



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:19 AM UTC

PDB ID : 5CUS / pdb\_00005cus  
Title : Crystal Structure of sErbB3-Fab3379 Complex  
Authors : Lee, S.; Schlessinger, J.  
Deposited on : 2015-07-25  
Resolution : 3.20 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](mailto: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>.

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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)  
Xtrriage (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

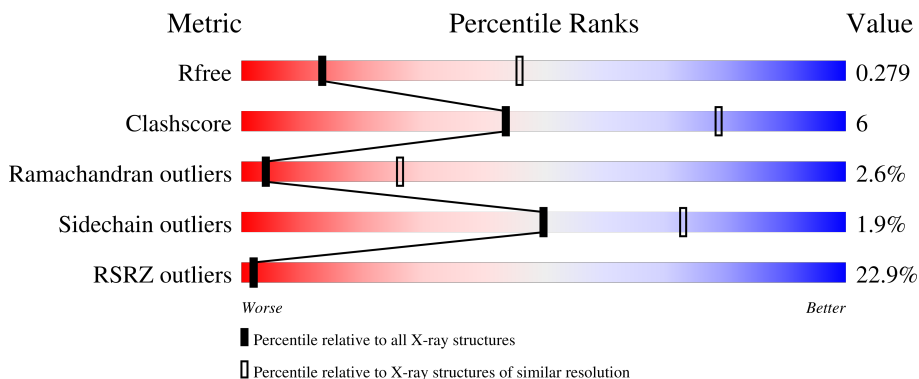
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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  $\geq 3$ , 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	627	 16% 77% 12% 11%
1	B	627	 17% 72% 12% 15%
1	C	627	 19% 69% 16% 14%
1	D	627	 24% 70% 10% 19%
2	H	221	 15% 65% 18% 18%

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Mol	Chain	Length	Quality of chain
2	I	221	<p>19% 67% 22% • 10%</p>
2	J	221	<p>13% 61% 18% 21%</p>
2	K	221	<p>19% 68% 13% 19%</p>
3	L	216	<p>17% 73% 12% 14%</p>
3	M	216	<p>26% 76% 16% • 6%</p>
3	N	216	<p>25% 69% 15% • 15%</p>
3	O	216	<p>31% 75% 17% • 7%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25896 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 Receptor tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	561	3927	2451	698	724	54	23	0	0
1	B	530	3720	2317	654	698	51	28	0	0
1	C	539	3839	2400	667	720	52	14	0	0
1	D	509	3521	2188	617	666	50	12	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	623	HIS	-	expression tag	UNP P21860
A	624	HIS	-	expression tag	UNP P21860
A	625	HIS	-	expression tag	UNP P21860
A	626	HIS	-	expression tag	UNP P21860
A	627	HIS	-	expression tag	UNP P21860
B	623	HIS	-	expression tag	UNP P21860
B	624	HIS	-	expression tag	UNP P21860
B	625	HIS	-	expression tag	UNP P21860
B	626	HIS	-	expression tag	UNP P21860
B	627	HIS	-	expression tag	UNP P21860
C	623	HIS	-	expression tag	UNP P21860
C	624	HIS	-	expression tag	UNP P21860
C	625	HIS	-	expression tag	UNP P21860
C	626	HIS	-	expression tag	UNP P21860
C	627	HIS	-	expression tag	UNP P21860
D	623	HIS	-	expression tag	UNP P21860
D	624	HIS	-	expression tag	UNP P21860
D	625	HIS	-	expression tag	UNP P21860
D	626	HIS	-	expression tag	UNP P21860
D	627	HIS	-	expression tag	UNP P21860

- Molecule 2 is a protein called IgG H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	182	1348	852	226	263	7	0	0	0
2	I	198	1431	902	239	283	7	0	0	0
2	J	175	1270	796	214	253	7	0	0	0
2	K	180	1294	816	216	255	7	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	10	GLY	ASP	conflict	UNP S6B291
H	31	TYR	THR	conflict	UNP S6B291
H	33	TYR	ALA	conflict	UNP S6B291
H	35	GLN	SER	conflict	UNP S6B291
H	50	TYR	GLY	conflict	UNP S6B291
H	53	SER	ASP	conflict	UNP S6B291
H	56	GLY	HIS	conflict	UNP S6B291
H	57	VAL	SER	conflict	UNP S6B291
H	58	THR	ILE	conflict	UNP S6B291
H	59	ASN	TYR	conflict	UNP S6B291
H	98	ARG	-	insertion	UNP S6B291
H	99	VAL	THR	conflict	UNP S6B291
H	101	LEU	SER	conflict	UNP S6B291
H	102	GLY	GLN	conflict	UNP S6B291
H	103	ASP	TRP	conflict	UNP S6B291
H	104	ALA	PRO	conflict	UNP S6B291
H	105	PHE	GLY	conflict	UNP S6B291
H	107	ILE	TYR	conflict	UNP S6B291
H	113	MET	LEU	conflict	UNP S6B291
H	215	LYS	ARG	conflict	UNP S6B291
I	10	GLY	ASP	conflict	UNP S6B291
I	31	TYR	THR	conflict	UNP S6B291
I	33	TYR	ALA	conflict	UNP S6B291
I	35	GLN	SER	conflict	UNP S6B291
I	50	TYR	GLY	conflict	UNP S6B291
I	53	SER	ASP	conflict	UNP S6B291
I	56	GLY	HIS	conflict	UNP S6B291
I	57	VAL	SER	conflict	UNP S6B291
I	58	THR	ILE	conflict	UNP S6B291
I	59	ASN	TYR	conflict	UNP S6B291

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Chain	Residue	Modelled	Actual	Comment	Reference
I	98	ARG	-	insertion	UNP S6B291
I	99	VAL	THR	conflict	UNP S6B291
I	101	LEU	SER	conflict	UNP S6B291
I	102	GLY	GLN	conflict	UNP S6B291
I	103	ASP	TRP	conflict	UNP S6B291
I	104	ALA	PRO	conflict	UNP S6B291
I	105	PHE	GLY	conflict	UNP S6B291
I	107	ILE	TYR	conflict	UNP S6B291
I	113	MET	LEU	conflict	UNP S6B291
I	215	LYS	ARG	conflict	UNP S6B291
J	10	GLY	ASP	conflict	UNP S6B291
J	31	TYR	THR	conflict	UNP S6B291
J	33	TYR	ALA	conflict	UNP S6B291
J	35	GLN	SER	conflict	UNP S6B291
J	50	TYR	GLY	conflict	UNP S6B291
J	53	SER	ASP	conflict	UNP S6B291
J	56	GLY	HIS	conflict	UNP S6B291
J	57	VAL	SER	conflict	UNP S6B291
J	58	THR	ILE	conflict	UNP S6B291
J	59	ASN	TYR	conflict	UNP S6B291
J	98	ARG	-	insertion	UNP S6B291
J	99	VAL	THR	conflict	UNP S6B291
J	101	LEU	SER	conflict	UNP S6B291
J	102	GLY	GLN	conflict	UNP S6B291
J	103	ASP	TRP	conflict	UNP S6B291
J	104	ALA	PRO	conflict	UNP S6B291
J	105	PHE	GLY	conflict	UNP S6B291
J	107	ILE	TYR	conflict	UNP S6B291
J	113	MET	LEU	conflict	UNP S6B291
J	215	LYS	ARG	conflict	UNP S6B291
K	10	GLY	ASP	conflict	UNP S6B291
K	31	TYR	THR	conflict	UNP S6B291
K	33	TYR	ALA	conflict	UNP S6B291
K	35	GLN	SER	conflict	UNP S6B291
K	50	TYR	GLY	conflict	UNP S6B291
K	53	SER	ASP	conflict	UNP S6B291
K	56	GLY	HIS	conflict	UNP S6B291
K	57	VAL	SER	conflict	UNP S6B291
K	58	THR	ILE	conflict	UNP S6B291
K	59	ASN	TYR	conflict	UNP S6B291
K	98	ARG	-	insertion	UNP S6B291
K	99	VAL	THR	conflict	UNP S6B291

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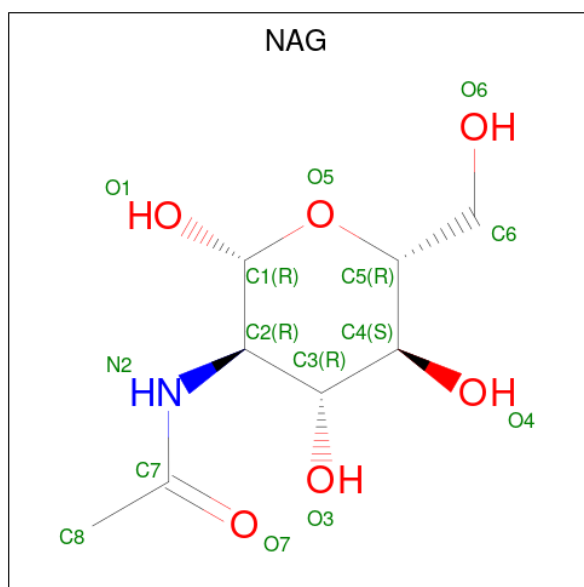
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Chain	Residue	Modelled	Actual	Comment	Reference
K	101	LEU	SER	conflict	UNP S6B291
K	102	GLY	GLN	conflict	UNP S6B291
K	103	ASP	TRP	conflict	UNP S6B291
K	104	ALA	PRO	conflict	UNP S6B291
K	105	PHE	GLY	conflict	UNP S6B291
K	107	ILE	TYR	conflict	UNP S6B291
K	113	MET	LEU	conflict	UNP S6B291
K	215	LYS	ARG	conflict	UNP S6B291

- Molecule 3 is a protein called Fab LC region of KTN3379.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	185	Total 1327	C 829	N 226	O 269	S 3	0	0	0
3	M	203	Total 1410	C 873	N 241	O 292	S 4	0	0	0
3	N	184	Total 1275	C 790	N 217	O 264	S 4	0	0	0
3	O	200	Total 1380	C 858	N 235	O 283	S 4	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

