



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:51 PM UTC

PDB ID : 8EL2 / pdb_00008el2
Title : SARS-CoV-2 RBD bound to neutralizing antibody Fab ICO-hu23
Authors : Besaw, J.E.; Kuo, A.; Morizumi, T.; Ernst, O.P.
Deposited on : 2022-09-22
Resolution : 2.89 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:

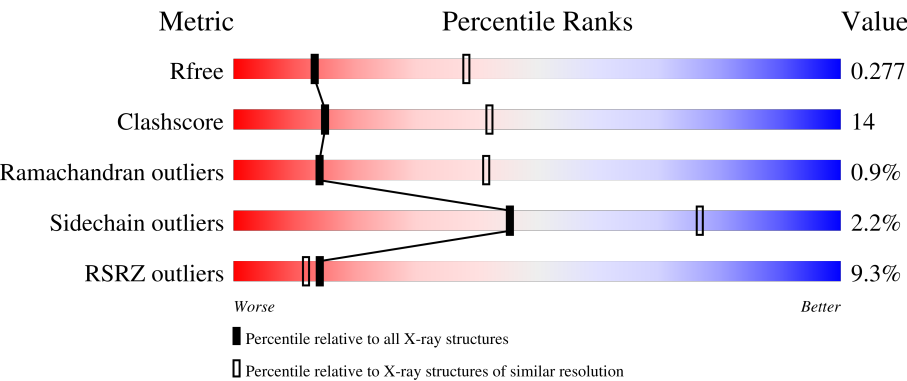
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	H	234	9% 70% 24% 6%
1	I	234	5% 73% 19% 6%
2	K	216	9% 75% 23% ..
2	L	216	6% 74% 24% ..
3	A	231	10% 59% 22% .. 16%

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Mol	Chain	Length	Quality of chain
3	B	231	12% 55% 21% •• 21%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9548 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 Fab ICO-hu23 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	219	Total	C	N	O	S	0	0	0
			1670	1066	277	319	8			
1	I	219	Total	C	N	O	S	0	0	0
			1672	1067	278	319	8			

- Molecule 2 is a protein called Fab ICO-hu23 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1580	987	260	328	5			
2	K	213	Total	C	N	O	S	0	0	0
			1573	984	256	328	5			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	194	Total	C	N	O	S	6	2	0
			1545	990	257	290	8			
3	B	183	Total	C	N	O	S	6	2	0
			1466	942	241	275	8			

There are 16 discrepancies between the modelled and reference sequences:

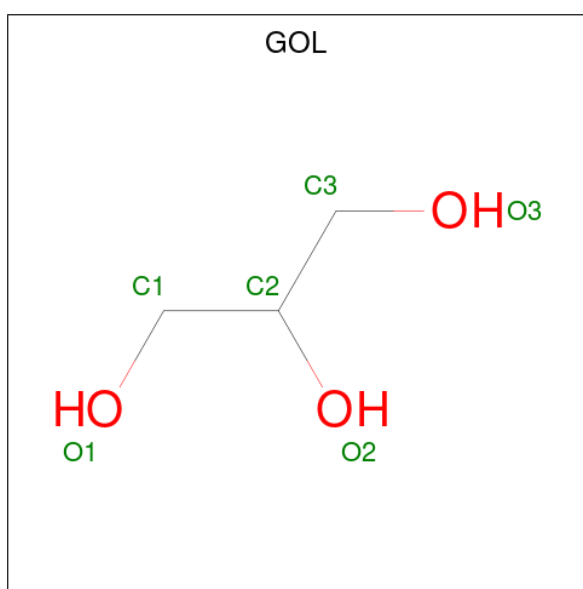
Chain	Residue	Modelled	Actual	Comment	Reference
A	317	ALA	-	expression tag	UNP P0DTC2
A	318	SER	-	expression tag	UNP P0DTC2
A	542	HIS	-	expression tag	UNP P0DTC2
A	543	HIS	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	317	ALA	-	expression tag	UNP P0DTC2
B	318	SER	-	expression tag	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



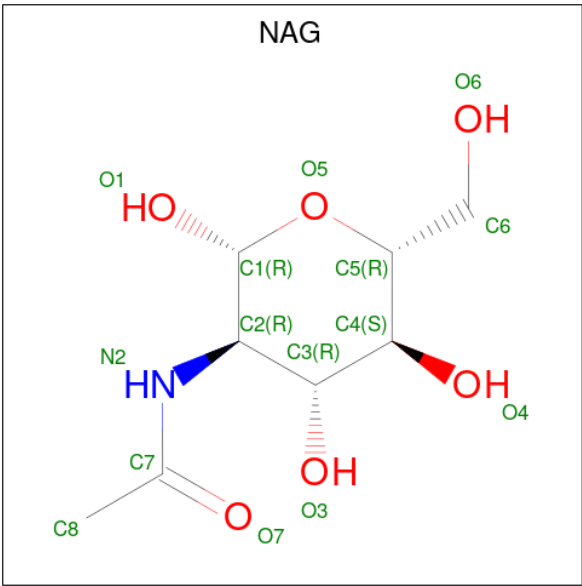
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total Zn 1 1	0	0
5	K	1	Total Zn 1 1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).

