



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2017 – 11:04 PM EST

PDB ID : 5CUS  
Title : Crystal Structure of sErbB3-Fab3379 Complex  
Authors : Lee, S.; Schlessinger, J.  
Deposited on : unknown  
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

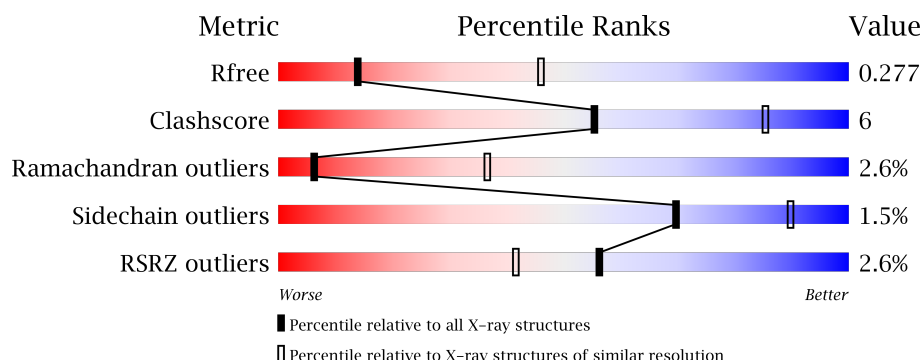
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	627	
1	C	627	
1	D	627	
2	H	221	

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Mol	Chain	Length	Quality of chain
2	I	221	
2	J	221	
2	K	221	
3	L	216	
3	M	216	
3	N	216	
3	O	216	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	M	301	-	-	-	X

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

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

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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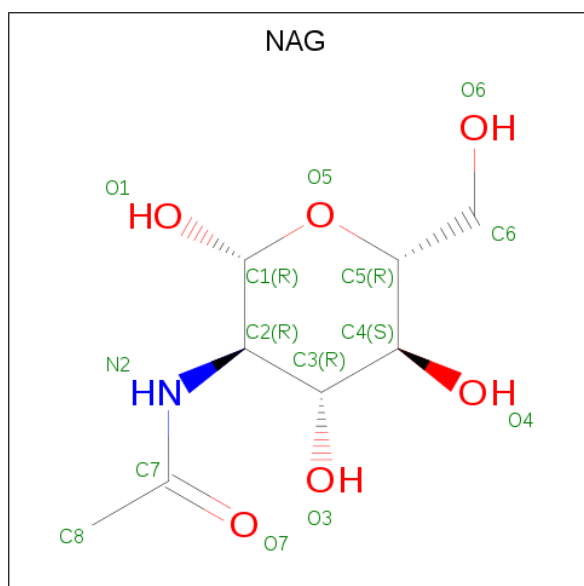
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Chain	Residue	Modelled	Actual	Comment	Reference
K	101	LEU	SER	conflict	UNP S6B291
K	102	GLY	GLN	conflict	UNP S6B291
K	103	ASP	TRP	conflict	UNP S6B291
K	104	ALA	PRO	conflict	UNP S6B291
K	105	PHE	GLY	conflict	UNP S6B291
K	107	ILE	TYR	conflict	UNP S6B291
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
3	L	185	Total	C	N	O	S	0	0	0
			1327	829	226	269	3			
3	M	203	Total	C	N	O	S	0	0	0
			1410	873	241	292	4			
3	N	184	Total	C	N	O	S	0	0	0
			1275	790	217	264	4			
3	O	200	Total	C	N	O	S	0	0	0
			1380	858	235	283	4			