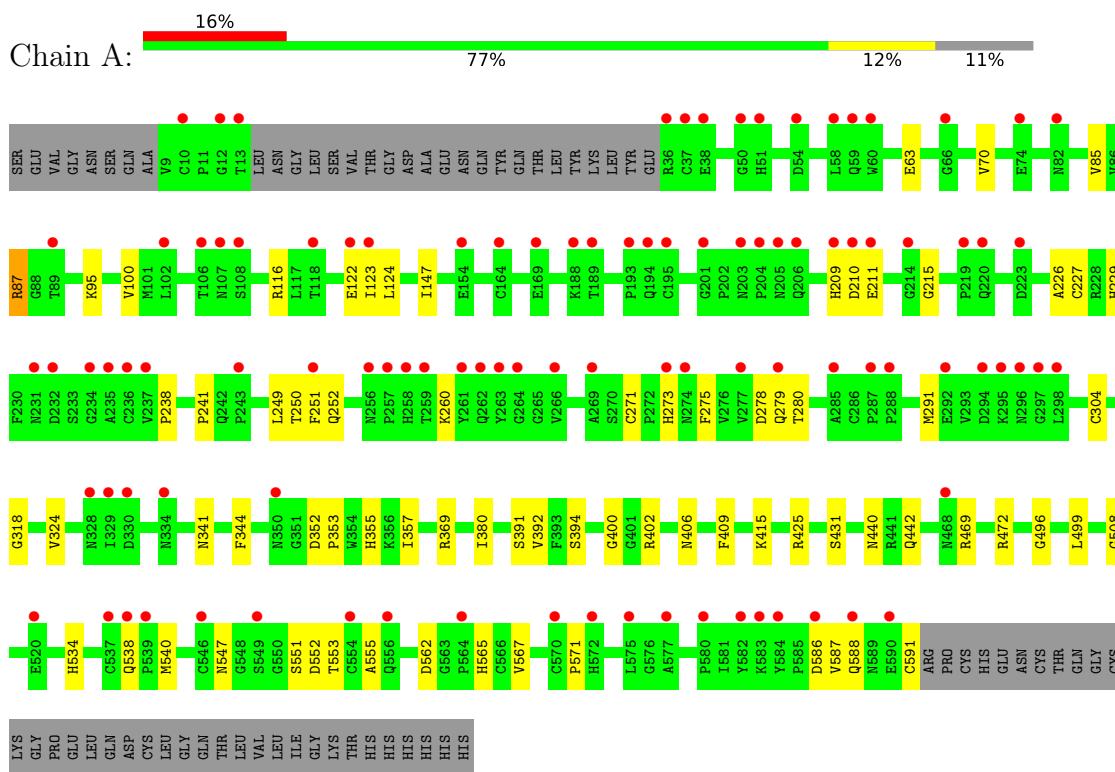


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1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

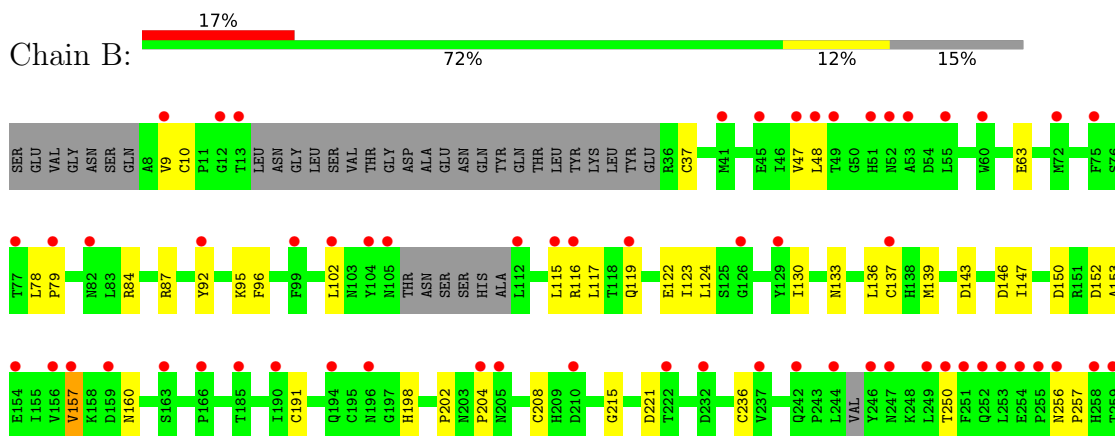
### 3 Residue-property plots [i](#)

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: Receptor tyrosine-protein kinase erbB-3

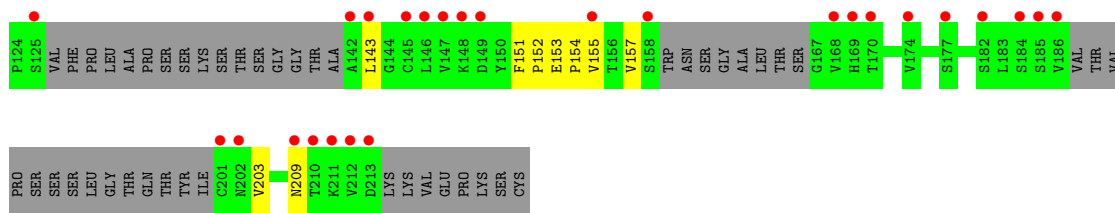


- Molecule 1: Receptor tyrosine-protein kinase erbB-3

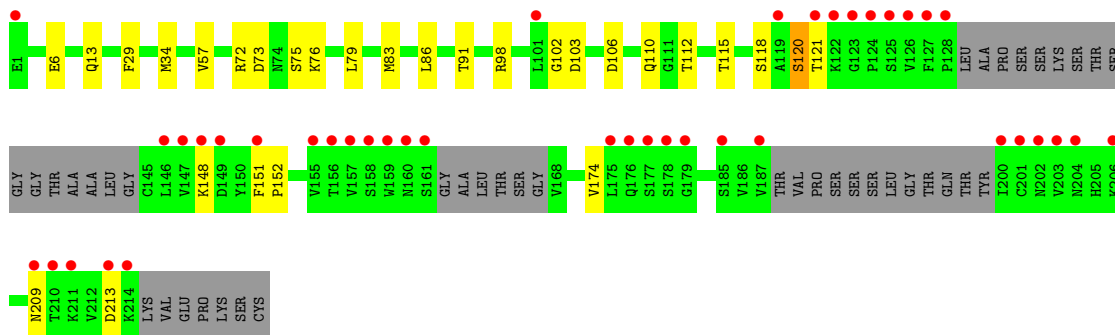




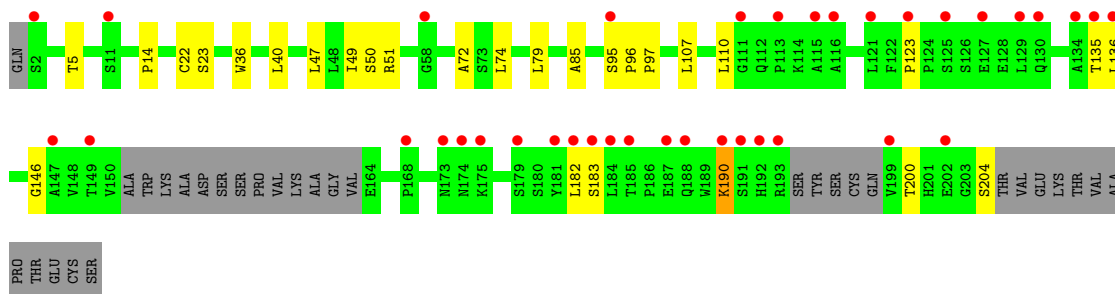




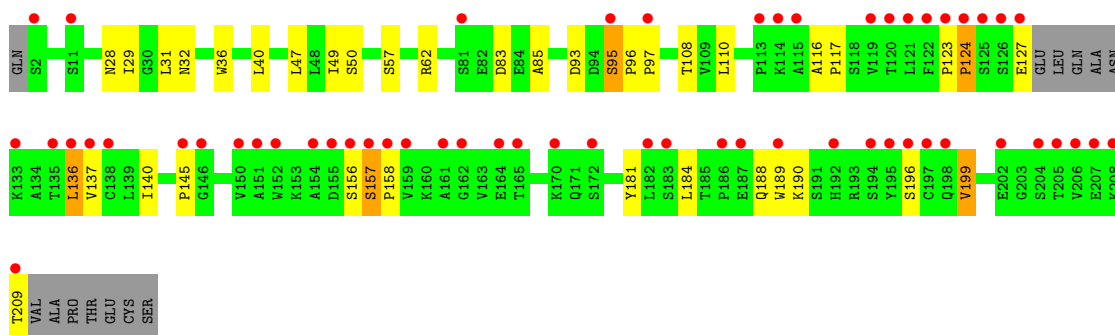
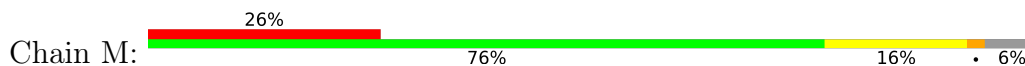
• Molecule 2: IgG H chain