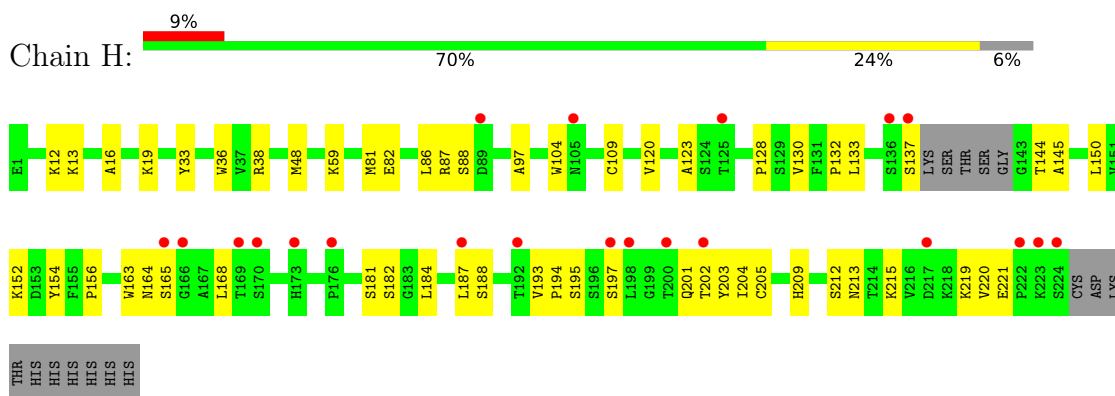


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

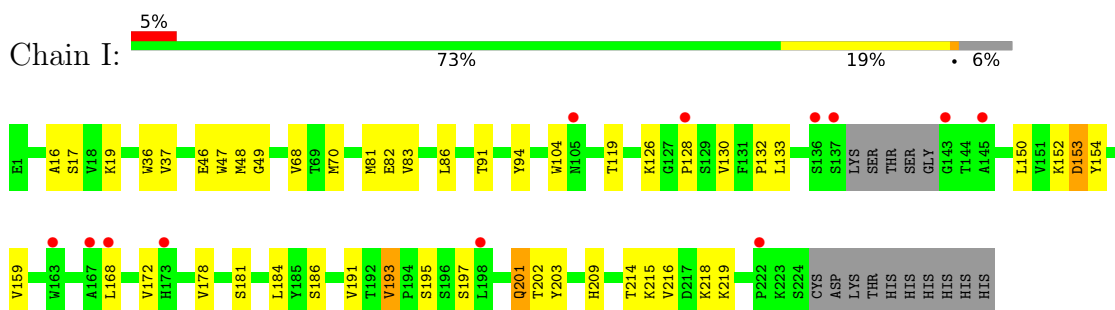
3 Residue-property plots

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.

