TYR:HB3	1.93	0.51
2:R:176:ALA:HA	2:R:187:LEU:HB3	1.93	0.51
3:J:153:ALA:HB2	1:E:355:ARG:HD2	1.93	0.51
2:P:100(L):PRO:HD2	3:O:36:PHE:HZ	1.76	0.51
2:R:100(L):PRO:HD2	3:Q:36:PHE:HZ	1.76	0.51
1:F:448:ASN:HA	2:R:98:TYR:HB3	1.93	0.51
2:R:100:GLY:N	2:R:100(C):CYS:SG	2.71	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:TYR:OH	2:P:100(I):ARG:O	2.17	0.50
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.46	0.50
3:G:33:LEU:HD22	3:G:71:PHE:CG	2.47	0.50
1:B:393:THR:HA	1:B:522:ALA:HA	1.94	0.50
2:K:108:LEU:HD22	2:K:151:PRO:HD3	1.93	0.50
1:D:350:VAL:HG22	1:D:422:ASN:HB3	1.92	0.50
1:C:384:PRO:HA	1:C:387:LEU:HD12	1.93	0.50
2:I:87:THR:HG23	2:I:110:THR:HA	1.94	0.50
3:J:140:TYR:CG	3:J:141:PRO:HA	2.46	0.50
1:A:384:PRO:HA	1:A:387:LEU:HD12	1.94	0.50
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.93	0.50
1:C:350:VAL:HG22	1:C:422:ASN:HB3	1.94	0.50
2:I:94:LYS:O	2:I:101:ASP:N	2.44	0.50
1:B:498:GLN:NE2	3:J:50:GLN:OE1	2.45	0.49
2:R:95:ASP:HA	2:R:100(L):PRO:HA	1.94	0.49
3:J:37:GLN:HB2	3:J:47:LEU:HD11	1.94	0.49
1:D:346:ARG:NH1	2:N:100(A):ASP:OD1	2.46	0.49
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.96	0.48
2:I:212:HIS:ND1	2:I:215:SER:OG	2.36	0.48
3:G:37:GLN:HB2	3:G:47:LEU:HD11	1.95	0.48
3:O:147:GLN:HB3	3:O:154:LEU:HD11	1.95	0.48
2:I:22:CYS:HB3	2:I:78:LEU:HB3	1.95	0.48
3:L:60:ASP:OD2	2:N:137:THR:OG1	2.32	0.48
3:O:37:GLN:NE2	3:O:86:TYR:OH	2.46	0.48
2:N:40:ALA:HB3	2:N:43:LYS:HB2	1.96	0.48
2:R:100(E):ILE:C	2:R:100(G):LEU:H	2.21	0.48
1:B:501:ASN:ND2	3:J:30:ASN:OD1	2.45	0.48
2:K:176:ALA:HB2	2:K:187:LEU:HD23	1.96	0.48
2:H:100(L):PRO:HD2	3:L:36:PHE:HZ	1.79	0.48
1:C:365:TYR:CD2	1:C:387:LEU:HB3	2.49	0.48
2:K:119:PRO:HB3	2:K:147:TYR:HB3	1.96	0.48
2:N:119:PRO:HB3	2:N:147:TYR:HB3	1.95	0.47
2:P:104:GLY:O	3:O:43:SER:OG	2.20	0.47
1:F:387:LEU:HA	1:F:390:LEU:HD12	1.95	0.47
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.95	0.47
1:C:342:PHE:HB2	4:C:601:NAG:H83	1.96	0.47
3:G:83:VAL:HG21	3:G:166:GLN:HB3	1.97	0.47
3:M:140:TYR:CG	3:M:141:PRO:HA	2.49	0.47
2:R:40:ALA:HB3	2:R:43:LYS:HB2	1.95	0.47
2:N:87:THR:HG23	2:N:110:THR:HA	1.96	0.47
1:A:365:TYR:H	1:A:388:ASN:HD21	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.96	0.47