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

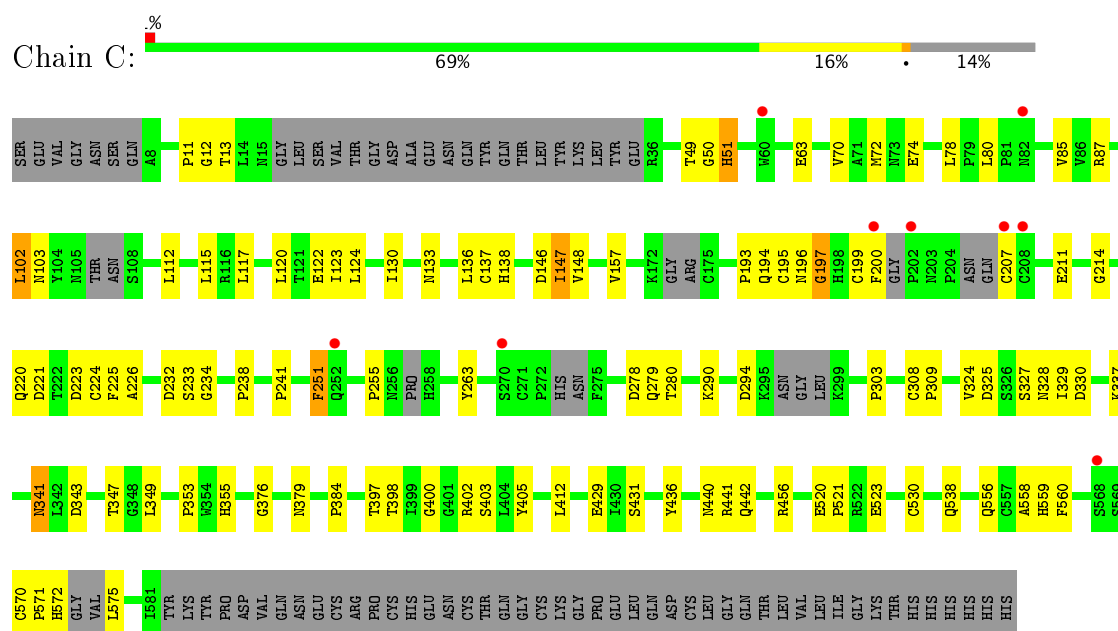
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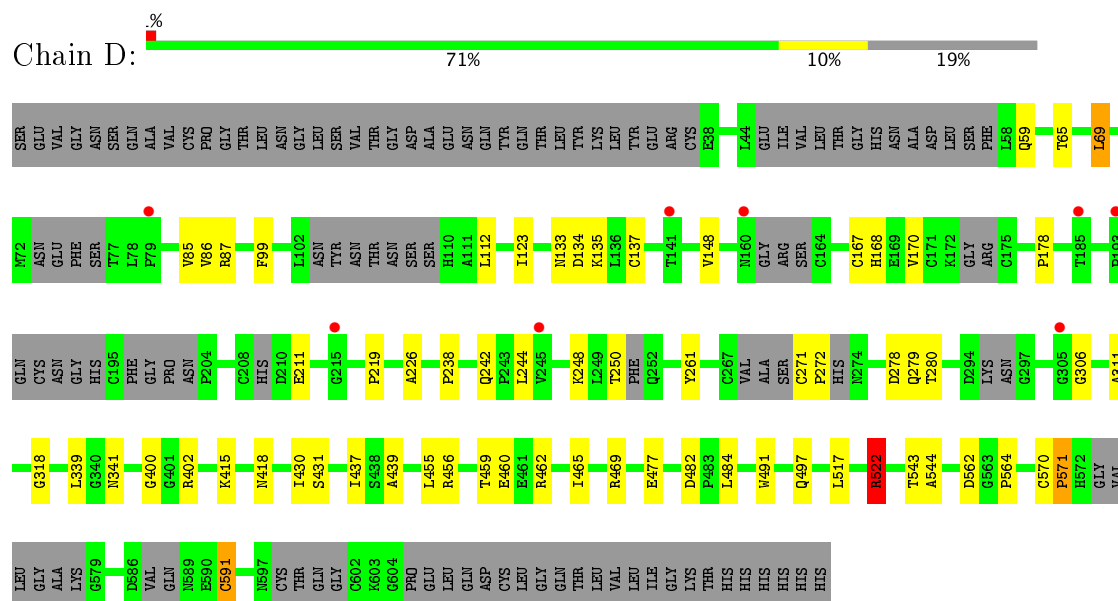
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1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