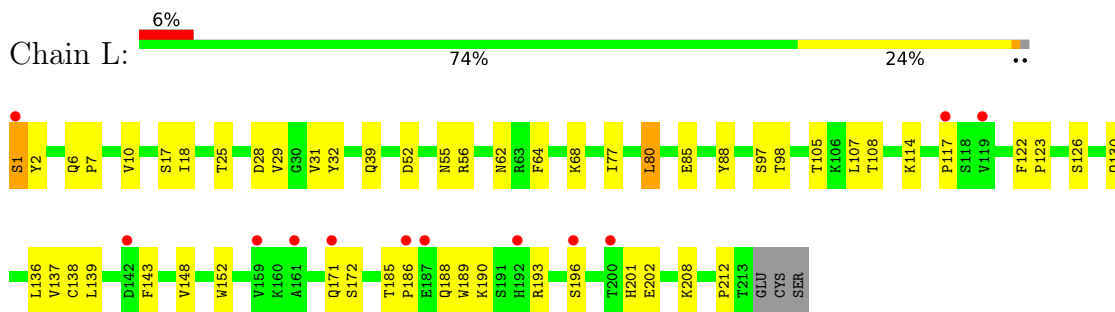
- Molecule 1: Fab ICO-hu23 Heavy Chain



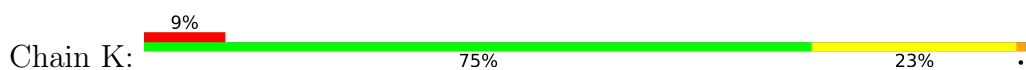
- Molecule 1: Fab ICO-hu23 Heavy Chain

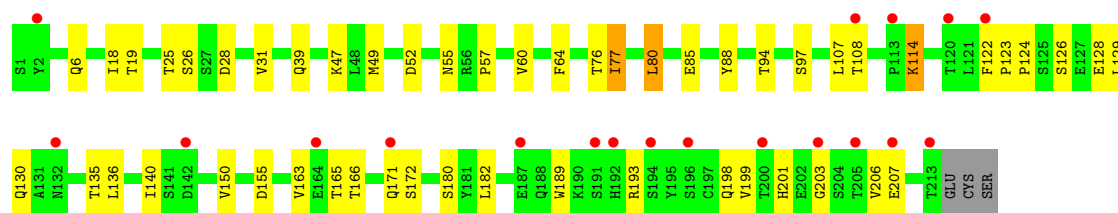


- Molecule 2: Fab ICO-hu23 Light Chain

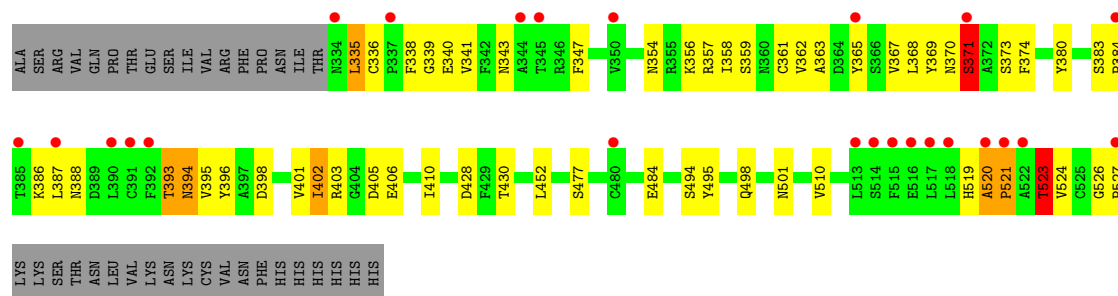


- Molecule 2: Fab ICO-hu23 Light Chain

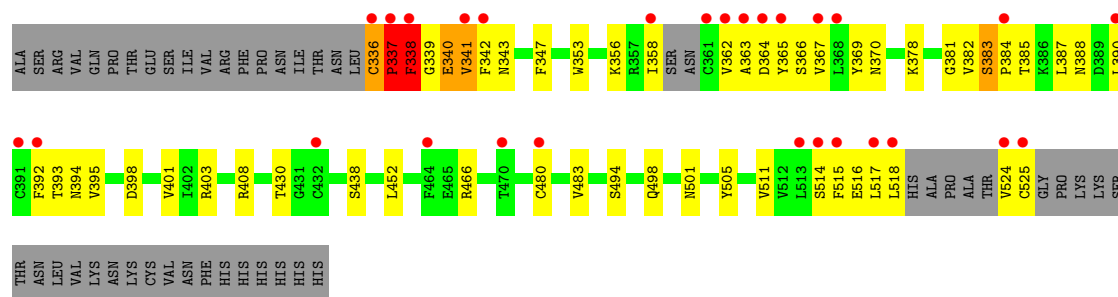




• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.30Å 140.30Å 202.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.78 – 2.89 46.78 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.78-2.89) 90.3 (46.78-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.53 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.239 , 0.281 0.237 , 0.277	Depositor DCC
R_{free} test set	2012 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å ²)	75.6	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9548	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, ZN, GOL

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	H	0.32	1/1718 (0.1%)	0.54	0/2345
1	I	0.31	0/1720	0.58	0/2347
2	K	0.30	0/1611	0.59	0/2202
2	L	0.27	0/1618	0.55	0/2210
3	A	0.40	0/1592	0.74	2/2167 (0.1%)
3	B	0.30	0/1508	0.67	2/2048 (0.1%)
All	All	0.32	1/9767 (0.0%)	0.61	4/13319 (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	A	0	1
3	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	165	SER	CB-OG	-6.34	1.29	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	338	PHE	CB-CA-C	-6.39	109.19	116.54
3	B	337	PRO	N-CA-CB	-6.24	96.69	103.25
3	A	335	LEU	CA-CB-CG	5.42	135.28	116.30
3	A	367	VAL	N-CA-C	-5.32	105.83	113.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	340	GLU	Peptide
3	B	383	SER	Peptide

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	H	1670	0	1615	36	1
1	I	1672	0	1622	43	1
2	K	1573	0	1513	38	0
2	L	1580	0	1529	34	0
3	A	1545	0	1463	56	5
3	B	1466	0	1380	56	1
4	B	6	0	8	0	0
4	L	6	0	8	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	14	0	13	0	0
6	B	14	0	13	3	0
All	All	9548	0	9164	256	6

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 14.

