Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 05:52 PM EDT

PDB ID	:	5CUS
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

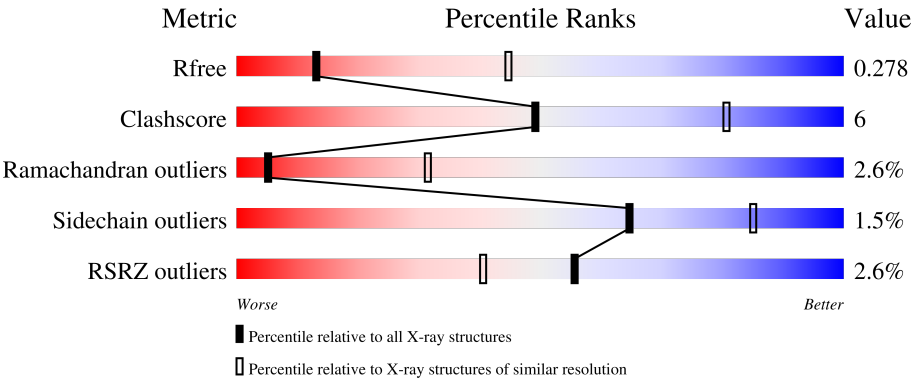
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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.



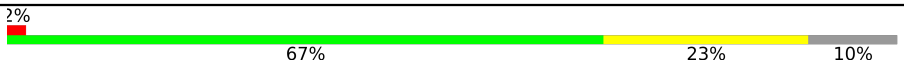
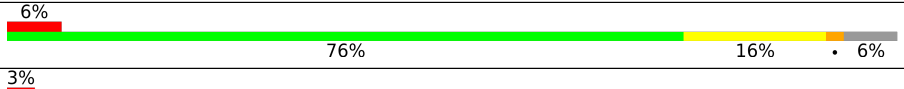
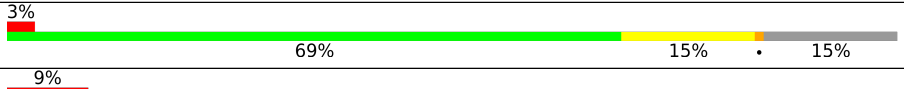
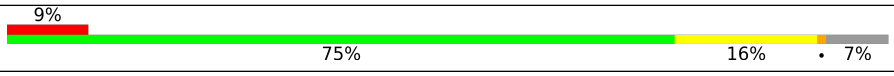
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 >=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 <=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	78% 11% 11%
1	B	627	72% 12% 15%
1	C	627	69% 16% 14%
1	D	627	71% 10% 19%
2	H	221	65% 17% 18%

Continued on next page...

Continued from previous page...

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	

2 Entry composition (i)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

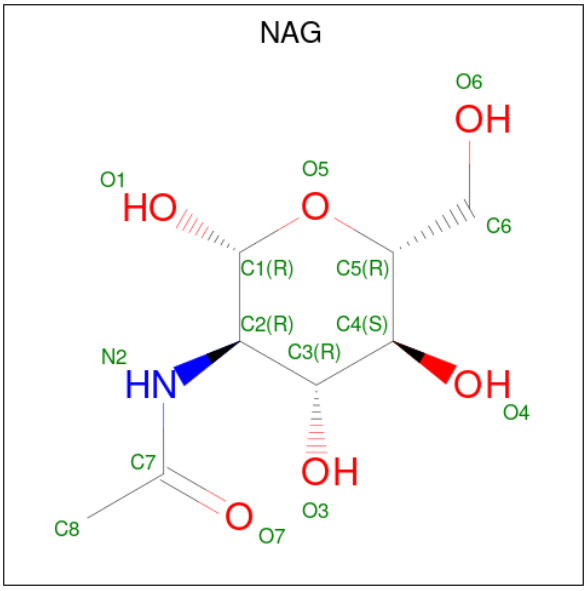
Continued from previous page...