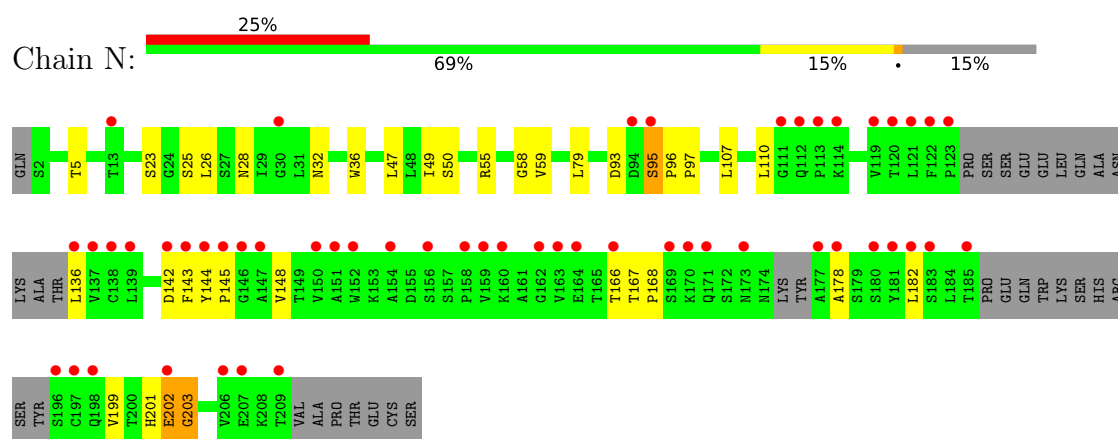
• Molecule 3: Fab LC region of KTN3379



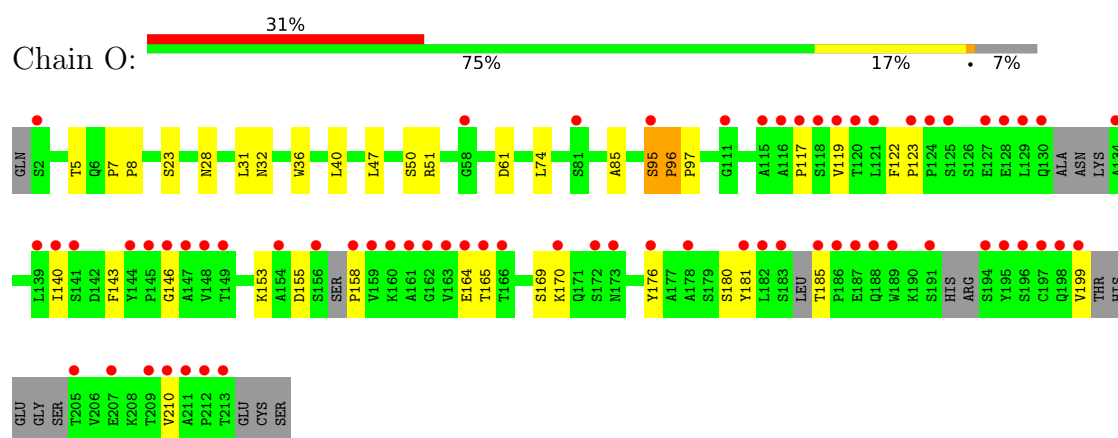
• Molecule 3: Fab LC region of KTN3379



• Molecule 3: Fab LC region of KTN3379



• Molecule 3: Fab LC region of KTN3379



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.38Å 127.14Å 138.08Å 87.10° 85.54° 89.92°	Depositor
Resolution (Å)	69.39 – 3.20 69.39 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (69.39-3.20) 98.3 (69.39-3.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 3.19Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.252 , 0.278 0.255 , 0.279	Depositor DCC
$R_{free}$ test set	4593 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtrriage
Anisotropy	0.367	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 82.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.048 for -h,k,-l	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	25896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/4023	0.75	0/5502
1	B	0.27	0/3801	0.74	2/5195 (0.0%)
1	C	0.27	0/3924	0.75	3/5355 (0.1%)
1	D	0.26	0/3596	0.74	2/4906 (0.0%)
2	H	0.27	0/1379	0.66	0/1878
2	I	0.28	0/1463	0.73	3/1994 (0.2%)
2	J	0.27	0/1295	0.67	0/1761
2	K	0.27	0/1321	0.66	0/1800
3	L	0.27	0/1359	0.72	1/1860 (0.1%)
3	M	0.29	0/1443	0.78	2/1984 (0.1%)
3	N	0.28	0/1301	0.77	2/1782 (0.1%)
3	O	0.28	0/1408	0.73	2/1926 (0.1%)
All	All	0.27	0/26313	0.74	17/35943 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	95	SER	CA-C-N	-9.07	111.04	120.38
3	N	95	SER	C-N-CA	-9.07	111.04	120.38
3	M	95	SER	CA-C-N	-8.73	111.39	120.38
3	M	95	SER	C-N-CA	-8.73	111.39	120.38
1	D	570	CYS	CA-C-N	8.11	129.98	119.84
1	D	570	CYS	C-N-CA	8.11	129.98	119.84
2	I	189	VAL	CA-C-N	6.63	128.13	119.84
2	I	189	VAL	C-N-CA	6.63	128.13	119.84
1	C	287	PRO	CA-C-N	5.92	127.25	119.84
1	C	287	PRO	C-N-CA	5.92	127.25	119.84
2	I	191	SER	CB-CA-C	-5.77	109.39	117.23
1	B	286	CYS	CA-C-N	5.64	123.78	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	CYS	C-N-CA	5.64	123.78	119.66
3	O	185	THR	CA-C-N	5.43	126.63	119.84
3	O	185	THR	C-N-CA	5.43	126.63	119.84
3	L	123	PRO	O-C-N	5.37	123.78	121.31
1	C	287	PRO	O-C-N	5.17	123.69	121.31