2:I:119:PRO:HB3	2:I:147:TYR:HB3	1.96	0.47
2:K:52:SER:HB2	2:K:100(C):CYS:SG	2.55	0.47
2:H:53:SER:HB3	2:H:100(A):ASP:HA	1.96	0.47
2:P:100(E):ILE:C	2:P:100(G):LEU:H	2.23	0.47
2:R:96:THR:OG1	3:Q:46:ARG:NH1	2.48	0.47
2:I:145:LYS:NZ	3:G:131:SER:OG	2.41	0.46
1:A:405:ASP:HA	1:A:408:ARG:HH22	1.80	0.46
2:I:176:ALA:HA	2:I:187:LEU:HB3	1.97	0.46
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.96	0.46
2:H:87:THR:HG23	2:H:110:THR:HA	1.96	0.46
2:P:100(F):LYS:HA	3:O:94:TRP:CD1	2.50	0.46
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.48	0.46
3:J:54:ARG:NH1	3:J:62:PHE:O	2.46	0.46
2:N:176:ALA:HB2	2:N:187:LEU:HD23	1.96	0.46
1:F:401:VAL:HG22	1:F:509:ARG:HG2	1.98	0.46
3:O:140:TYR:CG	3:O:141:PRO:HA	2.51	0.46
2:K:95:ASP:HA	2:K:100(L):PRO:HA	1.96	0.46
1:D:502:GLY:O	1:D:506:GLN:HG3	2.16	0.46
2:N:176:ALA:HA	2:N:187:LEU:HB3	1.98	0.46
2:R:52:SER:HB2	2:R:100(C):CYS:SG	2.56	0.46
1:D:439:ASN:HD21	1:D:499:PRO:HA	1.81	0.46
3:M:25:SER:O	3:M:69:THR:OG1	2.31	0.46
1:A:379:CYS:HA	1:A:432:CYS:HA	1.98	0.45
3:J:21:ILE:HD12	3:J:73:LEU:HD23	1.99	0.45
2:R:116:THR:HG22	2:R:215:SER:HB3	1.98	0.45
2:H:193:VAL:HG21	2:H:206:TYR:OH	2.17	0.45
3:G:140:TYR:CG	3:G:141:PRO:HA	2.52	0.45
2:N:100(E):ILE:C	2:N:100(G):LEU:H	2.24	0.45
2:H:212:HIS:ND1	2:H:215:SER:OG	2.42	0.45
3:G:147:GLN:HB3	3:G:154:LEU:HD11	1.99	0.45
2:N:52(A):GLY:HA3	2:N:100:GLY:HA2	1.98	0.45
3:L:103:LYS:HE2	3:L:105:GLU:HB3	1.98	0.45
3:L:140:TYR:CG	3:L:141:PRO:HA	2.51	0.45
2:I:126:PRO:HD3	2:I:140:LEU:HB3	1.97	0.45
2:R:222:ARG:HE	2:R:226:GLU:CD	2.25	0.45
2:K:176:ALA:HA	2:K:187:LEU:HB3	1.98	0.45
1:F:350:VAL:HG22	1:F:422:ASN:HB3	1.98	0.45
1:A:408:ARG:HH11	2:K:198:LEU:C	2.20	0.45
2:K:52(A):GLY:HA3	2:K:100:GLY:HA2	1.99	0.45
2:R:52(A):GLY:HA3	2:R:100:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:157:TRP:CH2	2:I:208:CYS:HB3	2.53	0.44
1:D:387:LEU:HA	1:D:390:LEU:HD12	1.99	0.44
3:Q:113:PRO:HB3	3:Q:139:PHE:HB3	1.99	0.44
1:A:498:GLN:H	1:A:501:ASN:ND2	2.14	0.44
2:H:68:THR:HG23	2:H:81:GLN:HB3	2.00	0.44
2:H:100(F):LYS:HA	3:L:94:TRP:CD1	2.52	0.44
2:K:68:THR:HG23	2:K:81:GLN:HB3	1.99	0.44
1:E:366:SER:O	1:E:370:ASN:HB2	2.17	0.44
3:J:156:SER:HB3	1:E:467:ASP:HA	2.00	0.44
1:F:418:ILE:HA	1:F:422:ASN:HD22	1.83	0.44