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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

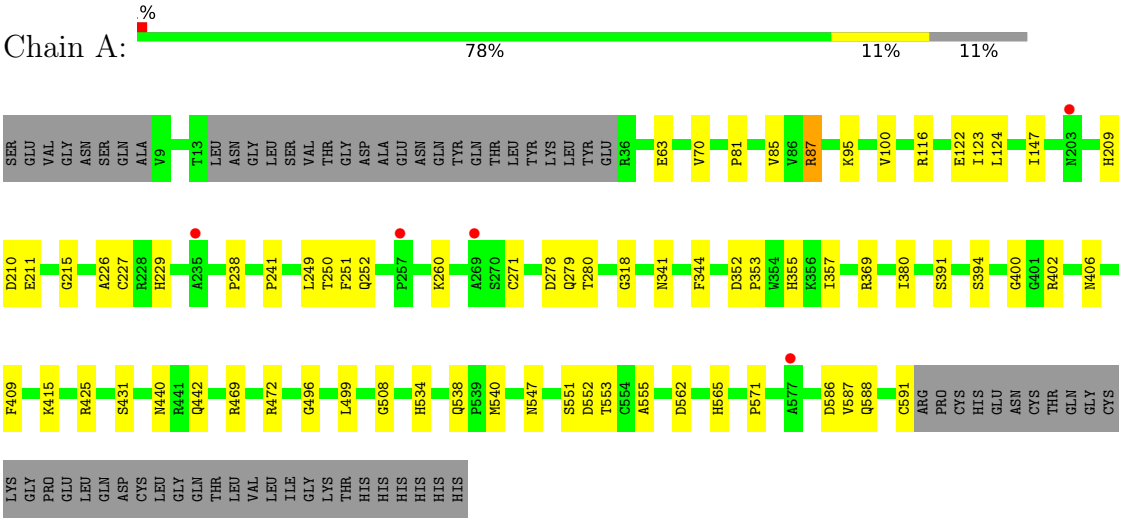


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1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

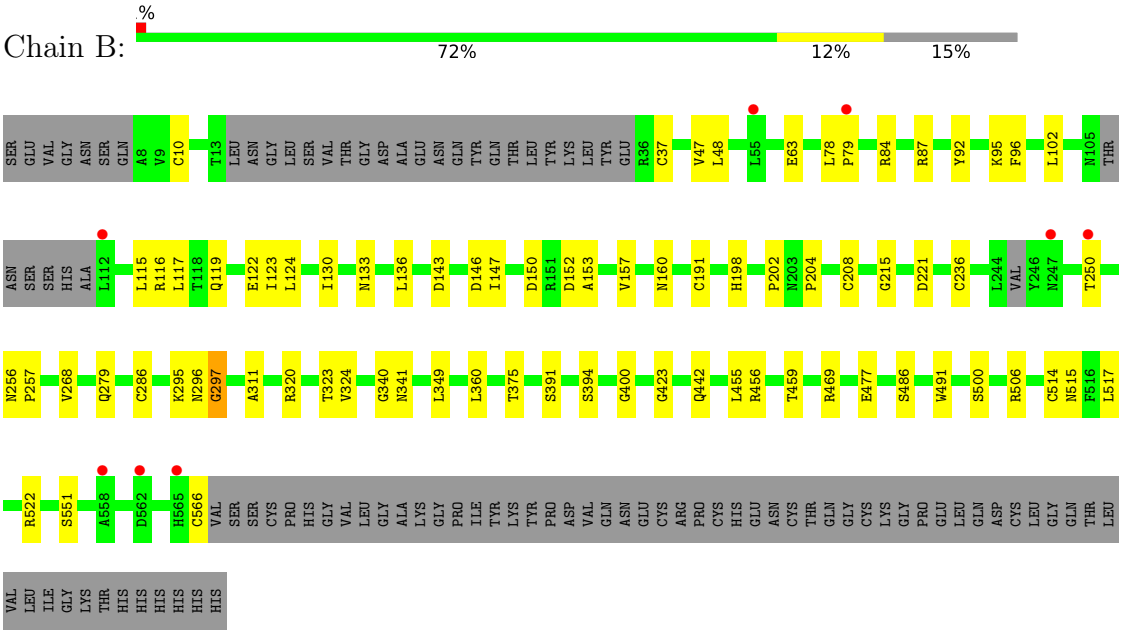
3 Residue-property plots (i)