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	3927	0	3437	39	0
1	B	3720	0	3310	36	0
1	C	3839	0	3426	50	0
1	D	3521	0	2985	36	0
2	H	1348	0	1268	23	0
2	I	1431	0	1329	26	0
2	J	1270	0	1174	23	0
2	K	1294	0	1175	16	0
3	L	1327	0	1253	16	0
3	M	1410	0	1283	20	0
3	N	1275	0	1170	18	0
3	O	1380	0	1258	21	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
4	C	42	0	39	1	0
4	D	42	0	39	2	0
4	M	14	0	13	0	0
All	All	25896	0	23211	297	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 (297) 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:D:517:LEU:O	1:D:522:ARG:NH1	2.11	0.83
1:B:63:GLU:OE2	1:B:87:ARG:NE	2.16	0.77
2:K:98:ARG:NH2	2:K:106:ASP:OD2	2.12	0.74
2:H:19:ARG:NH2	2:J:11:LEU:O	2.23	0.71
2:H:52:GLY:O	2:H:72:ARG:NH1	2.23	0.71
1:A:122:GLU:OE2	1:A:215:GLY:N	2.18	0.70
1:A:425:ARG:HH12	1:A:508:GLY:HA3	1.56	0.70
3:L:5:THR:HB	3:L:23:SER:HB3	1.75	0.69
1:C:341:ASN:HD22	1:C:376:GLY:HA3	1.57	0.67
3:N:5:THR:HB	3:N:23:SER:HB3	1.77	0.67
1:C:290:LYS:HA	1:C:303:PRO:HA	1.77	0.66
1:A:87:ARG:NH1	1:A:227:CYS:O	2.24	0.66
1:B:122:GLU:OE2	1:B:215:GLY:N	2.23	0.66
1:A:547:ASN:HB3	1:A:553:THR:HB	1.79	0.64
2:J:20:LEU:HD12	2:J:81:LEU:HD23	1.80	0.64
1:C:324:VAL:HA	1:C:328:ASN:HD21	1.63	0.63
1:A:425:ARG:NH2	1:A:496:GLY:O	2.32	0.62
3:L:79:LEU:HD11	3:L:107:LEU:HD21	1.81	0.62
3:N:79:LEU:HD11	3:N:107:LEU:HD21	1.82	0.62
3:N:47:LEU:HD21	3:N:50:SER:HB3	1.81	0.62
3:O:5:THR:HB	3:O:23:SER:HB3	1.81	0.61
2:H:91:THR:HG23	2:H:115:THR:HA	1.82	0.61
3:N:25:SER:HB3	3:N:28:ASN:HD21	1.66	0.61
3:O:47:LEU:HD21	3:O:50:SER:HB3	1.82	0.61
2:H:159:TRP:HA	2:H:201:CYS:HA	1.83	0.61
2:I:145:CYS:SG	2:I:146:LEU:N	2.74	0.60
3:M:157:SER:H	3:M:158:PRO:HD2	1.65	0.60
1:D:86:VAL:HB	1:D:123:ILE:HG12	1.82	0.60
1:C:51:HIS:H	1:C:74:GLU:HB2	1.66	0.59
2:J:34:MET:HB3	2:J:79:LEU:HD22	1.85	0.59
1:D:133:ASN:O	1:D:135:LYS:N	2.29	0.59
2:J:98:ARG:NH2	2:J:106:ASP:OD2	2.27	0.58
2:J:91:THR:HG23	2:J:115:THR:HA	1.85	0.58
1:C:341:ASN:ND2	1:C:403:SER:OG	2.35	0.58
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.83	0.58
2:H:98:ARG:NH2	2:H:106:ASP:OD2	2.30	0.58
2:J:22:CYS:HB3	2:J:79:LEU:HB3	1.85	0.58
3:N:36:TRP:HB2	3:N:49:ILE:HB	1.86	0.58
2:I:91:THR:HG23	2:I:115:THR:HA	1.85	0.58
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.86	0.58
2:I:34:MET:HB3	2:I:79:LEU:HD22	1.84	0.58
2:I:142:ALA:HB3	2:I:189:VAL:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:GLN:NE2	1:A:540:MET:SD	2.71	0.58
1:C:130:ILE:HB	1:C:157:VAL:HG13	1.84	0.57
1:D:469:ARG:NH2	1:D:477:GLU:OE2	2.37	0.57
1:A:425:ARG:NH1	1:A:508:GLY:HA3	2.19	0.57
1:D:562:ASP:HA	1:D:591:CYS:HB2	1.86	0.57
1:A:318:GLY:HA3	2:H:101:LEU:HD21	1.85	0.57
1:C:11:PRO:HB2	1:C:13:THR:HG23	1.86	0.57
2:K:91:THR:HG23	2:K:115:THR:HA	1.87	0.57
1:D:69:LEU:HD12	1:D:99:PHE:HB3	1.86	0.57
1:A:63:GLU:OE1	1:A:87:ARG:NE	2.36	0.57
3:L:47:LEU:HD21	3:L:50:SER:HB3	1.87	0.56
1:C:329:ILE:HG12	1:C:330:ASP:H	1.69	0.56
3:N:93:ASP:OD2	3:N:96:PRO:HD2	2.05	0.56
1:D:42:GLY:H	1:D:65:THR:HG1	1.53	0.56
1:A:70:VAL:HB	1:A:100:VAL:HG22	1.87	0.56
2:K:6:GLU:O	2:K:110:GLN:NE2	2.39	0.56
3:N:143:PHE:HB3	3:N:144:TYR:HA	1.88	0.56
1:B:157:VAL:O	1:B:160:ASN:ND2	2.39	0.55
1:C:137:CYS:SG	1:C:138:HIS:N	2.79	0.55
2:I:184:SER:HG	3:M:181:TYR:HH	1.53	0.55
1:B:47:VAL:HG12	1:B:48:LEU:HG	1.89	0.55
1:A:291:MET:HE3	1:A:304:CYS:HA	1.89	0.55
1:B:340:GLY:H	1:B:375:THR:HB	1.71	0.55
3:L:135:THR:HG22	3:L:183:SER:HA	1.88	0.55
1:C:440:ASN:O	1:C:442:GLN:N	2.40	0.55
1:A:318:GLY:O	3:L:51:ARG:NH1	2.37	0.55
2:I:6:GLU:O	2:I:110:GLN:NE2	2.40	0.54
1:B:150:ASP:HB3	1:B:153:ALA:HB2	1.88	0.54
2:J:14:PRO:HG2	2:J:118:SER:HB2	1.88	0.54
3:M:62:ARG:NH1	3:M:83:ASP:OD2	2.40	0.54
1:B:469:ARG:NH2	1:B:477:GLU:OE1	2.38	0.54
3:O:119:VAL:HG11	3:O:199:VAL:HG21	1.88	0.54
2:K:118:SER:O	2:K:120:SER:N	2.36	0.54
1:D:456:ARG:NH1	2:K:57:VAL:HA	2.23	0.54
2:H:17:SER:N	2:J:21:SER:OG	2.39	0.54
1:C:412:LEU:HD12	1:C:436:TYR:HB3	1.90	0.54
2:I:22:CYS:HB3	2:I:79:LEU:HB3	1.90	0.54
2:K:34:MET:HB3	2:K:79:LEU:HD22	1.89	0.53
3:M:40:LEU:HD23	3:M:85:ALA:HB2	1.91	0.53
1:A:440:ASN:O	1:A:442:GLN:N	2.35	0.53
2:H:148:LYS:NZ	3:L:135:THR:HG21	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:GLY:O	3:O:51:ARG:NH1	2.28	0.53
3:M:36:TRP:HB2	3:M:49:ILE:HB	1.91	0.53
3:O:146:GLY:HA3	3:O:176:TYR:HD2	1.74	0.53
1:C:397:THR:HG22	1:C:398:THR:HG23	1.91	0.53
2:I:14:PRO:HG2	2:I:118:SER:HB3	1.89	0.53
2:I:152:PRO:HD2	2:I:207:PRO:HG2	1.90	0.53
3:N:145:PRO:HD2	3:N:202:GLU:OE2	2.08	0.53
2:I:124:PRO:HB3	2:I:147:VAL:HG13	1.90	0.53
3:M:47:LEU:HD21	3:M:50:SER:HB3	1.89	0.53
1:B:517:LEU:O	1:B:522:ARG:NE	2.42	0.52
1:C:123:ILE:HG13	1:C:147:ILE:HD11	1.91	0.52
4:C:702:NAG:H83	4:C:702:NAG:H3	1.90	0.52
3:N:136:LEU:N	3:N:182:LEU:O	2.42	0.52
2:I:29:PHE:O	2:I:72:ARG:NH2	2.43	0.52
2:K:83:MET:HB3	2:K:86:LEU:HD21	1.91	0.52
3:M:108:THR:HG21	3:M:145:PRO:HB3	1.91	0.52
1:A:540:MET:HG3	1:A:555:ALA:HB3	1.92	0.51
1:A:586:ASP:O	1:A:588:GLN:N	2.43	0.51
3:O:40:LEU:HD23	3:O:85:ALA:HB2	1.92	0.51
3:O:117:PRO:HB3	3:O:143:PHE:HB3	1.91	0.51
3:M:188:GLN:O	3:M:190:LYS:N	2.42	0.51
2:I:2:VAL:HA	2:I:26:GLY:HA3	1.92	0.51
3:O:119:VAL:HG12	3:O:140:ILE:HA	1.92	0.51
2:J:73:ASP:OD1	2:J:75:SER:OG	2.27	0.50
3:N:55:ARG:NH2	3:N:59:VAL:O	2.44	0.50
1:A:211:GLU:OE1	1:A:229:HIS:ND1	2.44	0.50
1:B:455:LEU:HD23	1:B:459:THR:HG22	1.94	0.50
1:D:242:GLN:HG2	1:D:244:LEU:H	1.76	0.50
2:J:6:GLU:OE2	2:J:109:GLY:HA3	2.11	0.50
1:C:103:ASN:ND2	1:C:133:ASN:OD1	2.40	0.50
3:N:148:VAL:HG13	3:N:199:VAL:HG13	1.94	0.50
1:B:295:LYS:O	1:B:297:GLY:N	2.45	0.50
1:B:506:ARG:HH21	1:B:514:CYS:HA	1.77	0.49
1:D:430:ILE:HB	1:D:455:LEU:HD23	1.94	0.49
2:J:83:MET:HB3	2:J:86:LEU:HD21	1.94	0.49
2:H:205:HIS:CD2	2:H:207:PRO:HD2	2.47	0.49
2:J:6:GLU:O	2:J:110:GLN:NE2	2.45	0.49
3:M:196:SER:HB2	3:M:209:THR:HB	1.94	0.49
3:O:169:SER:OG	3:O:170:LYS:N	2.43	0.49
1:C:122:GLU:OE2	1:C:214:GLY:HA3	2.12	0.49
1:D:491:TRP:HB2	1:D:497:GLN:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:HG13	1:A:147:ILE:HG22	1.93	0.49
2:I:73:ASP:OD1	2:I:75:SER:OG	2.23	0.49
2:H:202:ASN:ND2	2:H:213:ASP:OD1	2.33	0.49
1:D:456:ARG:HH12	2:K:57:VAL:HA	1.77	0.49
2:J:20:LEU:HB2	2:J:81:LEU:HB3	1.95	0.49
1:A:394:SER:HB2	1:A:425:ARG:HD3	1.94	0.48
1:C:224:CYS:O	1:C:226:ALA:N	2.46	0.48
3:L:40:LEU:HD23	3:L:85:ALA:HB2	1.95	0.48
2:K:29:PHE:O	2:K:72:ARG:NH2	2.46	0.48
2:I:25:SER:OG	2:K:13:GLN:NE2	2.42	0.48
3:L:136:LEU:HD12	3:L:182:LEU:HD23	1.96	0.48
1:D:311:ALA:HB2	3:O:31:LEU:HA	1.94	0.48
1:B:442:GLN:HA	1:B:469:ARG:HD2	1.95	0.48
1:B:115:LEU:O	1:B:117:LEU:N	2.46	0.48
1:A:400:GLY:O	1:A:431:SER:HB2	2.14	0.47
1:C:349:LEU:HD21	1:C:384:PRO:HD3	1.96	0.47
2:J:36:TRP:CE2	2:J:81:LEU:HB2	2.50	0.47
1:B:143:ASP:OD2	1:B:146:ASP:HB2	2.14	0.47
1:D:418:ASN:ND2	4:D:701:NAG:O7	2.48	0.47
2:I:47:TRP:HZ2	2:I:50:TYR:HD2	1.61	0.47
1:D:402:ARG:NH1	2:K:103:ASP:OD2	2.48	0.47
2:H:102:GLY:HA3	3:L:51:ARG:HG2	1.96	0.47
1:A:87:ARG:HG2	1:A:124:LEU:HD12	1.97	0.47
2:I:168:VAL:HB	2:I:187:VAL:HB	1.97	0.47
3:O:164:GLU:OE2	3:O:181:TYR:HD1	1.98	0.47
1:A:472:ARG:HB3	2:K:213:ASP:OD2	2.15	0.46
1:C:337:LYS:NZ	3:N:32:ASN:OD1	2.47	0.46
1:D:482:ASP:OD1	1:D:484:LEU:HB2	2.15	0.46
1:A:406:ASN:HB3	1:A:409:PHE:HD2	1.81	0.46
3:L:36:TRP:CE2	3:L:74:LEU:HB2	2.51	0.46
1:B:123:ILE:HG13	1:B:147:ILE:HG22	1.98	0.46
1:C:232:ASP:O	1:C:234:GLY:N	2.49	0.46
1:C:347:THR:HG23	1:C:353:PRO:HD3	1.98	0.46
1:A:369:ARG:NH1	1:A:391:SER:O	2.48	0.46
1:B:486:SER:OG	1:B:500:SER:OG	2.31	0.45
1:C:133:ASN:HB3	1:C:136:LEU:HB3	1.98	0.45
1:D:543:THR:OG1	1:D:544:ALA:N	2.49	0.45
1:C:558:ALA:O	1:C:560:PHE:N	2.49	0.45
1:D:248:LYS:O	1:D:250:THR:N	2.45	0.45
2:K:151:PHE:HA	2:K:152:PRO:HA	1.76	0.45
1:D:456:ARG:O	1:D:462:ARG:NH1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:37:VAL:O	2:J:95:TYR:N	2.42	0.45
3:L:200:THR:HA	3:L:204:SER:HB2	1.98	0.45
3:M:62:ARG:HH12	3:M:83:ASP:CG	2.24	0.45
1:A:250:THR:O	1:A:252:GLN:N	2.49	0.45
1:B:130:ILE:HB	1:B:157:VAL:HG13	1.98	0.45
1:D:339:LEU:HD21	3:O:32:ASN:HA	1.98	0.45
1:A:209:HIS:CD2	1:A:210:ASP:H	2.35	0.45
1:B:221:ASP:HB3	1:B:236:CYS:H	1.80	0.45
2:H:6:GLU:OE2	2:H:109:GLY:HA3	2.16	0.45
2:I:106:ASP:HA	3:M:47:LEU:HD22	1.99	0.45
1:A:85:VAL:HG21	1:A:226:ALA:HB2	1.98	0.45
1:C:325:ASP:OD1	1:C:327:SER:OG	2.28	0.45
3:N:201:HIS:O	3:N:203:GLY:N	2.49	0.45
3:L:22:CYS:N	3:L:72:ALA:O	2.50	0.45
1:B:10:CYS:N	1:B:37:CYS:SG	2.90	0.45
2:I:144:GLY:HA3	2:I:186:VAL:HA	1.99	0.45
2:I:11:LEU:HD21	2:K:76:LYS:HD3	1.98	0.44
2:J:153:GLU:HB2	2:J:154:PRO:HA	1.99	0.44
1:C:50:GLY:HA3	1:C:74:GLU:H	1.82	0.44
1:C:193:PRO:HA	1:C:194:GLN:HA	1.64	0.44
2:I:83:MET:HB3	2:I:86:LEU:HD21	2.00	0.44
3:M:123:PRO:HA	3:M:124:PRO:HD3	1.84	0.44
3:O:164:GLU:OE2	3:O:180:SER:HA	2.18	0.44
1:A:211:GLU:HG3	1:A:238:PRO:HD3	2.00	0.44
1:C:199:CYS:HA	1:C:200:PHE:HA	1.65	0.44
1:B:92:TYR:N	1:B:96:PHE:O	2.47	0.44
3:L:36:TRP:HB2	3:L:49:ILE:HB	1.99	0.44
2:K:73:ASP:OD1	2:K:75:SER:OG	2.28	0.44
1:B:84:ARG:HG2	1:B:119:GLN:HB3	2.00	0.44
2:H:148:LYS:HZ1	3:L:135:THR:HG21	1.83	0.44
1:B:191:CYS:HA	1:B:202:PRO:HA	1.99	0.44
1:B:323:THR:OG1	1:B:324:VAL:N	2.50	0.44
1:C:85:VAL:HG11	1:C:226:ALA:HB2	2.00	0.44
1:D:431:SER:HB3	2:K:57:VAL:HG21	2.00	0.44
3:L:136:LEU:HB2	3:L:182:LEU:HB3	2.00	0.44
2:J:151:PHE:HA	2:J:152:PRO:HA	1.72	0.44
3:O:28:ASN:O	3:O:32:ASN:HB2	2.17	0.44
1:C:195:CYS:O	1:C:197:GLY:N	2.51	0.44
2:I:208:SER:O	2:I:210:THR:N	2.50	0.44
3:N:25:SER:HB3	3:N:28:ASN:ND2	2.31	0.44
3:O:123:PRO:HG3	3:O:210:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:THR:OG1	1:C:50:GLY:N	2.50	0.44
1:C:117:LEU:HB3	1:C:120:LEU:HB2	2.00	0.44
1:D:133:ASN:C	1:D:135:LYS:H	2.22	0.44
1:D:415:LYS:H	1:D:439:ALA:HB3	1.81	0.44
1:C:70:VAL:HG21	1:C:78:LEU:HD22	2.00	0.43
2:H:33:TYR:HB2	2:H:99:VAL:HG21	2.00	0.43
3:O:95:SER:OG	3:O:96:PRO:HD3	2.18	0.43
1:A:344:PHE:HB2	1:A:380:ILE:HA	2.00	0.43
1:B:551:SER:HB3	1:B:566:CYS:H	1.82	0.43
1:C:343:ASP:HA	1:C:379:ASN:HB3	1.99	0.43
1:C:398:THR:HG22	1:C:429:GLU:HB3	2.01	0.43
2:H:148:LYS:HB3	2:H:148:LYS:HE2	1.76	0.43
2:I:33:TYR:HB2	2:I:99:VAL:HB	2.00	0.43
2:J:33:TYR:HB2	2:J:99:VAL:HB	1.99	0.43
1:C:112:LEU:HD21	1:C:115:LEU:HD21	2.01	0.43
3:M:156:SER:HA	3:M:157:SER:HA	1.54	0.43
3:N:25:SER:OG	3:N:26:LEU:N	2.51	0.43
1:B:391:SER:O	1:B:394:SER:OG	2.21	0.43
1:D:311:ALA:HB1	1:D:339:LEU:HD13	2.00	0.43
2:H:151:PHE:HA	2:H:152:PRO:HA	1.82	0.43
1:C:72:MET:HA	1:C:102:LEU:O	2.19	0.43
1:D:123:ILE:HB	1:D:148:VAL:HA	2.00	0.43
2:H:73:ASP:OD1	2:H:75:SER:OG	2.32	0.43
2:I:127:PHE:HB2	2:I:146:LEU:HD22	2.01	0.42
3:O:153:LYS:HA	3:O:158:PRO:HA	2.00	0.42
1:C:523:GLU:OE2	1:C:530:CYS:HB3	2.19	0.42
1:B:349:LEU:HD13	1:B:360:LEU:HD23	2.01	0.42
1:C:63:GLU:OE2	1:C:87:ARG:HD2	2.19	0.42
1:A:552:ASP:OD2	1:A:565:HIS:NE2	2.52	0.42
1:A:278:ASP:O	1:A:280:THR:N	2.52	0.42
1:A:402:ARG:HG2	2:H:33:TYR:CE1	2.55	0.42
1:B:133:ASN:HB3	1:B:136:LEU:HB3	2.02	0.42
1:C:122:GLU:HA	1:C:147:ILE:HG13	2.02	0.42
1:D:65:THR:HA	1:D:87:ARG:HD2	2.01	0.42
3:M:28:ASN:O	3:M:32:ASN:HB2	2.20	0.42
1:B:256:ASN:HA	1:B:257:PRO:HD3	1.85	0.42
1:D:437:ILE:HB	1:D:465:ILE:HG23	2.02	0.42
3:M:28:ASN:OD1	3:M:29:ILE:N	2.46	0.42
1:B:423:GLY:O	1:B:491:TRP:HB3	2.20	0.42
1:C:402:ARG:NE	2:J:103:ASP:OD1	2.33	0.42
1:A:534:HIS:CE1	1:A:551:SER:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:7:PRO:HA	3:O:8:PRO:HD3	1.89	0.42
1:A:273:HIS:C	1:A:275:PHE:H	2.27	0.41
3:M:140:ILE:HG12	3:M:199:VAL:HG21	2.02	0.41
3:O:61:ASP:OD1	3:O:61:ASP:N	2.53	0.41
1:A:211:GLU:OE2	1:A:238:PRO:HB3	2.20	0.41
1:B:311:ALA:HB2	3:M:31:LEU:HA	2.02	0.41
1:C:211:GLU:OE2	1:C:238:PRO:HA	2.20	0.41
3:N:168:PRO:HA	3:N:178:ALA:HB2	2.02	0.41
1:C:11:PRO:HA	1:C:12:GLY:HA3	1.80	0.41
1:C:538:GLN:HB3	1:C:556:GLN:HG2	2.02	0.41
1:D:168:HIS:ND1	1:D:170:VAL:HG22	2.36	0.41
3:L:190:LYS:HE3	3:L:190:LYS:HA	2.02	0.41
1:A:357:ILE:CG1	1:B:320:ARG:HH11	2.34	0.41
1:A:415:LYS:O	3:M:57:SER:OG	2.35	0.41
1:A:562:ASP:HA	1:A:591:CYS:HB2	2.02	0.41
1:D:570:CYS:HA	1:D:571:PRO:HD2	1.73	0.41
2:J:157:VAL:HG22	2:J:203:VAL:HG22	2.01	0.41
3:M:28:ASN:HA	3:M:93:ASP:HA	2.02	0.41
3:O:122:PHE:HA	3:O:123:PRO:HD3	1.90	0.41
3:N:28:ASN:O	3:N:32:ASN:HB2	2.21	0.41
1:D:85:VAL:HG21	1:D:226:ALA:HB2	2.03	0.41
3:M:116:ALA:HA	3:M:117:PRO:HD3	1.91	0.41
3:N:166:THR:OG1	3:N:167:THR:N	2.54	0.41
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.89	0.41
1:B:198:HIS:HB3	1:B:208:CYS:HB2	2.02	0.41
1:C:520:GLU:HA	1:C:521:PRO:HA	1.87	0.41
1:D:211:GLU:OE2	1:D:238:PRO:HG3	2.21	0.41
3:O:36:TRP:CE2	3:O:74:LEU:HB2	2.56	0.41
1:A:241:PRO:HB2	1:A:260:LYS:H	1.86	0.41
1:B:87:ARG:HG2	1:B:124:LEU:HD12	2.02	0.41
1:B:137:CYS:C	1:B:139:MET:H	2.29	0.41
1:C:278:ASP:O	1:C:280:THR:N	2.54	0.41
1:D:400:GLY:O	1:D:431:SER:HB2	2.21	0.41
1:D:418:ASN:HD21	4:D:701:NAG:C7	2.34	0.41
2:I:123:GLY:HA2	2:I:124:PRO:HD3	1.91	0.41
2:H:127:PHE:O	2:H:146:LEU:HB3	2.21	0.41
2:I:151:PHE:HA	2:I:152:PRO:HA	1.80	0.40
1:C:195:CYS:HB2	1:C:207:CYS:HB2	1.84	0.40
2:H:75:SER:HB2	2:J:120:SER:HB3	2.03	0.40
1:B:78:LEU:HA	1:B:79:PRO:HD3	1.92	0.40
1:B:456:ARG:HD3	2:I:57:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:GLY:O	1:C:431:SER:HB2	2.21	0.40
1:C:405:TYR:CE2	1:C:412:LEU:HD22	2.57	0.40
1:C:570:CYS:O	1:C:572:HIS:N	2.55	0.40
1:D:271:CYS:HA	1:D:272:PRO:HD3	1.96	0.40
1:D:278:ASP:O	1:D:280:THR:N	2.55	0.40
2:H:40:ALA:HB3	2:H:43:LYS:HB2	2.03	0.40
1:C:308:CYS:HA	1:C:309:PRO:HD3	1.95	0.40
1:C:456:ARG:HD3	2:J:57:VAL:HG22	2.03	0.40
2:J:29:PHE:O	2:J:72:ARG:NH2	2.55	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	557/627 (89%)	491 (88%)	58 (10%)	8 (1%)	9	39
1	B	522/627 (83%)	447 (86%)	65 (12%)	10 (2%)	6	33
1	C	519/627 (83%)	424 (82%)	76 (15%)	19 (4%)	2	18
1	D	478/627 (76%)	402 (84%)	60 (13%)	16 (3%)	3	21
2	H	174/221 (79%)	166 (95%)	6 (3%)	2 (1%)	11	43
2	I	190/221 (86%)	166 (87%)	17 (9%)	7 (4%)	2	18
2	J	167/221 (76%)	150 (90%)	14 (8%)	3 (2%)	6	34
2	K	172/221 (78%)	149 (87%)	17 (10%)	6 (4%)	3	20
3	L	179/216 (83%)	157 (88%)	17 (10%)	5 (3%)	4	25
3	M	199/216 (92%)	166 (83%)	25 (13%)	8 (4%)	2	17
3	N	176/216 (82%)	147 (84%)	23 (13%)	6 (3%)	3	20
3	O	188/216 (87%)	166 (88%)	19 (10%)	3 (2%)	7	36
All	All	3521/4256 (83%)	3031 (86%)	397 (11%)	93 (3%)	4	26