All (256) 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:155:ASP:CG	2:K:193:ARG:CD	1.79	1.51
3:B:336:CYS:HB3	3:B:337:PRO:CD	1.44	1.38
3:B:336:CYS:CB	3:B:337:PRO:HD3	1.61	1.26
3:A:523:THR:CG2	3:A:524:VAL:H	1.43	1.26
2:K:155:ASP:OD2	2:K:193:ARG:CG	1.86	1.22
3:A:336:CYS:SG	3:A:361:CYS:SG	1.46	1.18
3:A:523:THR:HG23	3:A:524:VAL:HG23	1.32	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:523:THR:CG2	3:A:524:VAL:N	2.09	1.07
3:A:523:THR:HG22	3:A:524:VAL:H	1.12	1.07
3:A:523:THR:HG23	3:A:524:VAL:N	1.68	1.04
3:B:336:CYS:SG	3:B:362:VAL:O	2.18	1.01
3:A:335:LEU:HB3	3:A:362:VAL:HG13	1.46	0.96
3:B:395:VAL:HG12	3:B:515:PHE:HA	1.51	0.92
1:I:126:LYS:HZ1	1:I:153:ASP:HB3	1.33	0.91
3:A:359:SER:HB3	3:A:394:ASN:HD21	1.37	0.87
3:A:363:ALA:O	3:A:526:GLY:HA2	1.75	0.87
2:K:155:ASP:OD2	2:K:193:ARG:CD	0.56	0.86
1:I:16:ALA:O	1:I:86:LEU:HD12	1.79	0.82
3:A:359:SER:CB	3:A:394:ASN:HD21	1.94	0.80
3:B:394:ASN:O	3:B:516:GLU:HB3	1.81	0.80
2:K:85:GLU:HG3	2:K:108:THR:HA	1.64	0.79
3:B:385:THR:HA	3:B:387:LEU:HG	1.66	0.77
1:H:144:THR:OG1	1:H:193:VAL:O	2.02	0.77
2:K:193:ARG:CD	2:K:193:ARG:H	1.98	0.76
3:A:335:LEU:HB2	3:A:362:VAL:O	1.87	0.74
3:A:380:TYR:O	3:A:430:THR:HA	1.88	0.74
3:B:358:ILE:HB	3:B:395:VAL:O	1.87	0.73
3:A:523:THR:HG23	3:A:524:VAL:CG2	2.15	0.73
3:A:358:ILE:O	3:A:395:VAL:HG22	1.89	0.72
3:B:343:ASN:OD1	6:B:601:NAG:C1	2.38	0.71
1:I:128:PRO:HD2	1:I:214:THR:HG21	1.74	0.70
3:B:358:ILE:CG2	3:B:395:VAL:HG23	2.23	0.69
1:I:36:TRP:HB2	1:I:70:MET:HE2	1.75	0.69
2:L:122:PHE:HB2	2:L:137:VAL:HG22	1.73	0.68
3:B:393:THR:HG21	3:B:518:LEU:H	1.58	0.68
1:I:128:PRO:HB3	1:I:154:TYR:HB3	1.76	0.67
3:A:393:THR:C	3:A:523:THR:HG21	2.19	0.67
1:H:19:LYS:HG3	1:H:82:GLU:HB2	1.76	0.66
1:I:126:LYS:NZ	1:I:153:ASP:HB3	2.10	0.66
2:L:196:SER:OG	2:L:208:LYS:O	2.10	0.66
1:H:201:GLN:HG3	1:H:202:THR:H	1.60	0.66
2:L:10:VAL:HG23	2:L:107:LEU:HD12	1.77	0.65
3:A:393:THR:O	3:A:523:THR:CB	2.45	0.65
3:B:364:ASP:OD2	3:B:388:ASN:ND2	2.30	0.65
3:B:393:THR:CG2	3:B:518:LEU:H	2.09	0.65
1:H:204:ILE:HG22	1:H:219:LYS:HB2	1.79	0.64
3:B:336:CYS:HB3	3:B:337:PRO:HD3	0.67	0.64
3:A:359:SER:CB	3:A:394:ASN:ND2	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:163:VAL:HG22	2:K:182:LEU:HD13	1.80	0.62
3:B:408:ARG:HH11	3:B:408:ARG:HG3	1.64	0.62
1:I:132:PRO:HD3	1:I:218:LYS:HZ2	1.64	0.62
1:H:13:LYS:NZ	1:H:123:ALA:O	2.32	0.62
3:A:335:LEU:HA	3:A:361:CYS:HB2	1.81	0.62
3:B:358:ILE:HG21	3:B:395:VAL:HG23	1.81	0.61
3:B:366:SER:HA	3:B:369:TYR:HB3	1.82	0.61
2:K:47:LYS:HD3	2:K:49:MET:SD	2.41	0.61
1:H:150:LEU:HD21	1:H:152:LYS:HB2	1.83	0.61
3:B:385:THR:C	3:B:387:LEU:H	2.07	0.60
2:K:126:SER:O	2:K:130:GLN:HB2	2.01	0.60
3:B:385:THR:OG1	3:B:388:ASN:OD1	2.20	0.60
1:I:16:ALA:C	1:I:86:LEU:HD12	2.27	0.60
3:A:388:ASN:HB3	3:A:527:PRO:HD2	1.84	0.60
2:L:1:SER:O	2:L:1:SER:OG	2.11	0.59
2:K:39:GLN:HB2	2:K:88:TYR:CE2	2.37	0.59
2:K:150:VAL:HG12	2:K:199:VAL:HG12	1.83	0.59
3:A:361:CYS:O	3:A:524:VAL:HA	2.01	0.59
3:A:403:ARG:HG2	3:A:495:TYR:CE1	2.37	0.59
3:A:410:ILE:HD13	3:A:510:VAL:HG11	1.84	0.59
1:I:215:LYS:H	1:I:215:LYS:HD3	1.68	0.59
2:K:123:PRO:HA	2:K:136:LEU:HD23	1.85	0.59
3:A:393:THR:O	3:A:523:THR:OG1	2.21	0.58
3:A:402:ILE:CD1	3:A:410:ILE:HD11	2.33	0.58
1:H:150:LEU:CD2	1:H:152:LYS:HB2	2.34	0.58
2:L:126:SER:O	2:L:130:GLN:HG3	2.04	0.58
1:I:209:HIS:HB3	1:I:214:THR:HG23	1.84	0.58
1:I:150:LEU:HD21	1:I:152:LYS:HB2	1.85	0.58
2:K:171:GLN:HG3	2:K:172:SER:H	1.68	0.57
1:H:150:LEU:HD12	2:L:137:VAL:HG11	1.85	0.57
3:A:523:THR:CG2	3:A:524:VAL:HG23	2.21	0.57
2:K:129:LEU:HD21	2:K:189:TRP:CD1	2.40	0.57
1:I:218:LYS:HZ3	1:I:218:LYS:HB3	1.69	0.57
1:I:130:VAL:HG11	1:I:216:VAL:HG21	1.87	0.56
2:L:32:TYR:O	2:L:68:LYS:NZ	2.39	0.56
1:I:202:THR:HA	1:I:219:LYS:HE3	1.87	0.56
