



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:21 AM EDT

PDB ID : 5Y2M / pdb_00005y2m
Title : Crystal structure of a group 2 HA binding antibody AF4H1K1 Fab in complex with the H4N6 duck isolate (H4-CZ/56) hemagglutinin
Authors : Xiao, H.; Qi, J.; Gao, F.G.
Deposited on : 2017-07-26
Resolution : 3.80 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

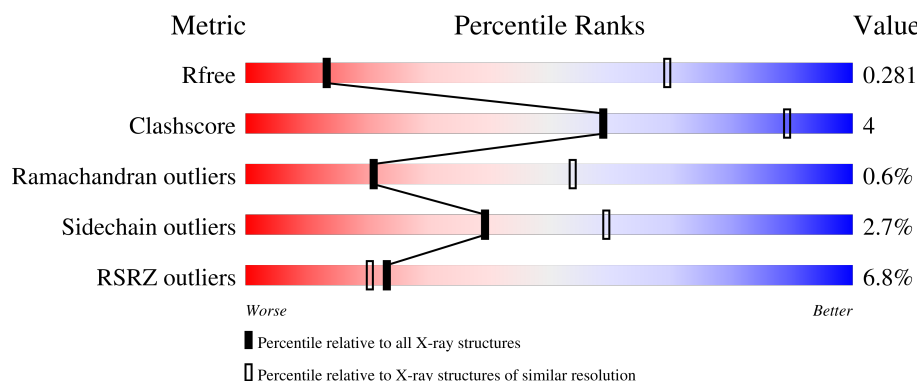
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	327	2% 87% 9% ..
1	B	327	% 86% 11% ..
1	C	327	2% 84% 12% ..
2	D	176	9% 88% 9% ..
2	E	176	11% 88% 10% ..

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Mol	Chain	Length	Quality of chain
2	F	176	12% 90% 7%
3	I	233	12% 76% 20%
3	K	233	15% 74% 21%
4	J	220	5% 80% 15%
4	L	220	8% 79% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18315 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2457	1538	437	470	12			
1	B	319	Total	C	N	O	S	0	0	0
			2457	1538	437	470	12			
1	C	319	Total	C	N	O	S	0	0	0
			2457	1538	437	470	12			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	172	Total	C	N	O	S	0	0	0
			1404	871	250	279	4			
2	E	172	Total	C	N	O	S	0	0	0
			1404	871	250	279	4			
2	F	172	Total	C	N	O	S	0	0	0
			1404	871	250	279	4			

- Molecule 3 is a protein called a group 2 HA binding antibody AF4H1K1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	224	Total	C	N	O	S	0	0	0
			1694	1077	286	325	6			
3	K	224	Total	C	N	O	S	0	0	0
			1694	1077	286	325	6			

- Molecule 4 is a protein called a group 2 HA binding antibody AF4H1K1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	212	Total	C	N	O	S	0	0	0
			1630	1018	278	329	5			
4	L	212	Total	C	N	O	S	0	0	0
			1630	1018	278	329	5			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

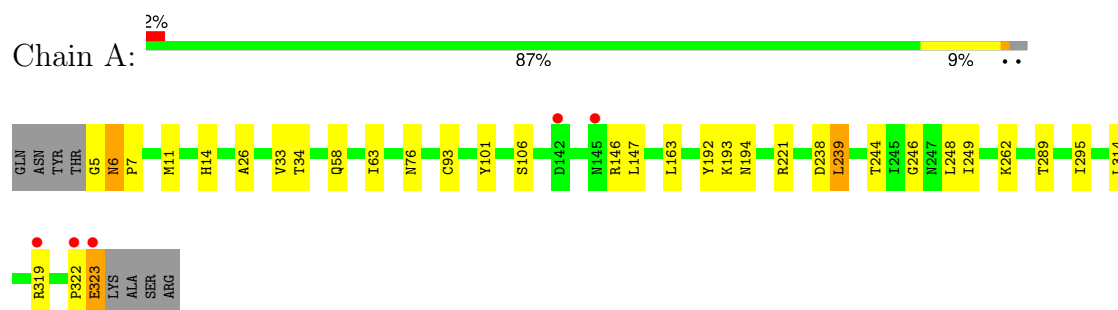


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

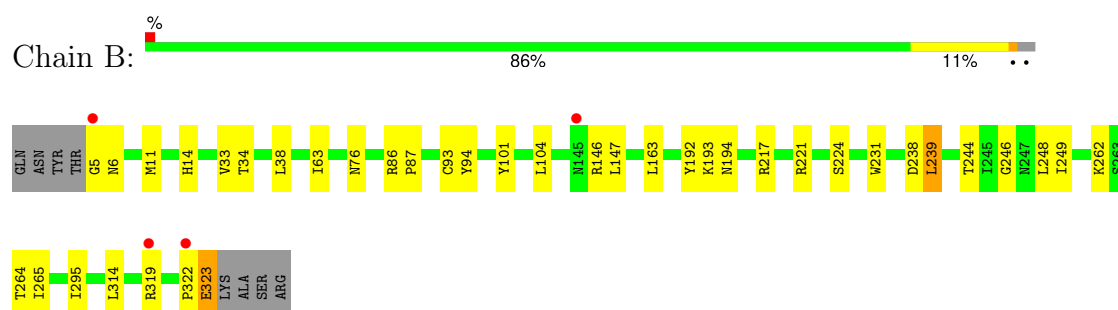
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