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	148	VAL
1	C	255	PRO
1	D	134	ASP
1	D	167	CYS
1	D	571	PRO
2	H	112	THR
2	I	112	THR
2	I	190	PRO
2	I	209	ASN
2	J	112	THR
2	K	209	ASN
3	M	124	PRO
1	B	116	ARG
1	B	296	ASN
1	C	51	HIS
1	C	233	SER
1	C	279	GLN
1	C	559	HIS
1	D	178	PRO
1	D	459	THR
2	H	160	ASN
3	L	110	LEU
2	J	209	ASN
2	K	112	THR
3	M	136	LEU
3	M	137	VAL
3	N	110	LEU
3	N	202	GLU
3	O	155	ASP
1	A	87	ARG
1	A	249	LEU
1	A	279	GLN
1	A	571	PRO
1	B	204	PRO
1	B	279	GLN
1	B	515	ASN
1	C	102	LEU
1	C	196	ASN
1	C	197	GLY
1	C	225	PHE
1	C	251	PHE
1	D	112	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	137	CYS
1	D	279	GLN
1	D	460	GLU
1	D	522	ARG
2	I	170	THR
3	M	110	LEU
3	M	189	TRP
3	N	203	GLY
3	O	96	PRO
1	A	116	ARG
1	A	251	PHE
1	A	587	VAL
1	B	95	LYS
1	C	124	LEU
1	C	146	ASP
1	C	220	GLN
1	C	221	ASP
1	C	294	ASP
1	C	441	ARG
1	D	59	GLN
1	D	261	TYR
3	L	14	PRO
2	J	143	LEU
2	K	120	SER
3	M	157	SER
3	O	97	PRO
1	A	95	LYS
1	B	102	LEU
1	B	297	GLY
1	B	400	GLY
1	D	564	PRO
1	D	591	CYS
3	L	96	PRO
2	I	149	ASP
2	K	102	GLY
2	K	121	THR
3	M	97	PRO
3	N	142	ASP
1	B	286	CYS
1	C	571	PRO
2	K	148	LYS
3	N	97	PRO

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Mol	Chain	Res	Type
1	D	219	PRO
1	D	306	GLY
3	N	58	GLY
1	C	241	PRO
3	L	97	PRO
3	L	146	GLY
2	I	195	GLY
3	M	96	PRO
2	I	152	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	379/543 (70%)	371 (98%)	8 (2%)	47	71
1	B	371/543 (68%)	365 (98%)	6 (2%)	55	75
1	C	390/543 (72%)	380 (97%)	10 (3%)	40	69
1	D	338/543 (62%)	330 (98%)	8 (2%)	43	70
2	H	144/183 (79%)	140 (97%)	4 (3%)	38	68
2	I	149/183 (81%)	147 (99%)	2 (1%)	61	78
2	J	131/183 (72%)	130 (99%)	1 (1%)	73	82
2	K	130/183 (71%)	129 (99%)	1 (1%)	73	82
3	L	143/180 (79%)	141 (99%)	2 (1%)	59	77
3	M	146/180 (81%)	141 (97%)	5 (3%)	32	64
3	N	131/180 (73%)	130 (99%)	1 (1%)	73	82
3	O	140/180 (78%)	138 (99%)	2 (1%)	59	77
All	All	2592/3624 (72%)	2542 (98%)	50 (2%)	50	73

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	271	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	324	VAL
1	A	341	ASN
1	A	355	HIS
1	A	392	VAL
1	A	469	ARG
1	A	499	LEU
1	A	567	VAL
1	B	9	VAL
1	B	152	ASP
1	B	157	VAL
1	B	250	THR
1	B	268	VAL
1	B	341	ASN
1	C	80	LEU
1	C	147	ILE
1	C	148	VAL
1	C	156	VAL
1	C	223	ASP
1	C	277	VAL
1	C	341	ASN
1	C	349	LEU
1	C	355	HIS
1	C	575	LEU
1	D	44	LEU
1	D	69	LEU
1	D	128	VAL
1	D	341	ASN
1	D	417	LEU
1	D	484	LEU
1	D	497	GLN
1	D	522	ARG
2	H	2	VAL
2	H	28	THR
2	H	58	THR
2	H	156	THR
3	L	95	SER
3	L	190	LYS
2	I	155	VAL
2	I	168	VAL
2	J	155	VAL
2	K	174	VAL
3	M	95	SER