3:B:358:ILE:HB	3:B:395:VAL:HG23	1.87	0.56
3:B:394:ASN:O	3:B:516:GLU:CB	2.51	0.56
3:B:343:ASN:CG	6:B:601:NAG:C1	2.79	0.56
3:B:358:ILE:CB	3:B:395:VAL:HG23	2.36	0.56
2:K:140:ILE:HG12	2:K:199:VAL:HG11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:381:GLY:HA3	3:B:430:THR:HG23	1.87	0.55
1:H:88:SER:HA	1:H:120:VAL:HG13	1.89	0.55
3:A:403:ARG:NH2	3:A:405:ASP:HB2	2.22	0.55
2:L:52:ASP:HB2	2:L:55:ASN:HD22	1.70	0.55
1:I:193:VAL:HG21	1:I:203:TYR:HE1	1.71	0.55
2:L:190:LYS:HG2	2:L:212:PRO:HB3	1.90	0.54
3:B:364:ASP:O	3:B:367:VAL:HG12	2.08	0.54
1:H:164:ASN:HB2	1:H:168:LEU:HB2	1.90	0.54
3:A:371:SER:C	3:A:373:SER:H	2.15	0.54
1:I:172:VAL:HG22	1:I:191:VAL:HG22	1.89	0.53
2:K:128:GLU:OE2	2:K:135:THR:HG23	2.08	0.53
3:A:365:TYR:O	3:A:368:LEU:HB2	2.08	0.53
2:L:171:GLN:HG3	2:L:172:SER:H	1.74	0.53
2:K:57:PRO:HD2	2:K:60:VAL:HG21	1.91	0.52
3:B:366:SER:O	3:B:370:ASN:HB2	2.09	0.52
1:H:163:TRP:CH2	1:H:205:CYS:HB3	2.43	0.52
2:L:62:ASN:N	2:L:62:ASN:OD1	2.41	0.52
2:K:85:GLU:HA	2:K:107:LEU:O	2.08	0.52
3:B:480:CYS:O	3:B:483:VAL:HG22	2.10	0.52
3:B:353:TRP:O	3:B:466:ARG:NH2	2.42	0.52
3:B:338:PHE:N	3:B:338:PHE:CD1	2.77	0.52
1:H:16:ALA:O	1:H:86:LEU:HD22	2.09	0.52
1:H:16:ALA:O	1:H:86:LEU:CD2	2.58	0.52
1:H:133:LEU:HD21	1:H:150:LEU:HB2	1.91	0.52
2:L:123:PRO:HA	2:L:136:LEU:HD13	1.91	0.51
1:I:104:TRP:CZ3	2:K:97:SER:HB3	2.45	0.51
3:B:336:CYS:CB	3:B:337:PRO:CD	2.37	0.51
3:B:403:ARG:HG2	3:B:505:TYR:HA	1.92	0.51
3:B:393:THR:OG1	3:B:394:ASN:N	2.43	0.51
2:K:28:ASP:HB3	2:K:94:THR:HG22	1.91	0.51
1:H:137:SER:O	1:H:137:SER:OG	2.29	0.51
1:H:193:VAL:HG12	1:H:197:SER:HB2	1.93	0.51
2:L:39:GLN:HB2	2:L:88:TYR:CE2	2.45	0.50
1:I:36:TRP:HB3	1:I:48:MET:HE3	1.93	0.50
3:A:523:THR:HG22	3:A:524:VAL:N	1.96	0.50
2:K:52:ASP:HB2	2:K:55:ASN:HD22	1.77	0.50
2:K:155:ASP:CB	2:K:193:ARG:CD	2.81	0.50
1:H:132:PRO:HB2	1:H:220:VAL:HG13	1.94	0.50
1:I:193:VAL:HG21	1:I:203:TYR:CE1	2.47	0.50
1:H:128:PRO:HB3	1:H:154:TYR:HB3	1.94	0.49
1:H:33:TYR:OH	3:A:484:GLU:OE2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:LYS:HG3	1:I:82:GLU:HB2	1.94	0.49
3:A:354:ASN:O	3:A:398:ASP:HA	2.13	0.49
1:H:87:ARG:O	1:H:120:VAL:HG11	2.12	0.49
3:A:347:PHE:HB3	3:A:401:VAL:HG23	1.94	0.49
3:B:498:GLN:HG3	3:B:501:ASN:OD1	2.11	0.49
1:I:150:LEU:CD2	1:I:152:LYS:HB2	2.42	0.49
3:A:359:SER:OG	3:A:394:ASN:ND2	2.46	0.49
3:B:408:ARG:HH11	3:B:408:ARG:CG	2.26	0.49
3:A:356:LYS:HE3	3:A:358:ILE:HG23	1.94	0.48
1:I:49:GLY:CA	1:I:70:MET:HE1	2.43	0.48
1:H:187:LEU:HD23	1:H:188:SER:N	2.28	0.48
3:A:371:SER:HB3	3:A:374:PHE:HB2	1.93	0.48
3:B:392:PHE:H	3:B:524:VAL:HG13	1.78	0.48
1:H:104:TRP:CZ3	2:L:97:SER:HB3	2.48	0.48
1:H:221:GLU:OE1	1:H:221:GLU:N	2.46	0.48
2:K:26:SER:O	2:K:31:VAL:HG13	2.14	0.48
3:B:341:VAL:HG13	3:B:342:PHE:CD2	2.48	0.48
2:L:117:PRO:HA	2:L:143:PHE:HB3	1.95	0.48
3:A:357:ARG:HG3	3:A:396:TYR:CE1	2.49	0.47
3:B:358:ILE:HG21	3:B:395:VAL:CG2	2.44	0.47
3:A:339:GLY:O	3:A:343:ASN:HB2	2.14	0.47
2:K:6:GLN:NE2	2:K:88:TYR:O	2.44	0.47
2:K:199:VAL:CG2	2:K:206:VAL:HB	2.45	0.47
3:A:520:ALA:HB1	3:A:521:PRO:CD	2.44	0.47
3:B:363:ALA:N	3:B:525:CYS:O	2.38	0.47
2:L:148:VAL:HG12	2:L:201:HIS:HB2	1.97	0.47
3:A:498:GLN:HG3	3:A:501:ASN:OD1	2.15	0.47
3:B:382:VAL:HG21	3:B:515:PHE:HE2	1.80	0.47
3:A:335:LEU:HB3	3:A:362:VAL:CG1	2.32	0.47
2:L:138:CYS:HB2	2:L:152:TRP:CZ2	2.50	0.46
2:K:18:ILE:CD1	2:K:77:ILE:HG13	2.46	0.46
2:K:114:LYS:HD2	2:K:114:LYS:N	2.30	0.46
1:I:209:HIS:HB3	1:I:214:THR:CG2	2.45	0.46
1:I:218:LYS:HB3	1:I:218:LYS:NZ	2.30	0.46
2:K:80:LEU:HD23	2:K:80:LEU:HA	1.68	0.46
2:K:165:THR:HG22	2:K:180:SER:OG	2.15	0.46
2:K:64:PHE:CE2	2:K:77:ILE:HD13	2.50	0.46
3:A:403:ARG:HG3	3:A:406:GLU:HG3	1.97	0.46
2:L:185:THR:OG1	2:L:188:GLN:HG3	2.16	0.46
1:I:47:TRP:CZ2	1:I:49:GLY:HA2	2.51	0.46