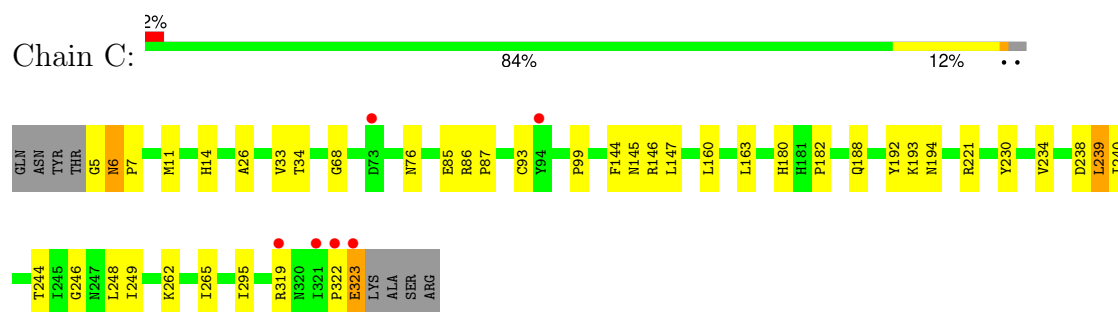
• Molecule 1: Hemagglutinin



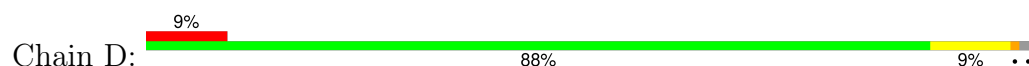
• Molecule 1: Hemagglutinin

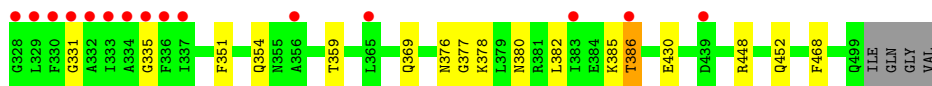


• Molecule 1: Hemagglutinin

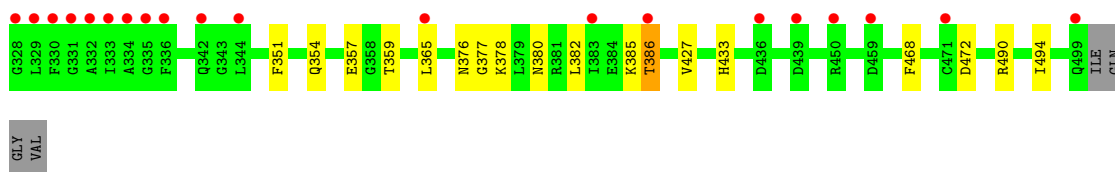
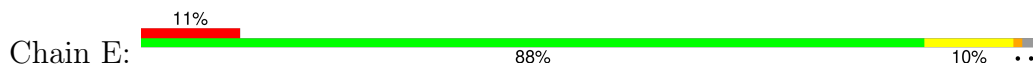


• Molecule 2: Hemagglutinin

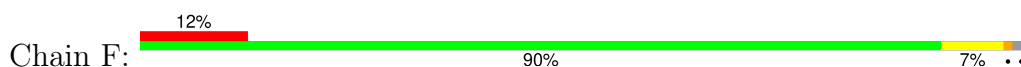




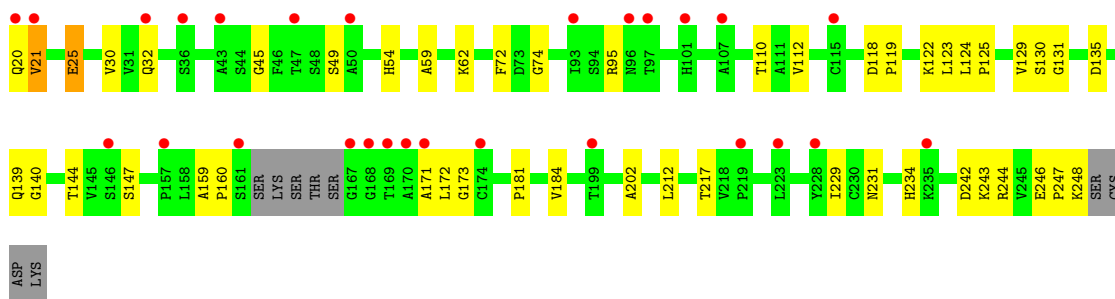
• Molecule 2: Hemagglutinin



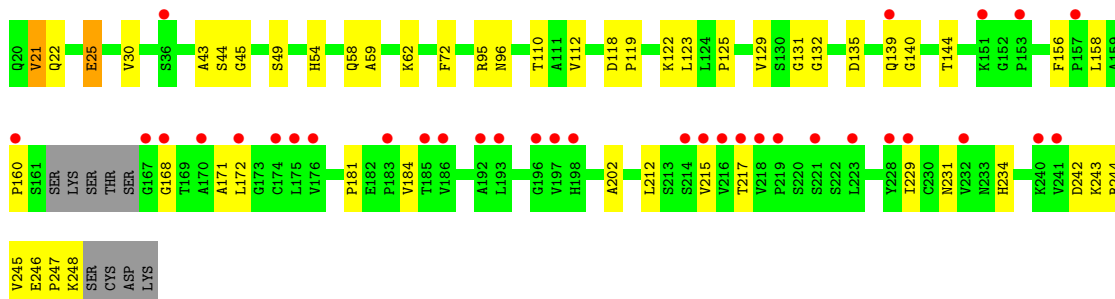
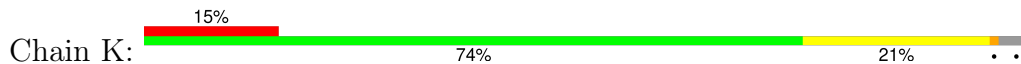
• Molecule 2: Hemagglutinin