2:H:193:VAL:HG22	2:H:194:PRO:HD2	1.99	0.44
2:I:40:ALA:HB3	2:I:43:LYS:HB2	1.99	0.44
2:N:22:CYS:HB3	2:N:78:LEU:HB3	2.00	0.44
2:I:58:TYR:OH	3:G:95:PRO:HB3	2.17	0.44
2:I:100(E):ILE:C	2:I:100(G):LEU:H	2.26	0.44
2:P:68:THR:HG23	2:P:81:GLN:HB3	2.00	0.44
1:F:365:TYR:CD2	1:F:387:LEU:HB3	2.53	0.44
2:H:100(E):ILE:C	2:H:100(G):LEU:H	2.25	0.44
2:I:52(A):GLY:HA3	2:I:100:GLY:HA2	2.00	0.44
2:P:52:SER:HB2	2:P:100(C):CYS:SG	2.58	0.44
1:F:449:TYR:OH	2:R:100(I):ARG:O	2.17	0.44
3:G:25:SER:O	3:G:69:THR:OG1	2.22	0.44
1:D:360:ASN:H	1:D:523:THR:HB	1.83	0.44
2:N:68:THR:HG23	2:N:81:GLN:HB3	1.99	0.44
2:N:100:GLY:N	2:N:100(C):CYS:SG	2.72	0.44
2:R:36:TRP:CD1	2:R:80:LEU:HB2	2.52	0.44
1:A:376:THR:HG23	1:A:378:LYS:HE2	1.99	0.43
2:H:47:TRP:CH2	2:H:100(L):PRO:HG3	2.45	0.43
2:I:56:SER:HB3	2:I:100(E):ILE:HG22	1.99	0.43
2:K:116:THR:HG22	2:K:215:SER:HB3	1.99	0.43
1:A:346:ARG:NH1	2:H:100(A):ASP:OD2	2.50	0.43
1:A:502:GLY:O	1:A:506:GLN:HG3	2.18	0.43
2:I:32:TYR:CG	2:I:94:LYS:HE2	2.53	0.43
3:G:120:PRO:HG3	3:G:130:ALA:HB1	2.00	0.43
2:N:93:ALA:HB1	2:N:100(L):PRO:HB3	2.00	0.43
3:M:33:LEU:HD22	3:M:71:PHE:CG	2.53	0.43
2:R:94:LYS:NZ	2:R:101:ASP:OD2	2.50	0.43
1:A:408:ARG:NH2	2:K:196:SER:HA	2.34	0.43
1:B:502:GLY:O	1:B:506:GLN:HG3	2.19	0.43
2:N:100(L):PRO:HD2	3:M:36:PHE:HZ	1.83	0.43
1:F:450:ASN:OD1	2:R:100(C):CYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:53:SER:HB3	2:I:100(A):ASP:HA	2.00	0.43
2:P:116:THR:HG22	2:P:149:PRO:HD3	2.00	0.43
1:C:360:ASN:H	1:C:523:THR:HB	1.84	0.43
2:I:63:VAL:HB	2:I:67:PHE:CD2	2.54	0.43
1:D:386:LYS:HD3	1:D:386:LYS:HA	1.82	0.43
1:F:386:LYS:HA	1:F:386:LYS:HD3	1.85	0.43
2:H:4:LEU:HD21	2:H:34:MET:HE1	2.02	0.42
2:N:63:VAL:HB	2:N:67:PHE:CD2	2.54	0.42
2:H:126:PRO:HG2	2:H:227:PRO:HB3	2.01	0.42
2:H:157:TRP:CH2	2:H:208:CYS:HB3	2.54	0.42
1:B:384:PRO:HA	1:B:387:LEU:HD12	2.01	0.42
2:K:100:GLY:N	2:K:100(C):CYS:SG	2.72	0.42
1:C:353:TRP:CD1	1:C:353:TRP:H	2.38	0.42
2:R:145:LYS:NZ	3:Q:131:SER:OG	2.49	0.42
1:E:386:LYS:HA	1:E:386:LYS:HD3	1.84	0.42
2:P:100(E):ILE:HG13	2:P:100(F):LYS:H	1.84	0.42
3:Q:120:PRO:HG3	3:Q:130:ALA:HB1	2.02	0.42
2:H:100(E):ILE:O	2:H:100(F):LYS:HB2	2.19	0.42
1:C:347:PHE:CE2	1:C:399:SER:HB2	2.54	0.42
2:R:100(F):LYS:HA	3:Q:94:TRP:CD1	2.55	0.42