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Mol	Chain	Res	Type
3	M	127	GLU
3	M	136	LEU
3	M	184	LEU
3	M	199	VAL
3	N	95	SER
3	O	95	SER
3	O	165	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
1	A	418	ASN
1	A	447	HIS
1	A	503	ASN
1	B	416	ASN
1	B	418	ASN
1	B	467	HIS
1	B	497	GLN
1	B	503	ASN
1	C	119	GLN
1	C	341	ASN
1	C	416	ASN
1	C	418	ASN
1	C	503	ASN
1	D	82	ASN
1	D	231	ASN
1	D	381	GLN
1	D	389	ASN
1	D	418	ASN
1	D	538	GLN
2	H	82	GLN
3	L	38	GLN
3	L	201	HIS
2	I	59	ASN
2	I	77	ASN
2	J	59	ASN
2	J	209	ASN
3	M	173	ASN
3	N	38	GLN
3	O	32	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 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	C	702	-	14,14,15	0.47	0	17,19,21	1.36	2 (11%)
4	NAG	D	702	-	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	M	301	-	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	A	702	-	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	A	701	-	14,14,15	0.31	0	17,19,21	0.35	0
4	NAG	D	703	-	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	C	701	-	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	B	702	-	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	B	701	-	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	D	701	-	14,14,15	0.26	0	17,19,21	0.40	0
4	NAG	C	703	-	14,14,15	0.24	0	17,19,21	0.41	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	702	-	-	6/6/23/26	0/1/1/1
4	NAG	D	702	-	-	2/6/23/26	0/1/1/1
4	NAG	M	301	-	-	2/6/23/26	0/1/1/1
4	NAG	A	702	-	-	0/6/23/26	0/1/1/1
4	NAG	A	701	-	-	2/6/23/26	0/1/1/1
4	NAG	D	703	-	-	0/6/23/26	0/1/1/1
4	NAG	C	701	-	-	2/6/23/26	0/1/1/1
4	NAG	B	702	-	-	2/6/23/26	0/1/1/1
4	NAG	B	701	-	-	4/6/23/26	0/1/1/1
4	NAG	D	701	-	-	2/6/23/26	0/1/1/1
4	NAG	C	703	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	702	NAG	C2-N2-C7	4.66	129.15	122.90
4	C	702	NAG	C1-C2-N2	2.13	113.80	110.43

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	702	NAG	O5-C5-C6-O6
4	B	701	NAG	O5-C5-C6-O6
4	C	701	NAG	O5-C5-C6-O6
4	B	702	NAG	O5-C5-C6-O6
4	C	702	NAG	O5-C5-C6-O6
4	D	701	NAG	O5-C5-C6-O6
4	M	301	NAG	O5-C5-C6-O6
4	M	301	NAG	C4-C5-C6-O6
4	B	701	NAG	C4-C5-C6-O6
4	D	702	NAG	C4-C5-C6-O6
4	C	703	NAG	O5-C5-C6-O6
4	C	701	NAG	C4-C5-C6-O6
4	C	703	NAG	C4-C5-C6-O6
4	C	702	NAG	C4-C5-C6-O6
4	D	701	NAG	C4-C5-C6-O6
4	B	702	NAG	C4-C5-C6-O6
4	B	701	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	701	NAG	O7-C7-N2-C2
4	C	702	NAG	C8-C7-N2-C2
4	C	702	NAG	O7-C7-N2-C2
4	A	701	NAG	O5-C5-C6-O6
4	A	701	NAG	C4-C5-C6-O6
4	C	702	NAG	C1-C2-N2-C7
4	C	702	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	702	NAG	1	0
4	D	701	NAG	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	561/627 (89%)	1.13	100 (17%) 4 3	15, 64, 126, 188	14 (2%)
1	B	530/627 (84%)	1.10	108 (20%) 3 2	13, 64, 122, 187	16 (3%)
1	C	539/627 (85%)	1.23	118 (21%) 2 2	12, 68, 139, 209	8 (1%)
1	D	509/627 (81%)	1.42	150 (29%) 1 1	12, 75, 142, 227	8 (1%)
2	H	182/221 (82%)	0.93	33 (18%) 3 3	15, 42, 144, 194	0
2	I	198/221 (89%)	0.95	42 (21%) 2 2	15, 40, 152, 176	0
2	J	175/221 (79%)	0.85	29 (16%) 4 3	16, 39, 129, 189	0
2	K	180/221 (81%)	1.00	41 (22%) 2 2	17, 41, 149, 187	0
3	L	185/216 (85%)	1.09	37 (20%) 3 2	19, 57, 145, 209	0
3	M	203/216 (93%)	1.39	57 (28%) 1 1	22, 62, 156, 215	0
3	N	184/216 (85%)	1.28	53 (28%) 1 1	15, 56, 144, 194	0
3	O	200/216 (92%)	1.47	67 (33%) 1 1	18, 65, 165, 221	0
All	All	3646/4256 (85%)	1.18	835 (22%) 2 2	12, 62, 143, 227	46 (1%)