3:A:393:THR:O	3:A:523:THR:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:428:ASP:OD1	3:A:428:ASP:N	2.39	0.46
3:B:340:GLU:OE1	3:B:340:GLU:HA	2.15	0.46
1:I:133:LEU:HD11	1:I:150:LEU:HB2	1.96	0.46
1:I:133:LEU:HD12	1:I:133:LEU:N	2.31	0.46
3:B:438:SER:O	3:B:438:SER:OG	2.33	0.46
1:H:38:ARG:HB3	1:H:48:MET:SD	2.56	0.45
2:L:2:TYR:OH	2:L:25:THR:HG23	2.16	0.45
3:B:430:THR:O	3:B:515:PHE:HB2	2.16	0.45
1:H:150:LEU:C	1:H:150:LEU:HD23	2.40	0.45
2:L:17:SER:HA	2:L:77:ILE:O	2.15	0.45
2:L:117:PRO:HD3	2:L:201:HIS:ND1	2.32	0.45
3:B:343:ASN:ND2	6:B:601:NAG:C1	2.80	0.45
3:A:359:SER:HB3	3:A:394:ASN:ND2	2.19	0.45
1:I:152:LYS:HA	1:I:186:SER:HB3	1.99	0.45
3:A:395:VAL:HG23	3:A:395:VAL:O	2.16	0.45
3:B:392:PHE:HD1	3:B:517:LEU:HD12	1.82	0.45
1:H:156:PRO:O	1:H:209:HIS:NE2	2.43	0.44
1:I:132:PRO:CD	1:I:218:LYS:HZ2	2.27	0.44
2:L:85:GLU:HG2	2:L:108:THR:HA	1.99	0.44
2:L:201:HIS:O	2:L:202:GLU:HB2	2.16	0.44
2:K:199:VAL:HG23	2:K:206:VAL:HB	2.00	0.44
3:A:338:PHE:HA	3:A:341:VAL:HG12	1.99	0.44
3:B:395:VAL:HA	3:B:514:SER:O	2.18	0.44
3:B:385:THR:C	3:B:387:LEU:N	2.75	0.44
1:I:37:VAL:HG23	1:I:46:GLU:O	2.18	0.43
2:K:198:GLN:OE1	2:K:207:GLU:HA	2.18	0.43
1:H:130:VAL:HA	1:H:150:LEU:O	2.18	0.43
1:I:48:MET:SD	1:I:81:MET:HE3	2.58	0.43
1:I:168:LEU:HD12	1:I:168:LEU:HA	1.59	0.43
3:A:369:TYR:CE2	3:A:384:PRO:HB2	2.53	0.43
3:A:403:ARG:HH21	3:A:405:ASP:HB2	1.84	0.43
1:H:144:THR:OG1	1:H:145:ALA:N	2.49	0.43
2:L:31:VAL:HG13	2:L:32:TYR:CD1	2.53	0.43
3:B:358:ILE:CG2	3:B:395:VAL:CG2	2.96	0.43
3:B:365:TYR:CD1	3:B:387:LEU:HB2	2.53	0.43
1:H:97:ALA:HB1	1:H:109:CYS:HB3	2.00	0.43
2:K:124:PRO:HD3	2:K:136:LEU:HD23	2.00	0.43
1:H:193:VAL:HG13	1:H:194:PRO:HD2	2.01	0.43
3:B:341:VAL:HG13	3:B:342:PHE:HD2	1.83	0.43
1:H:212:SER:O	1:H:213:ASN:HB2	2.19	0.43
1:H:59:LYS:HD3	2:L:98:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:126:LYS:HZ1	1:I:153:ASP:CB	2.17	0.43
1:I:133:LEU:HD11	1:I:150:LEU:CB	2.49	0.43
2:L:7:PRO:O	2:L:105:THR:OG1	2.31	0.42
2:K:193:ARG:CD	2:K:193:ARG:N	2.74	0.42
1:I:133:LEU:HD23	2:K:122:PHE:CB	2.49	0.42
1:I:159:VAL:HG12	1:I:209:HIS:HB2	2.01	0.42
1:H:36:TRP:CE2	1:H:81:MET:HB2	2.53	0.42
2:L:138:CYS:C	2:L:139:LEU:HD23	2.45	0.42
3:B:398:ASP:O	3:B:511:VAL:HA	2.19	0.42
3:B:452:LEU:HD22	3:B:494:SER:HB2	2.00	0.42
2:L:122:PHE:HB2	2:L:137:VAL:CG2	2.47	0.42
2:L:80:LEU:HD12	2:L:80:LEU:HA	1.79	0.42
3:A:394:ASN:HD22	3:A:394:ASN:HA	1.61	0.42
3:B:383:SER:HB3	3:B:384:PRO:HD2	2.01	0.42
1:I:48:MET:HE1	1:I:94:TYR:HD2	1.83	0.42
1:I:126:LYS:HZ3	1:I:184:LEU:HD22	1.84	0.42
3:B:347:PHE:HB3	3:B:401:VAL:HG23	2.02	0.42
3:B:408:ARG:CG	3:B:408:ARG:NH1	2.83	0.42
1:H:163:TRP:CZ3	1:H:205:CYS:HB3	2.55	0.42
3:A:452:LEU:HD23	3:A:494:SER:HB2	2.02	0.42
2:L:6:GLN:NE2	2:L:88:TYR:O	2.45	0.42
3:B:356:LYS:HD2	3:B:356:LYS:HA	1.82	0.42
2:K:19:THR:HG22	2:K:76:THR:HG23	2.02	0.41
3:A:369:TYR:CD2	3:A:384:PRO:HB2	2.55	0.41
2:L:28:ASP:OD1	2:L:29:VAL:N	2.45	0.41
1:I:68:VAL:HG12	1:I:83:VAL:HG22	2.00	0.41
1:I:128:PRO:HA	1:I:153:ASP:O	2.20	0.41
1:H:164:ASN:OD1	1:H:203:TYR:HA	2.21	0.41
2:L:186:PRO:HA	2:L:189:TRP:HB3	2.02	0.41
1:I:91:THR:HG23	1:I:119:THR:HA	2.01	0.41
2:K:201:HIS:C	2:K:203:GLY:H	2.29	0.41
3:A:386:LYS:O	3:A:386:LYS:HG3	2.19	0.41
1:I:49:GLY:C	1:I:70:MET:HE1	2.46	0.41
1:I:178:VAL:HG12	2:K:166:THR:HG23	2.02	0.41
3:A:383:SER:O	3:A:387:LEU:HD23	2.21	0.41
2:L:56:ARG:HD3	2:L:64:PHE:O	2.21	0.41
3:A:452:LEU:CD2	3:A:494:SER:HB2	2.51	0.41
3:A:357:ARG:NE	3:A:394:ASN:OD1	2.54	0.40
2:L:18:ILE:HD13	2:L:107:LEU:HD13	2.02	0.40
3:B:390:LEU:HD12	3:B:390:LEU:HA	1.70	0.40
1:H:12:LYS:O	1:H:120:VAL:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:25:THR:OG1	2:K:26:SER:N	2.54	0.40
3:A:394:ASN:N	3:A:523:THR:HG21	2.37	0.40
3:B:337:PRO:HG2	3:B:338:PHE:CD1	2.57	0.40