2:H:36:TRP:CD1	2:H:80:LEU:HB2	2.54	0.42
2:I:68:THR:HG23	2:I:81:GLN:HB3	2.00	0.42
2:R:100(K):GLY:HA3	3:Q:34:ASN:HD21	1.84	0.42
2:H:11:LEU:HD22	2:H:149:PRO:HD3	2.00	0.42
2:I:100(F):LYS:HA	3:G:94:TRP:CD1	2.55	0.42
2:K:63:VAL:HB	2:K:67:PHE:CD2	2.54	0.42
2:P:63:VAL:HB	2:P:67:PHE:CD2	2.55	0.42
1:A:387:LEU:HA	1:A:390:LEU:HD12	2.01	0.42
1:C:502:GLY:O	1:C:506:GLN:HG3	2.20	0.42
2:P:176:ALA:HA	2:P:187:LEU:HB3	2.01	0.42
2:R:36:TRP:NE1	2:R:80:LEU:HB2	2.35	0.42
3:M:37:GLN:HB2	3:M:47:LEU:HD11	2.02	0.42
2:I:82(C):LEU:HD23	2:I:82(C):LEU:HA	1.87	0.41
1:D:379:CYS:HA	1:D:432:CYS:HA	2.02	0.41
2:K:40:ALA:HB3	2:K:43:LYS:HB2	2.01	0.41
1:E:353:TRP:CD1	1:E:353:TRP:H	2.39	0.41
1:E:440:ASN:OD1	1:E:440:ASN:N	2.52	0.41
3:O:113:PRO:HB3	3:O:139:PHE:HB3	2.02	0.41
3:Q:140:TYR:CG	3:Q:141:PRO:HA	2.56	0.41
2:I:176:ALA:HB2	2:I:187:LEU:HD23	2.01	0.41
2:P:36:TRP:CD1	2:P:80:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:462:LYS:HB2	1:F:462:LYS:HE2	1.91	0.41
3:M:4:MET:SD	3:M:90:GLN:HB2	2.60	0.41
3:M:185:ASP:HA	3:M:188:LYS:HD3	2.02	0.41
2:P:82(C):LEU:HD23	2:P:82(C):LEU:HA	1.87	0.41
3:Q:37:GLN:HB2	3:Q:47:LEU:HD11	2.03	0.41
2:H:19:ARG:HB2	2:H:81:GLN:OE1	2.21	0.41
2:H:126:PRO:HD3	2:H:140:LEU:HB3	2.01	0.41
2:N:212:HIS:ND1	2:N:215:SER:OG	2.42	0.41
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.55	0.41
3:L:21:ILE:HD12	3:L:73:LEU:HD23	2.01	0.41
3:M:14:THR:HB	3:M:107:LYS:NZ	2.36	0.41
3:O:94:TRP:HE3	3:O:95:PRO:HA	1.86	0.41
1:C:498:GLN:H	1:C:501:ASN:ND2	2.19	0.41
1:D:384:PRO:HA	1:D:387:LEU:HD12	2.02	0.41
1:E:387:LEU:HA	1:E:390:LEU:HD12	2.02	0.41
1:F:360:ASN:H	1:F:523:THR:HB	1.86	0.41
2:R:82(C):LEU:HD23	2:R:82(C):LEU:HA	1.90	0.41
2:R:157:TRP:CH2	2:R:208:CYS:HB3	2.56	0.41
2:R:174:PHE:CD2	3:Q:164:THR:HG23	2.55	0.41
1:A:418:ILE:HA	1:A:422:ASN:HB2	2.03	0.41
3:L:136:LEU:HB2	3:L:175:LEU:HB3	2.03	0.41
3:Q:148:TRP:O	3:Q:154:LEU:HD12	2.21	0.41
1:A:462:LYS:HB2	1:A:462:LYS:HE2	1.96	0.40
2:K:212:HIS:ND1	2:K:215:SER:OG	2.41	0.40
2:K:222:ARG:HE	2:K:226:GLU:CD	2.29	0.40
3:J:37:GLN:NE2	3:J:86:TYR:OH	2.49	0.40
2:H:56:SER:HB3	2:H:100(E):ILE:HG22	2.03	0.40
2:R:63:VAL:HB	2:R:67:PHE:CD2	2.55	0.40
2:R:100(E):ILE:HG13	2:R:100(F):LYS:H	1.86	0.40