All (835) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	135	THR	9.9
1	C	200	PHE	7.9
1	C	15	ASN	7.5
1	A	294	ASP	7.0
1	D	189	THR	6.9
1	A	232	ASP	6.7
3	N	121	LEU	6.7
1	D	294	ASP	6.7
3	M	207	GLU	6.7
1	C	134	ASP	6.6
1	C	105	ASN	6.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	I	129	LEU	6.5
3	N	173	ASN	6.3
1	D	215	GLY	6.2
1	D	160	ASN	6.2
3	M	137	VAL	6.2
2	J	125	SER	6.1
2	I	185	SER	6.0
3	L	95	SER	6.0
2	J	212	VAL	5.9
3	O	148	VAL	5.9
2	K	159	TRP	5.7
1	D	72	MET	5.6
1	D	185	THR	5.6
1	C	270	SER	5.5
2	J	146	LEU	5.5
1	A	235	ALA	5.5
2	H	144	GLY	5.5
3	N	122	PHE	5.5
2	I	202	ASN	5.4
3	L	111	GLY	5.4
3	O	119	VAL	5.3
1	B	104	TYR	5.3
1	A	203	ASN	5.2
3	N	137	VAL	5.2
1	D	122	GLU	5.2
2	H	129	LEU	5.2
1	C	168	HIS	5.1
3	M	122	PHE	5.1
3	M	113	PRO	5.1
3	L	134	ALA	5.1
3	O	134	ALA	5.0
2	I	145	CYS	4.9
2	I	212	VAL	4.9
1	D	59	GLN	4.9
3	M	136	LEU	4.9
1	D	130	ILE	4.9
2	K	155	VAL	4.9
1	D	68	VAL	4.8
1	D	186	LEU	4.8
3	O	117	PRO	4.8
1	B	159	ASP	4.8
1	D	111	ALA	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	J	186	VAL	4.7
3	N	114	LYS	4.7
1	D	70	VAL	4.7
2	H	130	ALA	4.7
2	K	178	SER	4.7
1	D	44	LEU	4.7
1	A	590	GLU	4.6
1	B	556	GLN	4.6
1	C	202	PRO	4.6
3	M	123	PRO	4.6
2	K	127	PHE	4.6
1	C	549	SER	4.6
1	D	266	VAL	4.6
1	D	155	ILE	4.5
1	C	150	ASP	4.5
2	J	55	GLY	4.5
2	K	204	ASN	4.5
3	M	121	LEU	4.5
1	B	541	GLU	4.5
3	M	133	LYS	4.5
1	D	77	THR	4.5
1	D	114	GLN	4.5
3	N	183	SER	4.4
1	B	253	LEU	4.4
2	I	126	VAL	4.4
2	K	101	LEU	4.4
3	O	197	CYS	4.4
1	B	273	HIS	4.4
1	C	145	ARG	4.4
1	D	137	CYS	4.4
3	M	197	CYS	4.4
1	A	295	LYS	4.4
2	K	176	GLN	4.4
1	D	305	GLY	4.3
1	D	245	VAL	4.3
1	C	207	CYS	4.3
1	B	79	PRO	4.3
1	D	187	THR	4.3
3	N	145	PRO	4.3
1	B	246	TYR	4.3
1	C	208	CYS	4.3
3	M	158	PRO	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	L	136	LEU	4.2
3	O	161	ALA	4.2
3	M	120	THR	4.2
3	M	182	LEU	4.2
3	N	166	THR	4.2
2	K	177	SER	4.2
2	J	1	GLU	4.2
1	A	274	ASN	4.2
1	D	552	ASP	4.2
1	D	164	CYS	4.2
1	A	257	PRO	4.2
1	D	100	VAL	4.1
1	D	184	GLN	4.1
1	C	210	ASP	4.1
1	C	258	HIS	4.1
1	D	38	GLU	4.1
3	O	95	SER	4.1
1	A	572	HIS	4.1
1	C	216	CYS	4.1
1	C	252	GLN	4.1
1	B	247	ASN	4.1
1	C	109	SER	4.1
3	O	183	SER	4.1
1	C	164	CYS	4.1
1	A	582	TYR	4.1
3	O	165	THR	4.1
1	D	190	ILE	4.1
3	O	198	GLN	4.1
1	C	159	ASP	4.1
2	J	185	SER	4.1
1	B	292	GLU	4.1
1	C	169	GLU	4.1
1	A	285	ALA	4.1
1	C	272	PRO	4.1
2	H	187	VAL	4.0
1	C	166	PRO	4.0
1	C	247	ASN	4.0
1	B	232	ASP	4.0
3	O	195	TYR	4.0
2	I	142	ALA	4.0
2	K	161	SER	4.0
1	B	536	GLU	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	79	PRO	4.0
3	L	168	PRO	4.0
1	B	13	THR	4.0
2	H	185	SER	4.0
3	M	209	THR	4.0
3	O	185	THR	4.0
1	D	590	GLU	4.0
1	A	269	ALA	4.0
1	D	141	THR	4.0
1	C	264	GLY	3.9
2	K	202	ASN	3.9
3	L	125	SER	3.9
1	C	152	ASP	3.9
2	H	131	PRO	3.9
3	M	114	LYS	3.9
1	D	118	THR	3.9
3	O	163	VAL	3.9
1	D	204	PRO	3.9
3	M	124	PRO	3.9
2	H	127	PHE	3.9
1	C	199	CYS	3.9
3	N	151	ALA	3.9
1	B	105	ASN	3.9
1	D	274	ASN	3.9
1	A	273	HIS	3.8
1	C	60	TRP	3.8
3	M	95	SER	3.8
3	M	183	SER	3.8
1	D	142	ILE	3.8
3	O	124	PRO	3.8
3	N	156	SER	3.8
2	K	187	VAL	3.8
2	J	201	CYS	3.8
1	B	274	ASN	3.8
1	C	82	ASN	3.8
1	D	547	ASN	3.7
1	B	258	HIS	3.7
1	D	165	PRO	3.7
1	C	295	LYS	3.7
2	K	214	LYS	3.7
2	I	127	PHE	3.7
3	M	186	PRO	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	I	170	THR	3.7
3	N	136	LEU	3.7
1	C	330	ASP	3.7
1	D	193	PRO	3.7
2	I	147	VAL	3.7
3	O	130	GLN	3.7
1	A	60	TRP	3.7
2	I	146	LEU	3.7
3	O	123	PRO	3.6
3	O	194	SER	3.6
1	B	256	ASN	3.6
1	B	194	GLN	3.6
1	C	265	GLY	3.6
1	D	170	VAL	3.6
3	O	125	SER	3.6
1	A	54	ASP	3.6
2	H	214	LYS	3.6
1	D	116	ARG	3.6
1	A	584	TYR	3.6
2	H	169	HIS	3.6
3	N	123	PRO	3.6
1	C	195	CYS	3.5
1	C	113	ARG	3.5
2	K	125	SER	3.5
3	N	139	LEU	3.5
1	D	129	TYR	3.5
3	O	210	VAL	3.5
1	D	102	LEU	3.5
3	L	193	ARG	3.5
1	D	63	GLU	3.5
3	O	127	GLU	3.5
1	C	220	GLN	3.5
1	C	556	GLN	3.5
3	M	161	ALA	3.5
3	O	141	SER	3.5
2	H	123	GLY	3.4
1	A	279	GLN	3.4
1	D	139	MET	3.4
3	N	152	TRP	3.4
3	O	164	GLU	3.4
1	B	263	TYR	3.4
2	K	126	VAL	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	O	149	THR	3.4
1	A	37	CYS	3.4
1	D	212	CYS	3.4
1	C	577	ALA	3.4
2	I	156	THR	3.4
2	K	209	ASN	3.4
2	H	145	CYS	3.4
3	N	147	ALA	3.4
1	A	206	GLN	3.4
1	C	543	THR	3.4
1	B	196	ASN	3.4
1	C	251	PHE	3.4
3	N	142	ASP	3.4
1	D	579	GLY	3.4
1	D	166	PRO	3.4
3	L	135	THR	3.4
3	N	209	THR	3.4
1	D	205	ASN	3.3
3	N	163	VAL	3.3
1	B	559	HIS	3.3
1	C	193	PRO	3.3
2	H	209	ASN	3.3
1	D	157	VAL	3.3
2	I	164	LEU	3.3
2	J	168	VAL	3.3
3	O	187	GLU	3.3
1	B	12	GLY	3.3
1	C	146	ASP	3.3
3	M	155	ASP	3.3
2	I	189	VAL	3.3
2	H	211	LYS	3.3
1	B	530	CYS	3.3
1	D	208	CYS	3.3
2	H	149	ASP	3.3
1	A	231	ASN	3.3
3	O	128	GLU	3.3
1	D	582	TYR	3.3
1	B	250	THR	3.3
1	A	266	VAL	3.3
1	A	277	VAL	3.3
2	K	160	ASN	3.3
3	M	189	TRP	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	169	GLU	3.3
2	I	158	SER	3.2
1	C	175	CYS	3.2
3	O	139	LEU	3.2
1	B	266	VAL	3.2
3	O	120	THR	3.2
1	D	71	ALA	3.2
2	H	204	ASN	3.2
1	A	38	GLU	3.2
1	A	261	TYR	3.2
3	O	186	PRO	3.2
3	N	143	PHE	3.2
1	C	293	VAL	3.2
1	D	85	VAL	3.2
1	D	90	GLN	3.2
3	N	162	GLY	3.2
1	C	249	LEU	3.2
2	K	211	LYS	3.2
3	L	184	LEU	3.2
1	A	219	PRO	3.2
1	D	99	PHE	3.2
3	M	2	SER	3.2
3	N	196	SER	3.2
2	K	200	ILE	3.2
1	A	169	GLU	3.2
1	D	231	ASN	3.2
3	M	208	LYS	3.2
1	C	575	LEU	3.2
3	L	123	PRO	3.2
1	C	51	HIS	3.2
1	C	137	CYS	3.2
3	L	202	GLU	3.2
3	L	199	VAL	3.2
1	D	138	HIS	3.2
1	B	242	GLN	3.2
3	M	126	SER	3.2
1	A	330	ASP	3.1
2	H	213	ASP	3.1
1	A	10	CYS	3.1
3	O	189	TRP	3.1
2	J	147	VAL	3.1
1	A	193	PRO	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	168	HIS	3.1
1	B	543	THR	3.1
2	J	142	ALA	3.1
3	N	180	SER	3.1
1	A	236	CYS	3.1
1	B	566	CYS	3.1
2	K	1	GLU	3.1
2	I	155	VAL	3.1
1	A	468	ASN	3.1
2	K	124	PRO	3.1
1	B	252	GLN	3.1
3	O	213	THR	3.1
3	M	157	SER	3.1
1	D	93	ASP	3.1
3	L	192	HIS	3.1
1	A	59	GLN	3.1
1	D	206	GLN	3.1
1	D	39	VAL	3.1
3	L	187	GLU	3.1
3	O	207	GLU	3.1
1	B	296	ASN	3.1
1	D	272	PRO	3.1
2	I	143	LEU	3.0
3	O	116	ALA	3.0
1	D	172	LYS	3.0
1	C	204	PRO	3.0
1	D	171	CYS	3.0
1	A	256	ASN	3.0
3	L	149	THR	3.0
1	B	45	GLU	3.0
1	B	72	MET	3.0
3	O	2	SER	3.0
1	D	535	PRO	3.0
1	B	129	TYR	3.0
1	A	107	ASN	3.0
2	J	155	VAL	3.0
3	O	205	THR	3.0
1	C	165	PRO	3.0
1	C	217	SER	3.0
2	H	158	SER	3.0
3	L	175	LYS	3.0
1	C	271	CYS	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	J	174	VAL	3.0
1	B	518	ASN	3.0
1	B	77	THR	3.0
1	A	580	PRO	3.0
1	B	48	LEU	3.0
3	L	127	GLU	3.0
1	D	217	SER	3.0
3	O	118	SER	3.0
3	O	172	SER	3.0
3	N	160	LYS	3.0
1	C	513	HIS	3.0
2	K	179	GLY	3.0
3	O	146	GLY	3.0
3	O	173	ASN	3.0
1	B	51	HIS	2.9
1	B	126	GLY	2.9
1	B	41	MET	2.9
1	D	123	ILE	2.9
1	B	271	CYS	2.9
1	B	280	THR	2.9
2	K	175	LEU	2.9
1	C	213	ALA	2.9
3	L	2	SER	2.9
1	A	89	THR	2.9
1	D	133	ASN	2.9
3	M	138	CYS	2.9
1	C	266	VAL	2.9
3	N	159	VAL	2.9
1	A	214	GLY	2.9
1	D	264	GLY	2.9
3	O	111	GLY	2.9
3	N	120	THR	2.9
2	J	177	SER	2.9
3	M	170	LYS	2.9
1	A	210	ASP	2.9
1	A	296	ASN	2.9
3	L	174	ASN	2.9
3	M	119	VAL	2.9
1	B	563	GLY	2.9
1	C	299	LYS	2.9
1	D	249	LEU	2.9
1	B	269	ALA	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	M	151	ALA	2.8
3	N	177	ALA	2.8
1	D	543	THR	2.8
1	C	162	ARG	2.8
3	O	129	LEU	2.8
1	D	101	MET	2.8
1	B	279	GLN	2.8
3	N	171	GLN	2.8
3	N	113	PRO	2.8
1	A	118	THR	2.8
2	I	201	CYS	2.8
1	D	220	GLN	2.8
3	O	191	SER	2.8
3	O	196	SER	2.8
1	A	259	THR	2.8
3	L	129	LEU	2.8
1	B	285	ALA	2.8
3	L	147	ALA	2.8
1	D	62	ARG	2.8
1	D	40	VAL	2.8
2	K	147	VAL	2.8
3	M	196	SER	2.8
1	A	13	THR	2.8
1	A	575	LEU	2.8
1	B	254	GLU	2.8
3	M	164	GLU	2.8
1	B	75	PHE	2.8
1	C	101	MET	2.8
1	A	195	CYS	2.8
3	O	145	PRO	2.8
1	A	108	SER	2.8
1	A	298	LEU	2.8
1	C	250	THR	2.8
1	D	131	GLU	2.8
1	A	251	PHE	2.7
1	D	98	ILE	2.8
2	H	156	THR	2.8
2	K	213	ASP	2.7
1	D	110	HIS	2.7
1	D	188	LYS	2.7
3	O	154	ALA	2.7
1	B	137	CYS	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	537	CYS	2.7