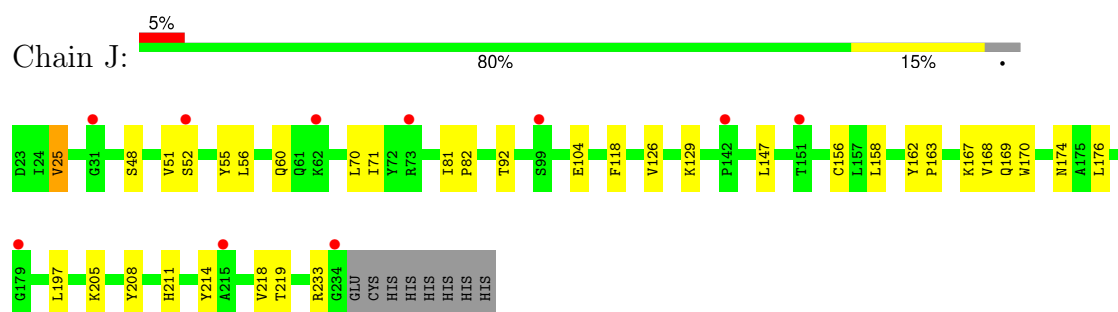
• Molecule 3: a group 2 HA binding antibody AF4H1K1 Fab heavy chain



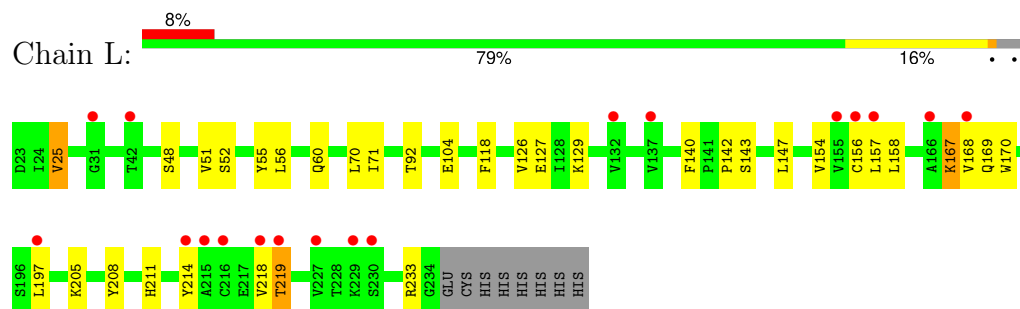
• Molecule 3: a group 2 HA binding antibody AF4H1K1 Fab heavy chain



• Molecule 4: a group 2 HA binding antibody AF4H1K1 Fab light chain



- Molecule 4: a group 2 HA binding antibody AF4H1K1 Fab 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	114.17Å 140.94Å 138.10Å 90.00° 95.31° 90.00°	Depositor
Resolution (Å)	49.21 – 3.80 49.21 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.21-3.80) 99.8 (49.21-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.235 , 0.277 0.243 , 0.281	Depositor DCC
R_{free} test set	2168 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	18315	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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	0.30	0/2511	0.76	1/3418 (0.0%)
1	B	0.31	0/2511	0.75	0/3418
1	C	0.29	0/2511	0.74	0/3418
2	D	0.32	0/1428	0.72	1/1922 (0.1%)
2	E	0.31	0/1428	0.71	1/1922 (0.1%)
2	F	0.33	0/1428	0.73	1/1922 (0.1%)
3	I	0.32	0/1739	0.76	4/2372 (0.2%)
3	K	0.32	0/1739	0.73	2/2372 (0.1%)
4	J	0.30	0/1665	0.73	0/2258
4	L	0.32	0/1665	0.72	0/2258
All	All	0.31	0/18625	0.74	10/25280 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	246	GLU	CA-C-N	6.14	127.51	119.84
3	I	246	GLU	C-N-CA	6.14	127.51	119.84
3	K	246	GLU	CA-C-N	6.04	127.39	119.84
3	K	246	GLU	C-N-CA	6.04	127.39	119.84
2	D	386	THR	N-CA-C	5.50	117.14	111.03
2	F	386	THR	N-CA-C	5.43	117.06	111.03
2	E	386	THR	N-CA-C	5.33	116.95	111.03
3	I	173	GLY	N-CA-C	5.16	118.08	110.80
1	A	58	GLN	CB-CA-C	-5.08	110.32	117.23
3	I	74	GLY	N-CA-C	-5.06	108.27	115.30

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	2457	0	2402	19	0
1	B	2457	0	2402	23	0
1	C	2457	0	2402	22	0
2	D	1404	0	1320	14	0
2	E	1404	0	1320	14	0
2	F	1404	0	1320	9	0
3	I	1694	0	1644	25	0
3	K	1694	0	1644	27	0
4	J	1630	0	1581	14	0
4	L	1630	0	1581	18	0
5	A	28	0	26	0	0
5	B	28	0	26	0	0
5	C	28	0	26	0	0
All	All	18315	0	17694	159	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 4.