2:N:100(E):ILE:HG13	2:N:100(F):LYS:H	1.86	0.40
1:E:462:LYS:HE2	1:E:462:LYS:HB2	1.89	0.40
3:Q:147:GLN:HB3	3:Q:154:LEU:HD11	2.02	0.40
2:N:36:TRP:NE1	2:N:80:LEU:HB2	2.37	0.40
1:E:379:CYS:HA	1:E:432:CYS:HA	2.02	0.40
1:A:440:ASN:OD1	1:A:440:ASN:N	2.54	0.40
3:J:4:MET:SD	3:J:90:GLN:HB2	2.61	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	191/205 (93%)	186 (97%)	5 (3%)	0	100	100
1	B	183/205 (89%)	179 (98%)	4 (2%)	0	100	100
1	C	191/205 (93%)	187 (98%)	4 (2%)	0	100	100
1	D	191/205 (93%)	186 (97%)	5 (3%)	0	100	100
1	E	191/205 (93%)	187 (98%)	4 (2%)	0	100	100
1	F	191/205 (93%)	187 (98%)	4 (2%)	0	100	100
2	H	223/232 (96%)	217 (97%)	6 (3%)	0	100	100
2	I	220/232 (95%)	215 (98%)	5 (2%)	0	100	100
2	K	221/232 (95%)	215 (97%)	6 (3%)	0	100	100
2	N	219/232 (94%)	214 (98%)	5 (2%)	0	100	100
2	P	220/232 (95%)	215 (98%)	5 (2%)	0	100	100
2	R	221/232 (95%)	215 (97%)	6 (3%)	0	100	100
3	G	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
3	J	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
3	L	217/219 (99%)	212 (98%)	5 (2%)	0	100	100
3	M	217/219 (99%)	212 (98%)	5 (2%)	0	100	100
3	O	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
3	Q	216/219 (99%)	212 (98%)	4 (2%)	0	100	100
All	All	3762/3936 (96%)	3676 (98%)	86 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	166/177 (94%)	166 (100%)	0	100	100
1	B	162/177 (92%)	162 (100%)	0	100	100
1	C	166/177 (94%)	166 (100%)	0	100	100
1	D	165/177 (93%)	165 (100%)	0	100	100
1	E	166/177 (94%)	166 (100%)	0	100	100
1	F	166/177 (94%)	166 (100%)	0	100	100
2	H	186/190 (98%)	186 (100%)	0	100	100
2	I	183/190 (96%)	183 (100%)	0	100	100
2	K	183/190 (96%)	183 (100%)	0	100	100
2	N	182/190 (96%)	182 (100%)	0	100	100
2	P	183/190 (96%)	183 (100%)	0	100	100
2	R	181/190 (95%)	181 (100%)	0	100	100
3	G	195/195 (100%)	195 (100%)	0	100	100
3	J	193/195 (99%)	193 (100%)	0	100	100
3	L	195/195 (100%)	195 (100%)	0	100	100
3	M	195/195 (100%)	195 (100%)	0	100	100
3	O	195/195 (100%)	195 (100%)	0	100	100
3	Q	194/195 (100%)	194 (100%)	0	100	100
All	All	3256/3372 (97%)	3256 (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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	ASN
1	A	370	ASN
3	L	17	GLN
3	L	53	ASN