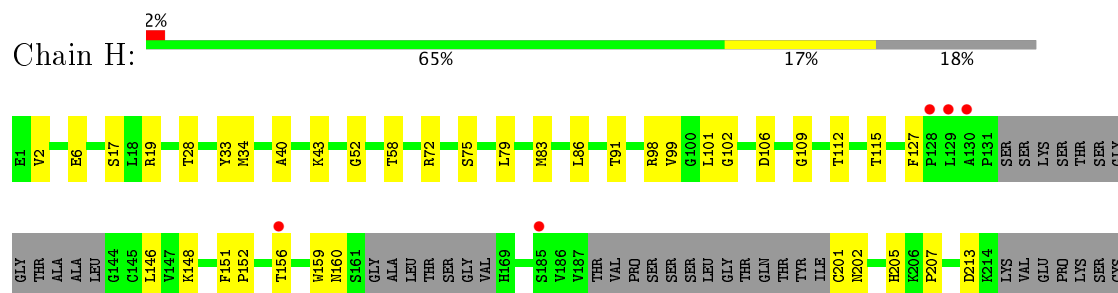




- Molecule 1: Receptor tyrosine-protein kinase erbB-3

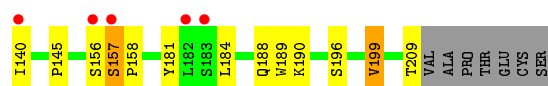


- Molecule 2: IgG H chain

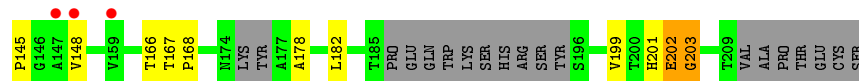


- Molecule 2: IgG H chain

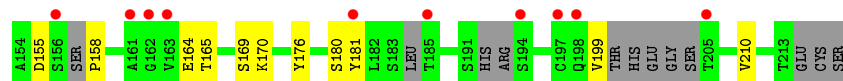
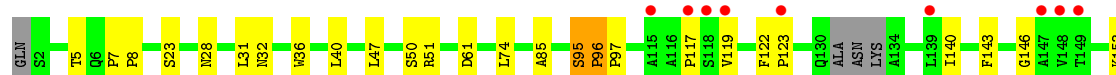
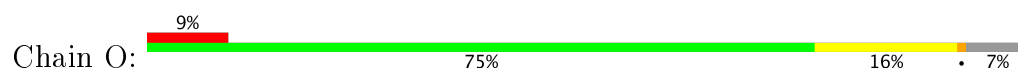




- Molecule 3: Fab LC region of KTN3379



- Molecule 3: Fab LC region of KTN3379



## 4 Data and refinement statistics

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) 96.7 (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)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.252 , 0.278 0.252 , 0.277	Depositor DCC
$R_{free}$ test set	4596 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	25896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage'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	0.20	0/4023	0.37	0/5502
1	B	0.20	0/3801	0.37	0/5195
1	C	0.20	0/3924	0.40	0/5355
1	D	0.20	0/3596	0.37	0/4906
2	H	0.22	0/1379	0.37	0/1878
2	I	0.21	0/1463	0.37	0/1994
2	J	0.21	0/1295	0.38	0/1761
2	K	0.21	0/1321	0.38	0/1800
3	L	0.20	0/1359	0.37	0/1860
3	M	0.20	0/1443	0.41	0/1984
3	N	0.20	0/1301	0.42	0/1782
3	O	0.20	0/1408	0.38	0/1926
All	All	0.20	0/26313	0.38	0/35943