All (159) 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)
1:B:244:THR:HG22	1:B:246:GLY:H	1.37	0.89
1:A:244:THR:HG22	1:A:246:GLY:H	1.40	0.86
1:C:244:THR:HG22	1:C:246:GLY:H	1.40	0.86
3:I:229:ILE:HG12	3:I:244:ARG:HG3	1.69	0.74
1:B:5:GLY:HA2	2:E:468:PHE:HA	1.68	0.74
1:C:5:GLY:HA2	2:F:468:PHE:HA	1.71	0.72
1:A:5:GLY:HA2	2:D:468:PHE:HA	1.72	0.70
4:L:211:HIS:O	4:L:233:ARG:NH2	2.26	0.69
3:K:229:ILE:HG12	3:K:244:ARG:HG3	1.75	0.68
4:J:211:HIS:O	4:J:233:ARG:NH2	2.27	0.66
4:L:60:GLN:HB2	4:L:70:LEU:HD11	1.78	0.66
1:C:322:PRO:O	1:C:323:GLU:HB2	1.95	0.66
1:B:322:PRO:O	1:B:323:GLU:HB2	1.95	0.66
3:K:231:ASN:ND2	3:K:242:ASP:OD1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:PRO:O	1:A:323:GLU:HB2	1.95	0.65
3:K:202:ALA:HB2	3:K:212:LEU:HD23	1.80	0.64
4:J:60:GLN:HB2	4:J:70:LEU:HD11	1.80	0.63
3:K:160:PRO:HG3	3:K:172:LEU:HB3	1.80	0.63
3:I:160:PRO:HG3	3:I:172:LEU:HB3	1.79	0.63
2:E:376:ASN:OD1	3:K:123:LEU:HB3	2.00	0.61
4:J:25:VAL:HG22	4:J:48:SER:HB2	1.83	0.61
2:E:354:GLN:HG3	2:E:359:THR:HG22	1.82	0.61
3:I:125:PRO:HD2	3:I:129:VAL:HG21	1.84	0.60
1:A:93:CYS:O	1:A:221:ARG:NH1	2.35	0.60
3:K:30:VAL:HG21	3:K:181:PRO:HG3	1.82	0.59
3:I:231:ASN:ND2	3:I:242:ASP:OD1	2.33	0.59
3:I:30:VAL:HG21	3:I:181:PRO:HG3	1.84	0.58
3:I:202:ALA:HB2	3:I:212:LEU:HD23	1.85	0.58
4:L:25:VAL:HG22	4:L:48:SER:HB2	1.86	0.58
2:D:354:GLN:HG3	2:D:359:THR:HG22	1.86	0.58
1:B:93:CYS:O	1:B:221:ARG:NH1	2.36	0.57
4:L:25:VAL:H	4:L:48:SER:HB3	1.70	0.57
1:C:33:VAL:HG12	1:C:34:THR:HG23	1.86	0.57
3:I:119:PRO:HD3	3:I:135:ASP:HB2	1.87	0.56
1:C:76:ASN:OD1	1:C:146:ARG:NH2	2.37	0.56
3:K:119:PRO:HD3	3:K:135:ASP:HB2	1.86	0.56
3:K:125:PRO:HD2	3:K:129:VAL:HG21	1.87	0.56
2:D:377:GLY:HA3	1:C:26:ALA:O	2.07	0.55
3:I:49:SER:O	3:I:72:PHE:HB2	2.07	0.55
2:F:354:GLN:HG3	2:F:359:THR:HG22	1.89	0.55
3:K:25:GLU:OE1	3:K:140:GLY:N	2.31	0.54
3:K:172:LEU:HB2	3:K:245:VAL:HG11	1.87	0.54
1:A:192:TYR:O	1:A:194:ASN:N	2.40	0.54
2:E:385:LYS:HD2	2:E:386:THR:N	2.23	0.54
3:K:158:LEU:HB3	4:L:140:PHE:CG	2.43	0.54
3:K:171:ALA:HB2	3:K:217:THR:HG22	1.89	0.54
1:A:26:ALA:O	2:E:377:GLY:HA3	2.08	0.53
3:I:171:ALA:HB2	3:I:217:THR:HG22	1.90	0.53
1:B:319:ARG:HG2	1:B:319:ARG:HH11	1.73	0.53
2:F:385:LYS:HD2	2:F:386:THR:N	2.24	0.53
1:B:33:VAL:HG12	1:B:34:THR:HG23	1.90	0.53
1:A:147:LEU:HD12	1:A:249:ILE:HG22	1.91	0.52
1:A:11:MET:HE1	2:D:351:PHE:CE2	2.44	0.52
3:I:25:GLU:OE1	3:I:139:GLN:N	2.43	0.52
2:F:385:LYS:HD2	2:F:386:THR:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:HG12	1:A:34:THR:HG23	1.91	0.52