3	G	17	GLN
3	G	53	ASN
1	B	370	ASN
1	B	448	ASN
2	K	211	ASN

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Mol	Chain	Res	Type
3	J	17	GLN
3	J	53	ASN
1	D	439	ASN
2	N	211	ASN
3	M	53	ASN
3	M	160	GLN
2	P	172	HIS
2	P	211	ASN
3	O	17	GLN
3	O	53	ASN
3	O	138	ASN
3	O	160	GLN
2	R	211	ASN
3	Q	50	GLN
3	Q	53	ASN
3	Q	160	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
4	NAG	F	1001	1	14,14,15	0.61	0	17,19,21	1.59	1 (5%)
4	NAG	E	1001	1	14,14,15	0.60	0	17,19,21	1.57	1 (5%)
4	NAG	D	1001	1	14,14,15	0.60	0	17,19,21	1.56	1 (5%)
4	NAG	B	1001	1	14,14,15	0.62	0	17,19,21	1.59	1 (5%)
4	NAG	A	1001	1	14,14,15	0.61	0	17,19,21	1.58	1 (5%)
4	NAG	C	601	1	14,14,15	0.69	0	17,19,21	2.18	4 (23%)

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	F	1001	1	-	4/6/23/26	0/1/1/1
4	NAG	E	1001	1	-	4/6/23/26	0/1/1/1
4	NAG	D	1001	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1001	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	4/6/23/26	0/1/1/1
4	NAG	C	601	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	NAG	C1-O5-C5	5.54	119.61	112.19
4	F	1001	NAG	C1-O5-C5	5.53	119.59	112.19
4	B	1001	NAG	C1-O5-C5	5.46	119.51	112.19
4	D	1001	NAG	C1-O5-C5	5.43	119.46	112.19
4	A	1001	NAG	C1-O5-C5	5.43	119.46	112.19
4	E	1001	NAG	C1-O5-C5	5.38	119.40	112.19
4	C	601	NAG	C2-N2-C7	4.03	128.30	122.90
4	C	601	NAG	C1-C2-N2	3.60	116.11	110.43
4	C	601	NAG	O7-C7-N2	2.17	125.81	121.98

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1001	NAG	O5-C5-C6-O6
4	A	1001	NAG	O5-C5-C6-O6
4	B	1001	NAG	O5-C5-C6-O6
4	D	1001	NAG	O5-C5-C6-O6
4	E	1001	NAG	O5-C5-C6-O6
4	A	1001	NAG	C4-C5-C6-O6
4	E	1001	NAG	C4-C5-C6-O6
4	F	1001	NAG	C4-C5-C6-O6
4	A	1001	NAG	C8-C7-N2-C2
4	A	1001	NAG	O7-C7-N2-C2
4	B	1001	NAG	C8-C7-N2-C2
4	B	1001	NAG	O7-C7-N2-C2
4	D	1001	NAG	C8-C7-N2-C2
4	D	1001	NAG	O7-C7-N2-C2
4	E	1001	NAG	C8-C7-N2-C2
4	E	1001	NAG	O7-C7-N2-C2
4	F	1001	NAG	C8-C7-N2-C2
4	F	1001	NAG	O7-C7-N2-C2
4	B	1001	NAG	C4-C5-C6-O6
4	D	1001	NAG	C4-C5-C6-O6
4	C	601	NAG	C3-C2-N2-C7
4	C	601	NAG	C4-C5-C6-O6
4	C	601	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	193/205 (94%)	-0.33	0 100 100	37, 76, 152, 197	0
1	B	187/205 (91%)	0.36	6 (3%) 50 36	88, 133, 191, 209	0