All (6) 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)
3:A:519:HIS:CE1	3:A:519:HIS:NE2[4_465]	1.32	0.88
3:A:519:HIS:ND1	3:A:519:HIS:CE1[4_465]	1.32	0.88
3:A:519:HIS:NE2	3:A:519:HIS:NE2[4_465]	1.50	0.70
1:I:201:GLN:OE1	3:B:378:LYS:NZ[6_554]	1.80	0.40
3:A:519:HIS:ND1	3:A:519:HIS:ND1[4_465]	1.83	0.37
1:H:215:LYS:N	3:A:370:ASN:ND2[6_554]	1.96	0.24

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	H	215/234 (92%)	203 (94%)	11 (5%)	1 (0%)	24	54
1	I	215/234 (92%)	205 (95%)	8 (4%)	2 (1%)	14	41
2	K	211/216 (98%)	196 (93%)	14 (7%)	1 (0%)	24	54
2	L	211/216 (98%)	200 (95%)	10 (5%)	1 (0%)	24	54
3	A	194/231 (84%)	181 (93%)	9 (5%)	4 (2%)	5	21
3	B	179/231 (78%)	163 (91%)	14 (8%)	2 (1%)	11	36
All	All	1225/1362 (90%)	1148 (94%)	66 (5%)	11 (1%)	14	41