1:B:63:ILE:HG13	1:B:101:TYR:CZ	2.43	0.52
4:J:169:GLN:HG2	4:J:176:LEU:HD11	1.92	0.52
2:E:385:LYS:HD2	2:E:386:THR:H	1.75	0.52
4:J:25:VAL:H	4:J:48:SER:HB3	1.76	0.51
4:L:169:GLN:HG2	4:L:176:LEU:HD11	1.93	0.51
2:D:385:LYS:HD2	2:D:386:THR:N	2.26	0.51
1:C:93:CYS:O	1:C:221:ARG:NH1	2.43	0.51
2:D:385:LYS:HD2	2:D:386:THR:H	1.76	0.50
3:K:25:GLU:OE1	3:K:139:GLN:N	2.43	0.50
3:K:49:SER:O	3:K:72:PHE:HB2	2.10	0.50
1:B:192:TYR:O	1:B:194:ASN:N	2.44	0.50
1:C:319:ARG:HG2	1:C:319:ARG:HH11	1.75	0.50
3:K:21:VAL:HA	3:K:45:GLY:HA3	1.92	0.50
3:I:184:VAL:HG12	3:I:234:HIS:HB2	1.94	0.50
4:L:142:PRO:HD3	4:L:154:VAL:HG22	1.93	0.50
3:K:215:VAL:HG21	4:L:157:LEU:HD13	1.93	0.50
1:A:238:ASP:OD1	1:A:239:LEU:N	2.40	0.50
1:A:319:ARG:HH11	1:A:319:ARG:HG2	1.76	0.50
1:B:11:MET:HE1	2:E:351:PHE:CE2	2.47	0.49
1:A:76:ASN:OD1	1:A:146:ARG:NH2	2.45	0.49
2:D:369:GLN:NE2	3:I:130:SER:OG	2.45	0.49
1:C:192:TYR:O	1:C:194:ASN:N	2.45	0.49
3:K:43:ALA:O	3:K:96:ASN:ND2	2.45	0.49
2:E:380:ASN:OD1	3:K:122:LYS:HG3	2.12	0.49
4:L:147:LEU:O	4:L:205:LYS:HD2	2.13	0.49
3:K:22:GLN:N	3:K:44:SER:O	2.45	0.48
3:K:184:VAL:HG12	3:K:234:HIS:HB2	1.94	0.48
1:B:314:LEU:HD22	2:E:382:LEU:HD23	1.94	0.48
3:I:32:GLN:HG2	3:I:147:SER:HA	1.94	0.48
1:C:11:MET:HE1	2:F:351:PHE:CE2	2.48	0.48
1:C:147:LEU:HD12	1:C:249:ILE:HG22	1.97	0.47
4:J:156:CYS:HB2	4:J:170:TRP:CH2	2.49	0.47
4:J:147:LEU:O	4:J:205:LYS:HD2	2.15	0.47
1:A:63:ILE:HG13	1:A:101:TYR:CZ	2.50	0.47
4:L:127:GLU:OE2	4:L:195:TYR:OH	2.28	0.47
1:C:238:ASP:OD1	1:C:239:LEU:N	2.44	0.46
1:C:182:PRO:HG2	1:C:188:GLN:OE1	2.15	0.46
1:B:76:ASN:OD1	1:B:146:ARG:NH2	2.49	0.46
2:D:331:GLY:O	2:D:335:GLY:HA3	2.15	0.46
1:B:11:MET:HE1	2:E:351:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:357:GLU:OE2	2:E:472:ASP:HB2	2.16	0.45
4:L:208:TYR:O	4:L:214:TYR:OH	2.32	0.45
1:C:244:THR:HG21	1:C:248:LEU:HB2	1.98	0.45
3:K:54:HIS:CD2	3:K:118:ASP:HB2	2.52	0.45
4:L:168:VAL:HG12	4:L:218:VAL:HG22	1.98	0.45
1:A:244:THR:HG21	1:A:248:LEU:HB2	1.98	0.44
1:B:147:LEU:HD12	1:B:249:ILE:HG22	1.99	0.44
1:C:85:GLU:HB2	1:C:265:ILE:HD11	1.99	0.44
1:C:68:GLY:HA3	1:C:145:ASN:OD1	2.16	0.44
2:D:376:ASN:OD1	3:I:123:LEU:HB3	2.17	0.44
3:I:21:VAL:HA	3:I:45:GLY:HA3	1.99	0.44
2:D:448:ARG:O	2:D:452:GLN:HG3	2.18	0.44
3:K:59:ALA:HB3	3:K:62:LYS:HB2	1.99	0.43
2:D:380:ASN:OD1	3:I:122:LYS:HG3	2.18	0.43
3:I:131:GLY:HA3	4:J:118:PHE:CE1	2.52	0.43
1:B:38:LEU:HD11	1:B:314:LEU:HB2	2.00	0.43
3:I:110:THR:HG23	3:I:144:THR:HA	2.00	0.43
1:A:6:ASN:H	1:A:7:PRO:CD	2.32	0.43
1:B:238:ASP:OD1	1:B:239:LEU:N	2.42	0.43