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3927	0	3437	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3720	0	3310	36	0
1	C	3839	0	3426	50	0
1	D	3521	0	2985	34	0
2	H	1348	0	1268	22	0
2	I	1431	0	1329	26	0
2	J	1270	0	1174	22	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	291	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 (291) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:98:ARG:NH2	2:H:106:ASP:OD2	2.30	0.58
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.83	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:142:ALA:HB3	2:I:189:VAL:H	1.69	0.58
2:I:34:MET:HB3	2:I:79:LEU:HD22	1.84	0.58
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:C:11:PRO:HB2	1:C:13:THR:HG23	1.86	0.57
1:A:318:GLY:HA3	2:H:101:LEU:HD21	1.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:H:17:SER:N	2:J:21:SER:OG	2.39	0.54
1:D:456:ARG:NH1	2:K:57:VAL:HA	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:117:PRO:HB3	3:O:143:PHE:HB3	1.91	0.51
3:O:40:LEU:HD23	3:O:85:ALA:HB2	1.92	0.51
1:B:486:SER:HG	1:B:500:SER:HG	1.58	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
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
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
2:K:29:PHE:O	2:K:72:ARG:NH2	2.46	0.48
3:L:40:LEU:HD23	3:L:85:ALA:HB2	1.95	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:B:391:SER:O	1:B:394:SER:OG	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:PRO:HA	1:C:194:GLN:HA	1.64	0.44
1:C:50:GLY:HA3	1:C:74:GLU:H	1.82	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
2:K:73:ASP:OD1	2:K:75:SER:OG	2.28	0.44
3:L:36:TRP:HB2	3:L:49:ILE:HB	1.99	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
2:J:151:PHE:HA	2:J:152:PRO:HA	1.72	0.44
3:L:136:LEU:HB2	3:L:182:LEU:HB3	2.00	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
1:C:117:LEU:HB3	1:C:120:LEU:HB2	2.00	0.44
1:C:49:THR:OG1	1:C:50:GLY:N	2.50	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:HE2	2:H:148:LYS:HB3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:O:7:PRO:HA	3:O:8:PRO:HD3	1.89	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:123:GLY:HA2	2:I:124:PRO:HD3	1.91	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: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:H:127:PHE:O	2:H:146:LEU:HB3	2.21	0.41
3:M:62:ARG:HH12	3:M:83:ASP:CG	2.24	0.40
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:A:415:LYS:O	3:M:57:SER:OG	2.35	0.40
1:B:78:LEU:HA	1:B:79:PRO:HD3	1.92	0.40
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:B:456:ARG:HD3	2:I:57:VAL:HG22	2.02	0.40
1:C:308:CYS:HA	1:C:309:PRO:HD3	1.95	0.40
2:J:29:PHE:O	2:J:72:ARG:NH2	2.55	0.40
1:C:456:ARG:HD3	2:J:57:VAL:HG22	2.03	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%)	13	53
1	B	522/627 (83%)	447 (86%)	65 (12%)	10 (2%)	9	46
1	C	519/627 (83%)	424 (82%)	76 (15%)	19 (4%)	4	26
1	D	478/627 (76%)	402 (84%)	60 (13%)	16 (3%)	4	29
2	H	174/221 (79%)	166 (95%)	6 (3%)	2 (1%)	17	58
2	I	190/221 (86%)	166 (87%)	17 (9%)	7 (4%)	4	26
2	J	167/221 (76%)	150 (90%)	14 (8%)	3 (2%)	10	47
2	K	172/221 (78%)	149 (87%)	17 (10%)	6 (4%)	4	28
3	L	179/216 (83%)	157 (88%)	17 (10%)	5 (3%)	6	34
3	M	199/216 (92%)	166 (83%)	25 (13%)	8 (4%)	3	24
3	N	176/216 (82%)	147 (84%)	23 (13%)	6 (3%)	4	28
3	O	188/216 (87%)	166 (88%)	19 (10%)	3 (2%)	11	50
All	All	3521/4256 (83%)	3031 (86%)	397 (11%)	93 (3%)	6	36

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	373 (98%)	6 (2%)	68	89
1	B	371/543 (68%)	367 (99%)	4 (1%)	78	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	390/543 (72%)	382 (98%)	8 (2%)	59	85
1	D	338/543 (62%)	335 (99%)	3 (1%)	82	94
2	H	144/183 (79%)	140 (97%)	4 (3%)	49	81
2	I	149/183 (81%)	147 (99%)	2 (1%)	73	91
2	J	131/183 (72%)	130 (99%)	1 (1%)	85	95
2	K	130/183 (71%)	130 (100%)	0	100	100
3	L	143/180 (79%)	141 (99%)	2 (1%)	71	90
3	M	146/180 (81%)	141 (97%)	5 (3%)	42	77
3	N	131/180 (73%)	130 (99%)	1 (1%)	85	95
3	O	140/180 (78%)	138 (99%)	2 (1%)	71	90
All	All	2592/3624 (72%)	2554 (98%)	38 (2%)	70	90