1	C	193/205 (94%)	-0.23	0 100 100	46, 89, 148, 187	0
1	D	193/205 (94%)	0.15	2 (1%) 79 65	73, 133, 200, 223	0
1	E	193/205 (94%)	0.06	0 100 100	91, 140, 204, 216	0
1	F	193/205 (94%)	0.31	4 (2%) 63 47	107, 146, 189, 215	0
2	H	227/232 (97%)	-0.44	0 100 100	30, 58, 91, 142	0
2	I	224/232 (96%)	-0.40	0 100 100	35, 59, 89, 114	0
2	K	225/232 (96%)	0.12	6 (2%) 56 41	83, 119, 145, 172	0
2	N	223/232 (96%)	-0.03	1 (0%) 88 80	84, 130, 171, 187	0
2	P	224/232 (96%)	0.29	7 (3%) 51 38	81, 130, 176, 203	0
2	R	225/232 (96%)	0.20	4 (1%) 67 52	86, 141, 171, 193	0
3	G	219/219 (100%)	-0.29	1 (0%) 87 77	45, 74, 103, 165	2 (0%)
3	J	218/219 (99%)	0.19	5 (2%) 61 45	73, 121, 150, 180	3 (1%)
3	L	219/219 (100%)	-0.31	0 100 100	38, 70, 110, 153	2 (0%)
3	M	219/219 (100%)	0.03	2 (0%) 81 68	84, 128, 158, 202	1 (0%)
3	O	219/219 (100%)	-0.04	2 (0%) 81 68	69, 115, 151, 184	2 (0%)
3	Q	218/219 (99%)	0.15	0 100 100	79, 151, 185, 194	0
All	All	3812/3936 (96%)	-0.01	40 (1%) 79 65	30, 117, 176, 223	10 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	432	CYS	4.9
2	K	128	SER	3.4
1	B	410	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	R	97	GLY	3.1
2	K	100(J)	GLY	3.0
2	K	100(H)	ILE	2.9
1	F	423	TYR	2.9
2	P	100(J)	GLY	2.8
2	P	97	GLY	2.7
2	R	100(J)	GLY	2.7
1	F	432	CYS	2.7
2	K	97	GLY	2.5
3	J	73	LEU	2.4
2	P	29	PHE	2.3
1	F	338	PHE	2.3
2	P	140	LEU	2.3
3	J	20	SER	2.3
3	J	62	PHE	2.3
2	R	96	THR	2.3
1	D	341	VAL	2.3
1	D	510	VAL	2.3
2	P	93	ALA	2.2
3	O	36	PHE	2.2
2	K	100(K)	GLY	2.2
3	J	21	ILE	2.2
3	J	64	GLY	2.2
3	M	133	VAL	2.1
1	F	492	LEU	2.1
2	K	33	ALA	2.1
2	R	33	ALA	2.1
3	M	205	VAL	2.1
3	O	47	LEU	2.1
1	B	423	TYR	2.1
2	P	205	THR	2.1
1	B	433	VAL	2.1
3	G	153	ALA	2.0
1	B	338	PHE	2.0
2	P	225	VAL	2.0
2	N	124	LEU	2.0
1	B	492	LEU	2.0

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

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($\text{\AA}^2$)	Q<0.9
4	NAG	F	1001	14/15	0.49	0.14	126,167,186,200	0
4	NAG	E	1001	14/15	0.69	0.10	142,162,186,189	0
4	NAG	C	601	14/15	0.72	0.10	102,156,177,179	0
4	NAG	D	1001	14/15	0.80	0.10	121,161,174,183	0
4	NAG	B	1001	14/15	0.85	0.08	156,181,193,195	0
4	NAG	A	1001	14/15	0.86	0.07	75,116,133,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.