1:A:289:THR:HG21	3:I:49:SER:C	2.44	0.43
1:B:93:CYS:SG	1:B:94:TYR:N	2.89	0.43
1:B:244:THR:HG21	1:B:248:LEU:HB2	2.01	0.43
3:I:124:LEU:HD12	3:I:129:VAL:HB	2.00	0.42
4:L:158:LEU:HB2	4:L:197:LEU:HB3	2.00	0.42
1:B:104:LEU:HB2	1:B:231:TRP:CZ3	2.53	0.42
3:K:202:ALA:HA	3:K:212:LEU:HB3	2.00	0.42
1:A:106:SER:OG	2:F:406:ASP:OD2	2.32	0.42
1:C:234:VAL:HG21	1:C:240:ILE:HB	2.01	0.42
3:I:54:HIS:CD2	3:I:118:ASP:HB2	2.55	0.42
4:J:208:TYR:O	4:J:214:TYR:OH	2.35	0.42
3:K:131:GLY:HA3	4:L:118:PHE:CE1	2.54	0.42
3:K:156:PHE:HB3	4:L:143:SER:OG	2.20	0.42
1:B:63:ILE:HG13	1:B:101:TYR:CE2	2.55	0.42
1:C:6:ASN:H	1:C:7:PRO:CD	2.33	0.42
3:I:202:ALA:HA	3:I:212:LEU:HB3	2.02	0.42
4:L:167:LYS:HB3	4:L:219:THR:HG23	2.01	0.42
3:I:25:GLU:OE1	3:I:140:GLY:N	2.33	0.42
1:C:180:HIS:ND1	1:C:192:TYR:OH	2.39	0.42
3:I:59:ALA:HB3	3:I:62:LYS:HB2	2.01	0.42
2:D:378:LYS:NZ	2:D:430:GLU:O	2.53	0.42
2:E:378:LYS:HZ1	2:E:433:HIS:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:331:GLY:O	2:F:335:GLY:HA3	2.20	0.41
1:B:264:THR:OG1	1:B:265:ILE:N	2.52	0.41
4:L:156:CYS:HB2	4:L:170:TRP:CH2	2.56	0.41
1:B:86:ARG:HA	1:B:87:PRO:HD3	1.95	0.41
2:E:490:ARG:O	2:E:494:ILE:HG12	2.21	0.41
4:J:81:ILE:HA	4:J:82:PRO:HD2	1.84	0.41
1:A:314:LEU:HD22	2:D:382:LEU:HD23	2.02	0.41
4:J:168:VAL:HG12	4:J:218:VAL:HG22	2.02	0.41
1:A:11:MET:HE1	2:D:351:PHE:CD2	2.55	0.41
2:F:448:ARG:O	2:F:452:GLN:HG3	2.20	0.41
4:J:147:LEU:H	4:J:147:LEU:HD12	1.83	0.41
1:C:86:ARG:HA	1:C:87:PRO:HD3	1.94	0.41
1:B:38:LEU:HD12	2:E:427:VAL:HG22	2.02	0.41
3:K:132:GLY:H	4:L:118:PHE:HE1	1.68	0.41
1:C:144:PHE:HB2	1:C:147:LEU:HB2	2.03	0.41
3:I:159:ALA:HA	3:I:160:PRO:HD3	1.82	0.41
4:J:158:LEU:HB2	4:J:197:LEU:HB3	2.03	0.41
1:B:217:ARG:HB2	1:B:224:SER:O	2.21	0.40
4:J:162:TYR:CG	4:J:163:PRO:HA	2.56	0.40
1:C:99:PRO:HG2	1:C:230:TYR:CE2	2.57	0.40
2:F:490:ARG:O	2:F:494:ILE:HG12	2.21	0.40
3:K:110:THR:HG23	3:K:144:THR:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/327 (97%)	304 (96%)	11 (4%)	2 (1%)	21	54
1	B	317/327 (97%)	304 (96%)	11 (4%)	2 (1%)	21	54
1	C	317/327 (97%)	304 (96%)	11 (4%)	2 (1%)	21	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	170/176 (97%)	161 (95%)	9 (5%)	0	100	100
2	E	170/176 (97%)	161 (95%)	9 (5%)	0	100	100
2	F	170/176 (97%)	160 (94%)	10 (6%)	0	100	100
3	I	220/233 (94%)	205 (93%)	14 (6%)	1 (0%)	24	57
3	K	220/233 (94%)	204 (93%)	14 (6%)	2 (1%)	14	45
4	J	210/220 (96%)	194 (92%)	13 (6%)	3 (1%)	9	37
4	L	210/220 (96%)	194 (92%)	13 (6%)	3 (1%)	9	37
All	All	2321/2415 (96%)	2191 (94%)	115 (5%)	15 (1%)	21	54