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	271	CYS
1	A	341	ASN
1	A	355	HIS
1	A	469	ARG
1	A	499	LEU
1	B	152	ASP
1	B	250	THR
1	B	268	VAL
1	B	341	ASN
1	C	80	LEU
1	C	147	ILE
1	C	223	ASP
1	C	251	PHE
1	C	263	TYR
1	C	341	ASN
1	C	355	HIS
1	C	575	LEU
1	D	69	LEU
1	D	341	ASN
1	D	522	ARG
2	H	2	VAL
2	H	28	THR

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Mol	Chain	Res	Type
2	H	58	THR
2	H	156	THR
3	L	95	SER
3	L	190	LYS
2	I	155	VAL
2	I	169	HIS
2	J	155	VAL
3	M	95	SER
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
1	A	418	ASN
1	A	503	ASN
1	B	503	ASN
1	C	341	ASN
1	C	418	ASN
1	C	503	ASN
1	D	381	GLN
1	D	418	ASN
3	L	38	GLN
3	L	201	HIS
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 carbohydrates 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	A	701	-	14,14,15	0.31	0	15,19,21	0.38	0
4	NAG	A	702	-	14,14,15	0.26	0	15,19,21	0.46	0
4	NAG	B	701	-	14,14,15	0.24	0	15,19,21	0.46	0
4	NAG	B	702	-	14,14,15	0.24	0	15,19,21	0.45	0
4	NAG	C	701	-	14,14,15	0.23	0	15,19,21	0.45	0
4	NAG	C	702	-	14,14,15	0.45	0	15,19,21	1.34	1 (6%)
4	NAG	C	703	-	14,14,15	0.24	0	15,19,21	0.45	0
4	NAG	D	701	-	14,14,15	0.26	0	15,19,21	0.44	0
4	NAG	D	702	-	14,14,15	0.25	0	15,19,21	0.46	0
4	NAG	D	703	-	14,14,15	0.26	0	15,19,21	0.40	0
4	NAG	M	301	-	14,14,15	0.31	0	15,19,21	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. '-' means no outliers of that kind were identified.

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	703	-	-	0/6/23/26	0/1/1/1
4	NAG	M	301	-	-	0/6/23/26	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(°)
4	C	702	NAG	C2-N2-C7	4.25	129.15	122.94