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	195	SER
3	A	371	SER
3	A	520	ALA
3	B	337	PRO
1	I	197	SER
3	A	523	THR
3	B	339	GLY
2	L	114	LYS
2	K	114	LYS
1	I	153	ASP
3	A	521	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	183/198 (92%)	180 (98%)	3 (2%)	55	83
1	I	184/198 (93%)	179 (97%)	5 (3%)	39	73
2	K	179/184 (97%)	177 (99%)	2 (1%)	65	88
2	L	181/184 (98%)	178 (98%)	3 (2%)	53	82
3	A	169/203 (83%)	162 (96%)	7 (4%)	27	61
3	B	160/203 (79%)	156 (98%)	4 (2%)	42	74
All	All	1056/1170 (90%)	1032 (98%)	24 (2%)	45	76

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	181	SER
1	H	182	SER
1	H	184	LEU
2	L	1	SER
2	L	80	LEU
2	L	193	ARG
1	I	17	SER
1	I	181	SER

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Mol	Chain	Res	Type
1	I	193	VAL
1	I	195	SER
1	I	201	GLN
2	K	77	ILE
2	K	80	LEU
3	A	371	SER
3	A	393	THR
3	A	394	ASN
3	A	402	ILE
3	A	477[A]	SER
3	A	477[B]	SER
3	A	523	THR
3	B	336	CYS
3	B	338	PHE
3	B	340	GLU
3	B	341	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	55	ASN
2	L	112	GLN
2	L	130	GLN
2	L	192	HIS
1	I	39	GLN
1	I	164	ASN
1	I	201	GLN
2	K	39	GLN
2	K	40	GLN
2	K	55	ASN
3	A	394	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	A	601	3	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	B	601	-	14,14,15	0.21	0	17,19,21	0.48	0
4	GOL	L	301	-	5,5,5	0.55	0	5,5,5	0.30	0
4	GOL	B	602	-	5,5,5	0.54	0	5,5,5	0.32	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
6	NAG	A	601	3	-	2/6/23/26	0/1/1/1
6	NAG	B	601	-	-	2/6/23/26	0/1/1/1
4	GOL	L	301	-	-	2/4/4/4	-
4	GOL	B	602	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	GOL	C1-C2-C3-O3
4	L	301	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	601	NAG	C4-C5-C6-O6
6	B	601	NAG	O5-C5-C6-O6
6	A	601	NAG	C4-C5-C6-O6
6	A	601	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	NAG	3	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	H	219/234 (93%)	0.55	21 (9%)	13 11	57, 80, 168, 190	0
1	I	219/234 (93%)	0.51	12 (5%)	30 24	59, 87, 149, 162	0
2	K	213/216 (98%)	0.73	19 (8%)	15 13	54, 95, 140, 155	0
2	L	213/216 (98%)	0.62	12 (5%)	30 23	53, 92, 141, 160	0
3	A	194/231 (83%)	0.90	24 (12%)	8 7	51, 103, 169, 222	2 (1%)
3	B	183/231 (79%)	1.03	28 (15%)	5 4	46, 101, 168, 186	2 (1%)
All	All	1241/1362 (91%)	0.71	116 (9%)	14 12	46, 95, 158, 222	4 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	168	LEU	6.0
3	B	338	PHE	4.9
3	B	392	PHE	4.7
3	B	524	VAL	4.7
3	B	361	CYS	4.5
3	B	341	VAL	4.3
3	B	362	VAL	4.2
3	B	518	LEU	4.1
3	A	517	LEU	4.1
2	L	161	ALA	4.0
3	A	515	PHE	3.8
3	B	384	PRO	3.8
1	H	224	SER	3.7
3	A	521	PRO	3.7
3	B	365	TYR	3.7
2	K	171	GLN	3.7
2	K	203	GLY	3.7
1	I	136	SER	3.6
2	L	196	SER	3.6

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Mol	Chain	Res	Type	RSRZ
3	A	371	SER	3.4
1	H	192	THR	3.4
3	A	334	ASN	3.4
2	L	187	GLU	3.4
3	B	525	CYS	3.4
3	A	390	LEU	3.4
1	H	197	SER	3.4
2	K	194	SER	3.3
3	A	514	SER	3.2
3	A	392	PHE	3.2
2	L	1	SER	3.1
3	B	517	LEU	3.1
1	H	137	SER	3.1
1	H	105	ASN	3.1
1	H	173	HIS	3.0
1	H	198	LEU	3.0
3	B	390	LEU	3.0
1	H	200	THR	3.0
3	B	342	PHE	3.0
3	B	432	CYS	2.9
1	I	137	SER	2.9
3	A	350	VAL	2.9
3	B	515	PHE	2.9
3	B	513	LEU	2.9
2	K	142	ASP	2.8
3	A	337	PRO	2.8
3	A	520	ALA	2.8
1	H	125	THR	2.8
1	H	165	SER	2.8
3	A	365	TYR	2.8
2	K	213	THR	2.8
1	H	169	THR	2.7
2	K	191	SER	2.7
3	A	518	LEU	2.7
3	A	522	ALA	2.7
1	I	173	HIS	2.6
1	H	223	LYS	2.6
1	H	166	GLY	2.6
3	A	527	PRO	2.6
3	B	367	VAL	2.6
1	H	170	SER	2.5
2	L	171	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	345	THR	2.5
3	B	514	SER	2.5
3	B	391	CYS	2.5
1	I	222	PRO	2.5
3	B	336	CYS	2.5
3	A	384	PRO	2.4
1	I	143	GLY	2.4
2	L	186	PRO	2.4
1	H	176	PRO	2.4
2	K	113	PRO	2.4
1	H	136	SER	2.3
1	H	202	THR	2.3
3	A	385	THR	2.3
1	I	198	LEU	2.3
3	A	344	ALA	2.3
2	L	142	ASP	2.3
2	K	192	HIS	2.3
3	B	358	ILE	2.3
2	K	108	THR	2.3
3	B	470	THR	2.3
2	L	117	PRO	2.3
2	L	200	THR	2.2
2	K	120	THR	2.2
1	I	163	TRP	2.2
3	B	337	PRO	2.2
2	K	196	SER	2.2
2	K	164	GLU	2.2
3	A	387	LEU	2.2
3	B	368	LEU	2.2
1	I	105	ASN	2.2
1	I	128	PRO	2.2
1	H	187	LEU	2.2
1	I	145	ALA	2.2
2	K	187	GLU	2.2
2	K	2	TYR	2.1
3	B	464	PHE	2.1
1	I	167	ALA	2.1
2	K	207	GLU	2.1
2	K	132	ASN	2.1
1	H	222	PRO	2.1
3	A	513	LEU	2.1
2	K	200	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	364	ASP	2.1
1	H	217	ASP	2.0
3	B	363	ALA	2.0
2	L	192	HIS	2.0
3	A	391	CYS	2.0
3	A	480	CYS	2.0
3	B	480	CYS	2.0
2	K	122	PHE	2.0
2	K	205	THR	2.0
1	H	89	ASP	2.0
3	A	516	GLU	2.0
2	L	119	VAL	2.0
2	L	159	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	L	301	6/6	0.57	0.27	140,140,140,140	0
6	NAG	B	601	14/15	0.76	0.16	134,148,153,156	0
6	NAG	A	601	14/15	0.78	0.12	127,132,139,144	0
4	GOL	B	602	6/6	0.83	0.13	113,113,113,113	0
5	ZN	L	302	1/1	0.91	0.10	147,147,147,147	0
5	ZN	K	301	1/1	0.94	0.09	144,144,144,144	0

6.5 Other polymers [i](#)

There are no such residues in this entry.