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	51	VAL
4	L	51	VAL
3	K	168	GLY
1	A	6	ASN
1	A	193	LYS
1	B	6	ASN
1	B	193	LYS
4	J	55	TYR
1	C	6	ASN
1	C	193	LYS
3	I	247	PRO
3	K	247	PRO
4	L	52	SER
4	L	55	TYR
4	J	52	SER

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	274/282 (97%)	268 (98%)	6 (2%)	45	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	274/282 (97%)	268 (98%)	6 (2%)	45	63
1	C	274/282 (97%)	267 (97%)	7 (3%)	40	60
2	D	147/150 (98%)	147 (100%)	0	100	100
2	E	147/150 (98%)	146 (99%)	1 (1%)	76	77
2	F	147/150 (98%)	147 (100%)	0	100	100
3	I	187/196 (95%)	180 (96%)	7 (4%)	30	54
3	K	187/196 (95%)	180 (96%)	7 (4%)	30	54
4	J	184/192 (96%)	174 (95%)	10 (5%)	20	45
4	L	184/192 (96%)	174 (95%)	10 (5%)	20	45
All	All	2005/2072 (97%)	1951 (97%)	54 (3%)	39	59

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

Mol	Chain	Res	Type
1	A	14	HIS
1	A	163	LEU
1	A	239	LEU
1	A	262	LYS
1	A	295	ILE
1	A	323	GLU
1	B	14	HIS
1	B	163	LEU
1	B	239	LEU
1	B	262	LYS
1	B	295	ILE
1	B	323	GLU
2	E	365	LEU
1	C	14	HIS
1	C	160	LEU
1	C	163	LEU
1	C	239	LEU
1	C	262	LYS
1	C	295	ILE
1	C	323	GLU
3	I	20	GLN
3	I	21	VAL
3	I	25	GLU
3	I	95	ARG
3	I	112	VAL

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Mol	Chain	Res	Type
3	I	243	LYS
3	I	248	LYS
4	J	25	VAL
4	J	56	LEU
4	J	71	ILE
4	J	92	THR
4	J	104	GLU
4	J	126	VAL
4	J	129	LYS
4	J	167	LYS
4	J	174	ASN
4	J	219	THR
3	K	21	VAL
3	K	25	GLU
3	K	58	GLN
3	K	95	ARG
3	K	112	VAL
3	K	243	LYS
3	K	248	LYS
4	L	25	VAL
4	L	56	LEU
4	L	71	ILE
4	L	92	THR
4	L	104	GLU
4	L	126	VAL
4	L	129	LYS
4	L	167	LYS
4	L	174	ASN
4	L	219	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
2	D	369	GLN
2	D	452	GLN
2	D	486	HIS
2	E	392	GLN
2	E	452	GLN
2	F	342	GLN
2	F	392	GLN
2	F	452	GLN