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

### 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, 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(Å²)	Q<0.9
1	A	561/627 (89%)	-0.04	6 (1%)	80	68	15, 64, 126, 188	14 (2%)
1	B	530/627 (84%)	-0.07	8 (1%)	74	61	18, 64, 122, 187	16 (3%)
1	C	539/627 (85%)	0.05	9 (1%)	70	57	16, 69, 139, 209	8 (1%)
1	D	509/627 (81%)	-0.00	8 (1%)	72	59	14, 75, 142, 227	8 (1%)
2	H	182/221 (82%)	0.06	5 (2%)	55	40	15, 42, 144, 194	0
2	I	198/221 (89%)	-0.00	4 (2%)	65	50	15, 40, 152, 176	0
2	J	175/221 (79%)	-0.10	3 (1%)	70	57	16, 39, 129, 189	0
2	K	180/221 (81%)	0.06	5 (2%)	53	39	17, 41, 149, 187	0
3	L	185/216 (85%)	0.18	9 (4%)	30	18	19, 57, 145, 209	0
3	M	203/216 (93%)	0.29	13 (6%)	20	11	22, 62, 156, 215	0
3	N	184/216 (85%)	0.19	7 (3%)	41	27	15, 56, 144, 194	0
3	O	200/216 (92%)	0.32	19 (9%)	9	5	18, 65, 165, 221	0
All	All	3646/4256 (85%)	0.04	96 (2%)	56	41	14, 62, 143, 227	46 (1%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	135	THR	7.7
3	O	119	VAL	6.3
3	O	123	PRO	5.5
3	M	136	LEU	5.1
3	L	134	ALA	4.9
1	A	235	ALA	4.7
3	L	111	GLY	4.5
3	N	121	LEU	4.3
1	D	160	ASN	4.1
2	I	185	SER	4.0
1	C	200	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	193	PRO	3.9
1	A	257	PRO	3.9
3	M	120	THR	3.8
3	O	163	VAL	3.7
3	O	149	THR	3.6
1	D	245	VAL	3.6
2	H	130	ALA	3.6
1	C	270	SER	3.6
3	M	137	VAL	3.6
3	O	205	THR	3.5
1	C	208	CYS	3.5
3	O	156	SER	3.2
3	N	119	VAL	3.2
3	L	199	VAL	3.2
3	L	136	LEU	3.2
1	A	269	ALA	3.2
3	N	120	THR	3.2
1	B	112	LEU	3.1
2	J	185	SER	3.1
3	M	121	LEU	3.0
1	C	202	PRO	3.0
3	O	197	CYS	3.0
3	M	156	SER	2.9
1	C	252	GLN	2.9
2	K	185	SER	2.9
1	B	79	PRO	2.8
3	M	123	PRO	2.8
3	L	193	ARG	2.8
2	H	185	SER	2.7
1	D	79	PRO	2.7
2	J	212	VAL	2.7
3	M	182	LEU	2.7
3	N	122	PHE	2.6
2	K	177	SER	2.6
3	N	159	VAL	2.6
1	C	207	CYS	2.5
1	D	185	THR	2.5
3	N	148	VAL	2.5
2	K	178	SER	2.5
1	A	203	ASN	2.4
3	O	161	ALA	2.4
3	N	147	ALA	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	O	198	GLN	2.4
3	O	147	ALA	2.4
3	O	118	SER	2.4
1	D	141	THR	2.4
3	O	117	PRO	2.3
2	I	145	CYS	2.3
3	L	123	PRO	2.3
1	A	236	CYS	2.3
3	M	157	SER	2.3
3	O	194	SER	2.3
3	O	181	TYR	2.3
1	C	568	SER	2.3
1	B	247	ASN	2.3
2	H	156	THR	2.3
3	L	185	THR	2.3
2	I	146	LEU	2.3
2	I	189	VAL	2.3
3	M	113	PRO	2.2
3	O	162	GLY	2.2
1	C	82	ASN	2.2
3	O	148	VAL	2.2
1	B	250	THR	2.2
2	H	128	PRO	2.2
3	O	115	ALA	2.2
1	B	562	ASP	2.2
3	M	119	VAL	2.2
2	H	129	LEU	2.2
1	A	580	PRO	2.2
1	B	55	LEU	2.1
3	L	116	ALA	2.1
3	O	139	LEU	2.1
3	M	183	SER	2.1
2	K	203	VAL	2.1
1	D	305	GLY	2.1
1	B	565	HIS	2.1
1	D	215	GLY	2.1
2	K	179	GLY	2.1
1	B	253	LEU	2.1
2	J	146	LEU	2.0
3	L	184	LEU	2.0
3	O	185	THR	2.0
3	M	140	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	60	TRP	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	M	301	14/15	0.74	0.32	4.39	85,94,103,106	0
4	NAG	A	701	14/15	0.92	0.22	1.48	35,45,54,56	0
4	NAG	C	702	14/15	0.82	0.26	1.45	26,46,57,59	0
4	NAG	D	702	14/15	0.90	0.23	1.15	30,37,49,53	0
4	NAG	B	702	14/15	0.88	0.25	0.61	54,59,85,91	0
4	NAG	D	701	14/15	0.92	0.20	-0.08	30,47,62,64	0
4	NAG	C	703	14/15	0.81	0.22	-0.21	37,58,70,87	0
4	NAG	B	701	14/15	0.89	0.19	-0.39	29,44,51,51	0
4	NAG	A	702	14/15	0.89	0.20	-1.21	21,34,53,71	0
4	NAG	C	701	14/15	0.92	0.19	-1.36	25,47,67,71	0
4	NAG	D	703	14/15	0.90	0.16	-1.86	23,45,56,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.