1	C	267	CYS	2.7
1	C	276	VAL	2.7
2	I	187	VAL	2.7
1	A	539	PRO	2.7
1	C	219	PRO	2.7
1	B	520	GLU	2.7
3	M	156	SER	2.7
3	O	140	ILE	2.7
3	O	156	SER	2.7
1	D	503	ASN	2.7
1	C	253	LEU	2.7
1	C	546	CYS	2.7
1	C	541	GLU	2.7
2	J	182	SER	2.7
2	K	121	THR	2.7
2	I	169	HIS	2.7
1	D	298	LEU	2.7
1	C	191	CYS	2.7
1	D	542	GLY	2.7
3	M	187	GLU	2.7
1	B	284	ARG	2.7
1	A	583	LYS	2.7
2	J	170	THR	2.7
3	M	11	SER	2.7
3	M	125	SER	2.7
1	A	586	ASP	2.7
3	O	144	TYR	2.7
1	C	186	LEU	2.7
1	C	142	ILE	2.7
3	N	198	GLN	2.7
1	C	576	GLY	2.7
1	D	191	CYS	2.7
1	D	520	GLU	2.7
1	D	536	GLU	2.7
2	H	125	SER	2.7
2	K	185	SER	2.7
1	D	153	ALA	2.7
1	D	58	LEU	2.7
2	H	157	VAL	2.7
2	J	213	ASP	2.7
1	B	205	ASN	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	597	ASN	2.7
1	B	166	PRO	2.6
1	C	571	PRO	2.6
3	M	145	PRO	2.6
1	C	275	PHE	2.6
3	N	170	LYS	2.6
3	N	207	GLU	2.6
1	B	60	TRP	2.6
1	B	55	LEU	2.6
1	D	97	ALA	2.6
1	D	148	VAL	2.6
1	D	327	SER	2.6
2	I	141	ALA	2.6
1	A	350	ASN	2.6
1	C	196	ASN	2.6
2	H	128	PRO	2.6
2	I	209	ASN	2.6
1	B	154	GLU	2.6
1	C	170	VAL	2.6
1	D	112	LEU	2.6
2	H	120	SER	2.6
3	O	160	LYS	2.6
1	A	82	ASN	2.6
1	B	52	ASN	2.6
1	D	43	ASN	2.6
2	I	55	GLY	2.6
3	N	202	GLU	2.6
1	A	58	LEU	2.6
1	B	259	THR	2.6
1	C	115	LEU	2.6
3	L	182	LEU	2.6
2	I	163	ALA	2.6
1	C	301	CYS	2.6
1	D	175	CYS	2.6
3	L	11	SER	2.6
3	M	204	SER	2.6
1	C	289	ASP	2.6
1	C	550	GLY	2.6
3	O	162	GLY	2.6
1	C	39	VAL	2.6
3	N	206	VAL	2.6
1	A	106	THR	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	I	159	TRP	2.6
1	A	164	CYS	2.6
1	D	96	PHE	2.6
2	I	125	SER	2.6
3	N	112	GLN	2.6
1	B	244	LEU	2.6
1	D	555	ALA	2.6
1	B	185	THR	2.6
2	H	151	PHE	2.5
1	C	209	HIS	2.5
1	C	212	CYS	2.5
1	D	539	PRO	2.5
2	I	178	SER	2.5
1	B	249	LEU	2.5
1	B	293	VAL	2.5
1	C	294	ASP	2.5
2	H	155	VAL	2.5
3	M	206	VAL	2.5
3	O	178	ALA	2.5
3	M	152	TRP	2.5
2	I	171	PHE	2.5
2	K	151	PHE	2.5
1	C	79	PRO	2.5
3	N	181	TYR	2.5
1	A	554	CYS	2.5
2	I	184	SER	2.5
2	J	143	LEU	2.5
3	N	30	GLY	2.5
3	N	169	SER	2.5
1	A	205	ASN	2.5
1	A	292	GLU	2.5
1	B	529	GLU	2.5
1	C	259	THR	2.5
1	D	459	THR	2.5
3	N	144	TYR	2.5
1	C	188	LYS	2.5
1	D	113	ARG	2.5
2	I	211	LYS	2.5
2	K	122	LYS	2.5
3	L	190	LYS	2.5
1	A	538	GLN	2.5
1	B	267	CYS	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	N	111	GLY	2.5
1	C	163	SER	2.5
2	K	158	SER	2.5
3	M	194	SER	2.5
2	I	204	ASN	2.5
2	K	149	ASP	2.5
1	D	144	TRP	2.5
3	L	185	THR	2.5
3	N	158	PRO	2.5
3	N	119	VAL	2.5
1	D	224	CYS	2.5
3	N	197	CYS	2.5
1	A	74	GLU	2.5
1	A	154	GLU	2.5
1	D	41	MET	2.5
1	A	223	ASP	2.5
1	C	225	PHE	2.5
1	D	325	ASP	2.5
2	K	148	LYS	2.5
2	I	190	PRO	2.5
1	A	201	GLY	2.5
3	M	146	GLY	2.5
2	K	203	VAL	2.5
3	N	150	VAL	2.5
1	A	556	GLN	2.5
1	B	538	GLN	2.5
3	M	154	ALA	2.4
3	O	115	ALA	2.4
1	B	282	CYS	2.4
2	J	158	SER	2.4
1	A	189	THR	2.4
2	I	188	THR	2.4
1	D	521	PRO	2.4
1	A	588	GLN	2.4
1	C	279	GLN	2.4
1	C	147	ILE	2.4
1	A	546	CYS	2.4
3	M	202	GLU	2.4
1	C	284	ARG	2.4
1	C	578	LYS	2.4
2	H	148	LYS	2.4
2	J	202	ASN	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	J	209	ASN	2.4
3	L	173	ASN	2.4
1	D	221	ASP	2.4
1	D	562	ASP	2.4
3	M	205	THR	2.4
1	A	564	PRO	2.4
2	I	193	SER	2.4
3	L	179	SER	2.4
1	B	112	LEU	2.4
1	B	564	PRO	2.4
2	K	128	PRO	2.4
1	B	482	ASP	2.4
1	A	263	TYR	2.4
1	B	261	TYR	2.4
1	D	559	HIS	2.4
1	A	220	GLN	2.4
1	D	78	LEU	2.4
2	H	177	SER	2.4
1	C	167	CYS	2.4
1	D	167	CYS	2.4
1	B	82	ASN	2.4
2	H	55	GLY	2.4
2	I	160	ASN	2.4
1	A	258	HIS	2.4
3	N	94	ASP	2.4
3	O	170	LYS	2.4
3	O	188	GLN	2.4
1	B	204	PRO	2.4
1	C	183	CYS	2.4
1	D	594	CYS	2.4
1	A	50	GLY	2.3
1	A	577	ALA	2.3
1	C	155	ILE	2.3
1	D	135	LYS	2.3
1	D	565	HIS	2.3
1	D	595	HIS	2.3
3	L	115	ALA	2.3
1	B	562	ASP	2.3
1	C	96	PHE	2.3
3	O	121	LEU	2.3
1	A	122	GLU	2.3
1	D	181	GLU	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	O	199	VAL	2.3
1	C	108	SER	2.3
1	C	243	PRO	2.3
2	I	207	PRO	2.3
3	O	158	PRO	2.3
1	A	36	ARG	2.3
1	D	121	THR	2.3
1	D	513	HIS	2.3
3	M	115	ALA	2.3
1	C	72	MET	2.3
1	A	102	LEU	2.3
1	C	194	GLN	2.3
1	D	154	GLU	2.3
1	D	91	VAL	2.3
1	A	204	PRO	2.3
1	D	178	PRO	2.3
1	B	270	SER	2.3
1	D	179	GLY	2.3
1	D	297	GLY	2.3
2	I	71	SER	2.3
3	L	191	SER	2.3
1	A	209	HIS	2.3
2	H	201	CYS	2.3
3	O	176	TYR	2.3
3	M	127	GLU	2.3
1	B	156	VAL	2.3
1	C	86	VAL	2.3
1	D	86	VAL	2.3
2	J	148	LYS	2.3
1	A	12	GLY	2.3
1	B	190	ILE	2.3
1	C	144	TRP	2.3
1	D	176	TRP	2.3
1	B	49	THR	2.3
1	D	568	SER	2.3
1	D	572	HIS	2.3
3	L	121	LEU	2.3
1	A	537	CYS	2.3
1	B	275	PHE	2.3
1	C	560	PHE	2.3
2	I	206	LYS	2.3
1	A	211	GLU	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	N	164	GLU	2.3
1	A	288	PRO	2.3
1	B	535	PRO	2.3
1	C	303	PRO	2.3
1	A	264	GLY	2.3
1	B	222	THR	2.3
2	J	210	THR	2.3
3	O	81	SER	2.3
1	D	67	TYR	2.3
1	A	262	GLN	2.3
3	L	188	GLN	2.3
1	C	245	VAL	2.3
1	A	520	GLU	2.2
1	C	94	GLY	2.2
1	D	593	PRO	2.2
3	O	58	GLY	2.2
2	K	156	THR	2.2
3	N	13	THR	2.2
3	O	209	THR	2.2
3	M	195	TYR	2.2
1	B	262	GLN	2.2
1	A	234	GLY	2.2
1	D	219	PRO	2.2
1	D	115	LEU	2.2
1	B	260	LYS	2.2
1	B	92	TYR	2.2
1	B	505	SER	2.2
1	B	157	VAL	2.2
1	D	128	VAL	2.2
1	A	328	ASN	2.2
1	D	82	ASN	2.2
1	A	329	ILE	2.2
1	C	533	CYS	2.2
1	D	586	ASP	2.2
1	A	297	GLY	2.2
1	C	11	PRO	2.2
3	M	162	GLY	2.2
3	O	182	LEU	2.2
1	C	151	ARG	2.2
2	I	165	THR	2.2
3	O	166	THR	2.2
1	A	237	VAL	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	237	VAL	2.2
1	B	268	VAL	2.2
1	A	549	SER	2.2
1	B	281	SER	2.2
2	J	145	CYS	2.2
3	L	113	PRO	2.2
3	O	147	ALA	2.2
1	A	188	LYS	2.2
1	B	565	HIS	2.2
1	C	121	THR	2.2
2	H	57	VAL	2.2
2	K	157	VAL	2.2
3	O	159	VAL	2.2
3	L	130	GLN	2.2
3	M	198	GLN	2.2
1	D	517	LEU	2.2
1	A	334	ASN	2.2
1	C	292	GLU	2.2
1	B	542	GLY	2.2
1	D	299	LYS	2.2
1	D	152	ASP	2.2
1	D	289	ASP	2.2
2	K	201	CYS	2.2
3	N	138	CYS	2.2
1	C	572	HIS	2.2
1	C	187	THR	2.1
2	K	210	THR	2.1
1	D	61	ILE	2.1
1	B	115	LEU	2.1
1	D	262	GLN	2.1
2	J	184	SER	2.1
2	J	211	LYS	2.1
3	L	183	SER	2.1
1	C	254	GLU	2.1
3	O	211	ALA	2.1
1	B	255	PRO	2.1
1	C	579	GLY	2.1
1	D	265	GLY	2.1
2	H	179	GLY	2.1
3	N	185	THR	2.1
1	D	117	LEU	2.1
2	K	146	LEU	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	K	206	LYS	2.1
1	C	8	ALA	2.1
3	L	116	ALA	2.1
3	N	178	ALA	2.1
1	B	297	GLY	2.1
2	I	192	SER	2.1
3	L	58	GLY	2.1
1	B	9	VAL	2.1
1	C	171	CYS	2.1
2	H	159	TRP	2.1
2	J	149	ASP	2.1
1	A	51	HIS	2.1
3	M	192	HIS	2.1
1	B	102	LEU	2.1
1	C	375	THR	2.1
2	H	122	LYS	2.1
3	O	181	TYR	2.1
1	A	194	GLN	2.1
1	B	53	ALA	2.1
1	B	119	GLN	2.1
2	K	119	ALA	2.1
2	I	179	GLY	2.1
1	B	276	VAL	2.1
1	A	123	ILE	2.1
1	C	117	LEU	2.1
2	J	169	HIS	2.1
3	N	182	LEU	2.1
1	D	242	GLN	2.1
1	A	66	GLY	2.1
1	C	563	GLY	2.1
2	J	123	GLY	2.1
2	K	123	GLY	2.1
1	A	287	PRO	2.1
1	D	257	PRO	2.1
2	H	171	PHE	2.1
3	M	150	VAL	2.1
1	B	210	ASP	2.1
1	A	570	CYS	2.1
3	L	181	TYR	2.1
1	B	264	GLY	2.1
1	B	99	PHE	2.1
1	B	560	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	M	97	PRO	2.1
1	D	511	VAL	2.0
3	M	159	VAL	2.0
1	B	163	SER	2.0
3	M	81	SER	2.0
1	B	116	ARG	2.0
3	M	165	THR	2.0
1	B	557	CYS	2.0
1	D	207	CYS	2.0
1	D	570	CYS	2.0
3	N	154	ALA	2.0
1	B	251	PHE	2.0
1	D	94	GLY	2.0
3	N	146	GLY	2.0
3	O	212	PRO	2.0
1	C	80	LEU	2.0
1	D	448	SER	2.0
3	M	172	SER	2.0
3	N	95	SER	2.0
1	B	554	CYS	2.0
1	D	563	GLY	2.0
1	A	243	PRO	2.0
1	B	47	VAL	2.0
1	C	520	GLU	2.0
1	D	83	LEU	2.0
2	I	183	LEU	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	C	702	14/15	0.64	0.22	26,46,57,59	0
4	NAG	M	301	14/15	0.75	0.22	85,94,103,106	0
4	NAG	C	703	14/15	0.77	0.17	37,58,70,87	0
4	NAG	A	702	14/15	0.79	0.16	21,34,53,71	0
4	NAG	B	701	14/15	0.79	0.16	29,44,51,51	0
4	NAG	B	702	14/15	0.79	0.17	54,59,85,91	0
4	NAG	C	701	14/15	0.80	0.16	25,47,67,71	0
4	NAG	D	702	14/15	0.82	0.17	30,37,49,53	0
4	NAG	D	703	14/15	0.85	0.12	23,45,56,68	0
4	NAG	A	701	14/15	0.86	0.14	35,45,54,56	0
4	NAG	D	701	14/15	0.87	0.14	30,47,62,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.