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Mol	Chain	Res	Type
2	F	486	HIS
3	I	20	GLN
3	I	205	GLN
3	K	20	GLN
4	L	160	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
5	NAG	B	601	1	14,14,15	0.35	0	17,19,21	0.34	0
5	NAG	B	602	1	14,14,15	0.29	0	17,19,21	0.49	0
5	NAG	C	602	1	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	C	601	1	14,14,15	0.39	0	17,19,21	0.34	0
5	NAG	A	602	1	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
5	NAG	A	601	1	14,14,15	0.28	0	17,19,21	0.38	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
5	NAG	B	601	1	-	2/6/23/26	0/1/1/1
5	NAG	B	602	1	-	2/6/23/26	0/1/1/1
5	NAG	C	602	1	-	2/6/23/26	0/1/1/1
5	NAG	C	601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	602	1	-	2/6/23/26	0/1/1/1
5	NAG	A	601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	NAG	C8-C7-N2-C2
5	A	602	NAG	O7-C7-N2-C2
5	B	602	NAG	C8-C7-N2-C2
5	B	602	NAG	O7-C7-N2-C2
5	C	602	NAG	C8-C7-N2-C2
5	C	602	NAG	O7-C7-N2-C2
5	C	601	NAG	O5-C5-C6-O6
5	B	601	NAG	O5-C5-C6-O6
5	C	601	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	B	601	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	319/327 (97%)	0.16	5 (1%) 70 48	33, 68, 102, 181	0
1	B	319/327 (97%)	0.13	4 (1%) 75 53	36, 71, 106, 205	0
1	C	319/327 (97%)	0.23	6 (1%) 66 45	41, 78, 110, 170	0
2	D	172/176 (97%)	0.66	15 (8%) 16 16	40, 90, 171, 309	0
2	E	172/176 (97%)	0.88	20 (11%) 9 12	45, 102, 173, 346	0
2	F	172/176 (97%)	0.90	21 (12%) 8 12	34, 110, 175, 299	0
3	I	224/233 (96%)	1.07	27 (12%) 8 12	41, 95, 171, 209	0
3	K	224/233 (96%)	0.87	34 (15%) 5 8	55, 101, 254, 347	0
4	J	212/220 (96%)	0.65	10 (4%) 36 27	55, 94, 148, 187	0
4	L	212/220 (96%)	0.95	18 (8%) 16 17	72, 143, 239, 296	0
All	All	2345/2415 (97%)	0.58	160 (6%) 23 20	33, 87, 191, 347	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	329	LEU	10.4
2	E	334	ALA	8.7
2	E	329	LEU	7.8
2	E	332	ALA	7.3
2	D	329	LEU	7.2
2	F	334	ALA	7.0
2	E	333	ILE	6.8
3	K	215	VAL	6.5
3	K	175	LEU	6.2
2	E	336	PHE	5.7
2	E	331	GLY	5.7
2	D	330	PHE	5.4
2	F	336	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
2	E	328	GLY	5.3
2	D	332	ALA	5.3
2	F	328	GLY	5.1
2	F	331	GLY	5.1
2	E	335	GLY	4.8
3	K	176	VAL	4.7
4	J	52	SER	4.6
3	K	228	TYR	4.5
2	D	328	GLY	4.5
2	F	330	PHE	4.4
2	D	331	GLY	4.4
1	B	322	PRO	4.3
2	F	332	ALA	4.3
4	L	137	VAL	4.2
2	D	333	ILE	4.2
3	I	170	ALA	4.2
1	A	145	ASN	4.1
3	K	214	SER	4.0
3	I	167	GLY	4.0
3	K	216	VAL	3.9
1	B	319	ARG	3.9
3	I	21	VAL	3.9
3	I	43	ALA	3.9
3	K	170	ALA	3.9
2	F	335	GLY	3.7
4	L	218	VAL	3.7
4	L	156	CYS	3.7
3	I	47	THR	3.6
2	D	336	PHE	3.6
1	C	319	ARG	3.5
3	K	193	LEU	3.5
3	I	168	GLY	3.4
2	E	365	LEU	3.4
2	E	330	PHE	3.3
1	B	145	ASN	3.3
2	E	383	ILE	3.3
4	L	227	VAL	3.3
2	E	386	THR	3.2
2	D	365	LEU	3.2
4	L	215	ALA	3.2
4	L	216	CYS	3.2
4	L	31	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	334	ALA	3.1
3	I	115	CYS	3.1
3	K	241	VAL	3.1
3	I	171	ALA	3.1
4	L	157	LEU	3.1
1	C	322	PRO	3.0
3	I	161	SER	3.0
4	L	166	ALA	3.0
2	F	348	TRP	3.0
2	D	439	ASP	3.0
3	K	153	PRO	2.9
3	K	167	GLY	2.9
2	F	386	THR	2.9
2	F	457	ALA	2.9
3	I	223	LEU	2.9
3	K	151	LYS	2.9
1	A	319	ARG	2.9
3	I	36	SER	2.9
3	K	172	LEU	2.9
1	A	322	PRO	2.9
3	K	229	ILE	2.8
3	I	174	CYS	2.8
2	D	386	THR	2.8
3	K	217	THR	2.8
3	K	223	LEU	2.7
3	K	160	PRO	2.7
4	L	229	LYS	2.7
3	I	169	THR	2.7
3	K	36	SER	2.7
3	I	157	PRO	2.7
3	I	50	ALA	2.7
3	I	97	THR	2.7
4	L	168	VAL	2.7
3	I	146	SER	2.7
3	I	107	ALA	2.7
4	L	219	THR	2.7
3	K	198	HIS	2.6
3	K	183	PRO	2.6
3	K	168	GLY	2.6
3	I	228	TYR	2.6
3	I	96	ASN	2.6
1	B	5	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	459	ASP	2.6
4	L	132	VAL	2.6
2	D	383	ILE	2.6
2	F	337	ILE	2.6
3	I	32	GLN	2.6
2	F	375	ILE	2.5
4	J	151	THR	2.5
3	K	174	CYS	2.5
2	F	333	ILE	2.5
4	L	197	LEU	2.5
2	E	439	ASP	2.5
3	I	93	ILE	2.5
2	D	335	GLY	2.5
2	E	450	ARG	2.5
2	F	471	CYS	2.5
2	F	383	ILE	2.4
2	D	356	ALA	2.4
3	K	197	VAL	2.4
3	K	219	PRO	2.4
2	E	499	GLN	2.4
2	E	436	ASP	2.4
4	J	73	ARG	2.4
4	J	215	ALA	2.4
2	F	463	GLY	2.4
3	I	20	GLN	2.3
3	K	221	SER	2.3
2	F	356	ALA	2.3
3	I	101	HIS	2.3
3	K	157	PRO	2.3
4	J	142	PRO	2.3
2	E	471	CYS	2.3
2	F	452	GLN	2.3
2	F	436	ASP	2.3
4	J	99	SER	2.3
2	D	337	ILE	2.3
1	C	73	ASP	2.2
3	I	235	LYS	2.2
3	K	240	LYS	2.2
3	I	219	PRO	2.2
2	F	439	ASP	2.2
2	E	342	GLN	2.2
4	L	214	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	323	GLU	2.2
4	J	62	LYS	2.2
4	L	230	SER	2.1
3	K	186	VAL	2.1
3	K	218	VAL	2.1
1	C	323	GLU	2.1
3	I	199	THR	2.1
2	E	344	LEU	2.1
3	K	232	VAL	2.1
4	L	155	VAL	2.1
1	A	142	ASP	2.1
4	J	31	GLY	2.1
3	K	185	THR	2.1
4	L	42	THR	2.1
1	C	321	ILE	2.1
1	C	94	TYR	2.1
4	J	234	GLY	2.0
3	K	196	GLY	2.0
3	K	139	GLN	2.0
4	J	179	GLY	2.0
3	K	192	ALA	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($\text{\AA}^2$)	Q<0.9
5	NAG	C	602	14/15	0.56	0.18	63,69,78,86	0
5	NAG	A	601	14/15	0.57	0.19	102,123,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	602	14/15	0.67	0.20	67,77,82,93	0
5	NAG	A	602	14/15	0.71	0.20	65,78,151,153	0
5	NAG	C	601	14/15	0.73	0.16	104,123,130,132	0
5	NAG	B	601	14/15	0.81	0.16	114,125,131,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.