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

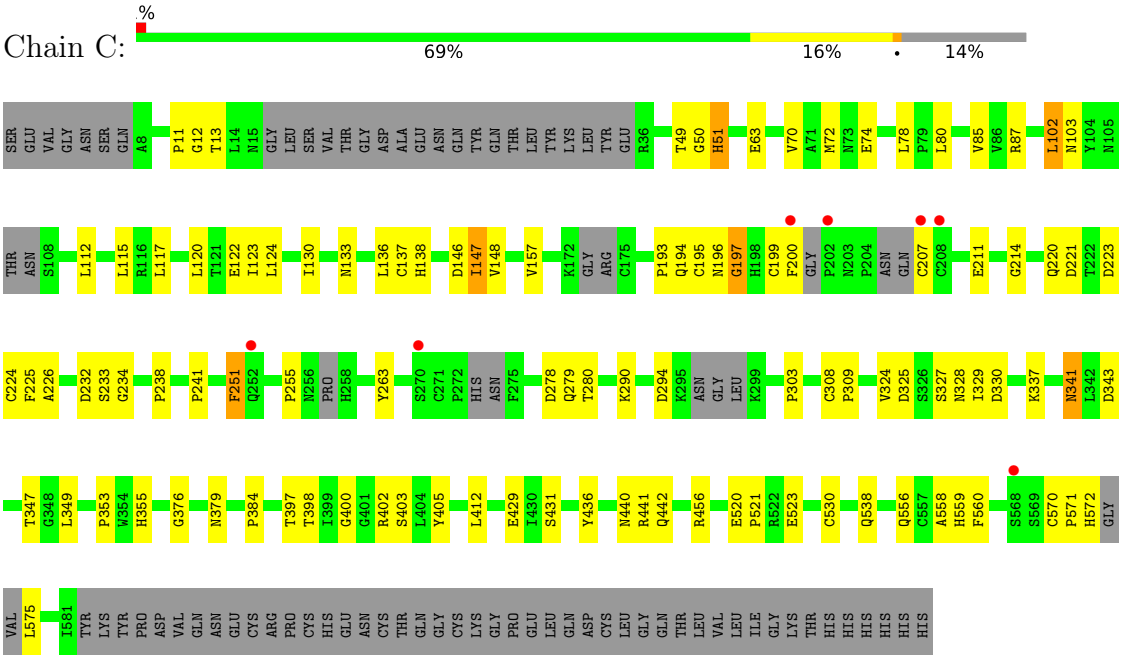


• Molecule 1: Receptor tyrosine-protein kinase erbB-3



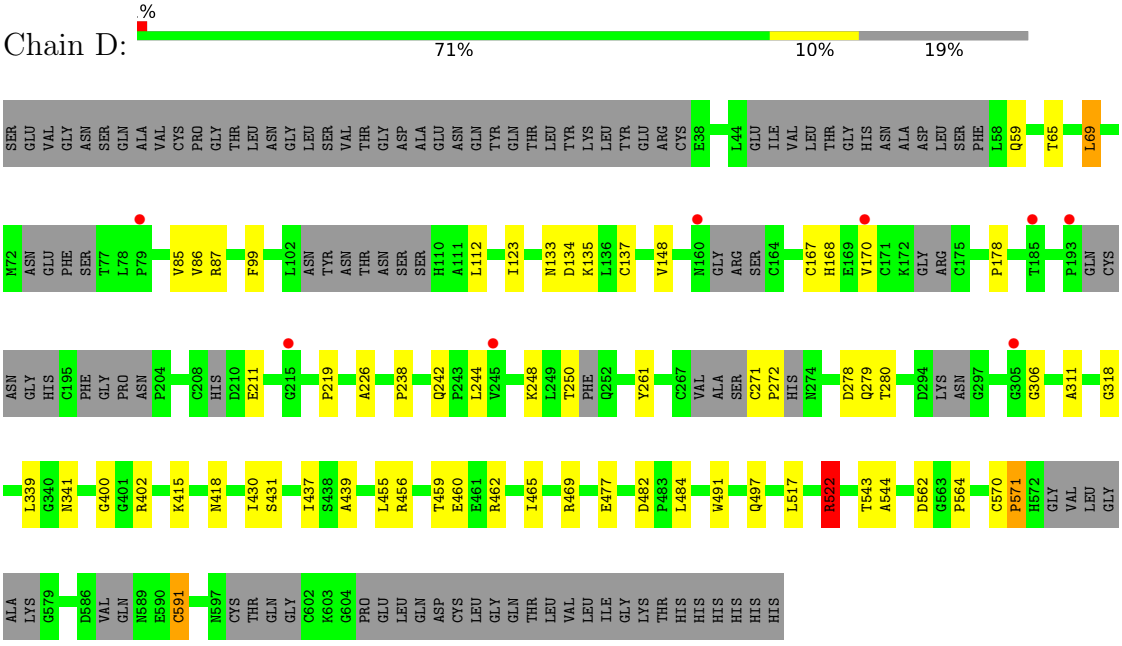
• Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain C:



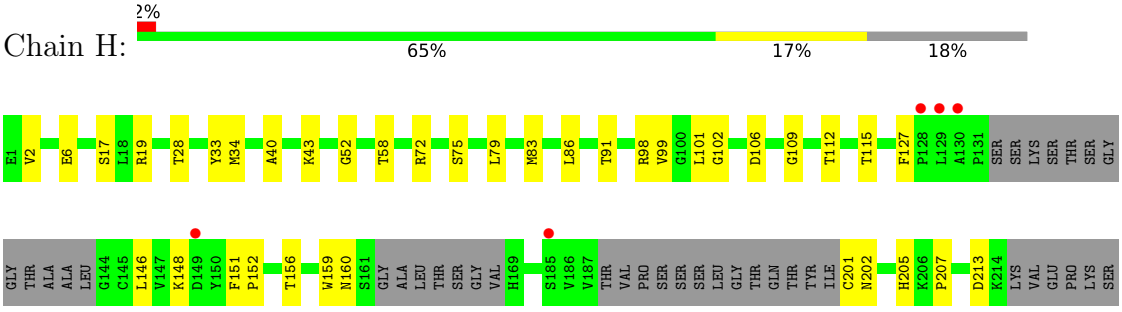
• Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain D:



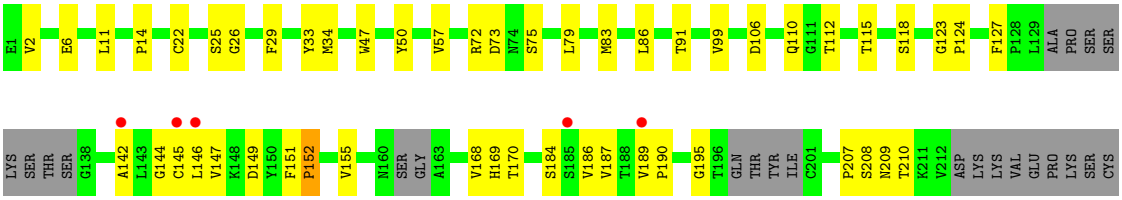
• Molecule 2: IgG H chain

Chain H:



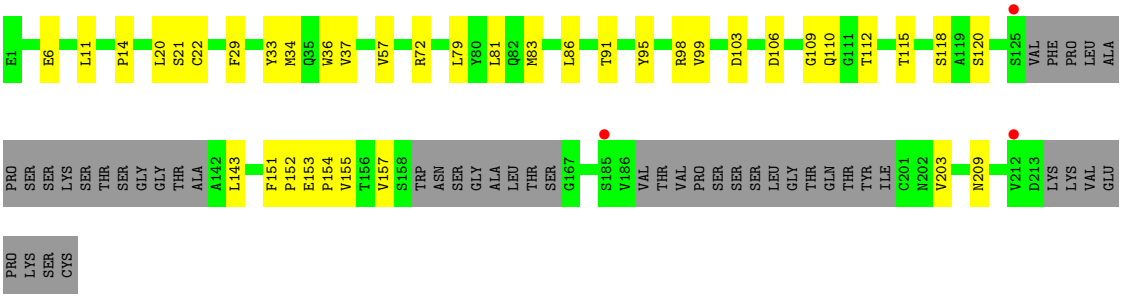
• Molecule 2: IgG H chain

Chain I:



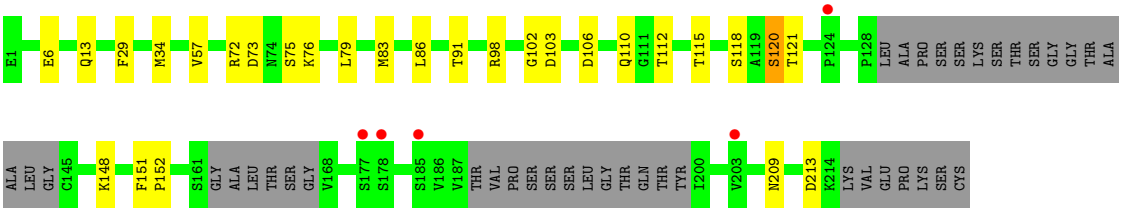
• Molecule 2: IgG H chain

Chain J:



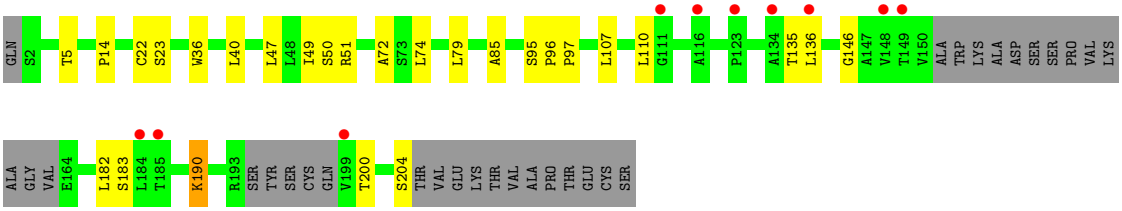
• Molecule 2: IgG H chain

Chain K:



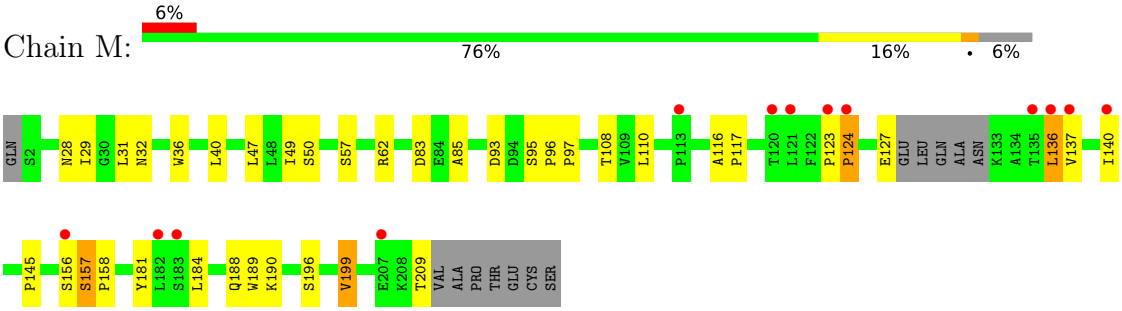
• Molecule 3: Fab LC region of KTN3379

Chain L:



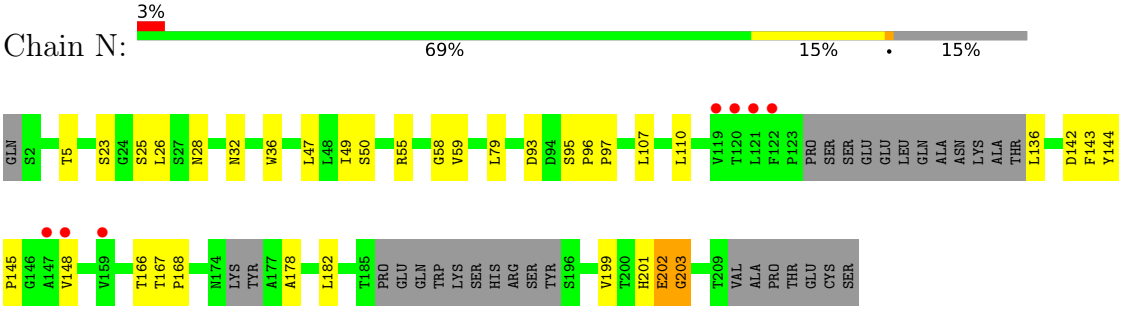
• Molecule 3: Fab LC region of KTN3379

Chain M:



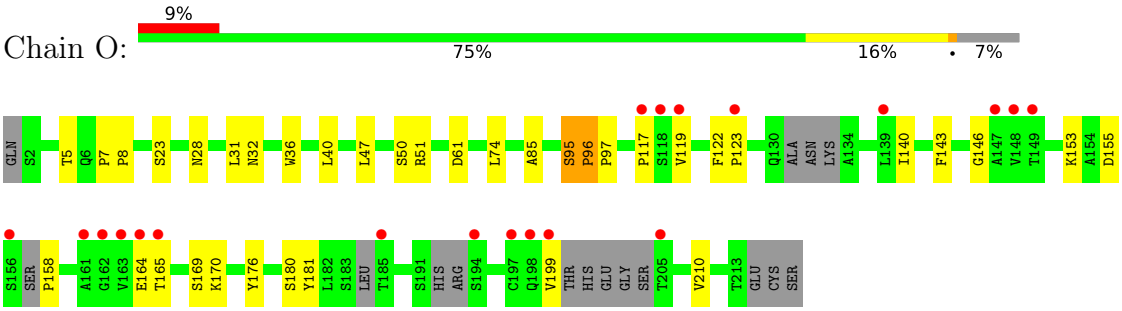
• Molecule 3: Fab LC region of KTN3379

Chain N:



• Molecule 3: Fab LC region of KTN3379

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.31 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.252 , 0.278 0.253 , 0.278	Depositor DCC
R_{free} test set	4593 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.20	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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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: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
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: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

Continued on next page...

Continued from previous page...

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
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
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
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: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
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:B:456:ARG:HD3	2:I:57:VAL:HG22	2.02	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: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%)	11	46
1	B	522/627 (83%)	447 (86%)	65 (12%)	10 (2%)	8	39
1	C	519/627 (83%)	424 (82%)	76 (15%)	19 (4%)	3	22
1	D	478/627 (76%)	402 (84%)	60 (13%)	16 (3%)	4	25
2	H	174/221 (79%)	166 (95%)	6 (3%)	2 (1%)	14	51
2	I	190/221 (86%)	166 (87%)	17 (9%)	7 (4%)	3	22
2	J	167/221 (76%)	150 (90%)	14 (8%)	3 (2%)	8	41
2	K	172/221 (78%)	149 (87%)	17 (10%)	6 (4%)	3	24
3	L	179/216 (83%)	157 (88%)	17 (10%)	5 (3%)	5	29
3	M	199/216 (92%)	166 (83%)	25 (13%)	8 (4%)	3	21
3	N	176/216 (82%)	147 (84%)	23 (13%)	6 (3%)	3	24
3	O	188/216 (87%)	166 (88%)	19 (10%)	3 (2%)	9	43
All	All	3521/4256 (83%)	3031 (86%)	397 (11%)	93 (3%)	5	31

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (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%)	373 (98%)	6 (2%)	62 84
1	B	371/543 (68%)	367 (99%)	4 (1%)	73 88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	390/543 (72%)	382 (98%)	8 (2%)	53 79
1	D	338/543 (62%)	335 (99%)	3 (1%)	78 91
2	H	144/183 (79%)	140 (97%)	4 (3%)	43 74
2	I	149/183 (81%)	147 (99%)	2 (1%)	69 87
2	J	131/183 (72%)	130 (99%)	1 (1%)	81 93
2	K	130/183 (71%)	130 (100%)	0	100 100
3	L	143/180 (79%)	141 (99%)	2 (1%)	67 86
3	M	146/180 (81%)	141 (97%)	5 (3%)	37 70
3	N	131/180 (73%)	130 (99%)	1 (1%)	81 93
3	O	140/180 (78%)	138 (99%)	2 (1%)	67 86
All	All	2592/3624 (72%)	2554 (98%)	38 (2%)	65 85

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

Continued on next page...

Continued from previous page...

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

Sometimes 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 monosaccharides 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	703	-	14,14,15	0.25	0	17,19,21	0.39	0
4	NAG	B	702	-	14,14,15	0.25	0	17,19,21	0.39	0
4	NAG	D	701	-	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	C	702	-	14,14,15	0.44	0	17,19,21	1.28	1 (5%)
4	NAG	A	701	-	14,14,15	0.32	0	17,19,21	0.33	0
4	NAG	D	703	-	14,14,15	0.27	0	17,19,21	0.36	0
4	NAG	D	702	-	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	C	701	-	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	M	301	-	14,14,15	0.32	0	17,19,21	0.36	0
4	NAG	B	701	-	14,14,15	0.24	0	17,19,21	0.40	0
4	NAG	A	702	-	14,14,15	0.27	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	703	-	-	2/6/23/26	0/1/1/1
4	NAG	B	702	-	-	2/6/23/26	0/1/1/1
4	NAG	D	701	-	-	2/6/23/26	0/1/1/1
4	NAG	C	702	-	-	5/6/23/26	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	D	702	-	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	701	-	-	2/6/23/26	0/1/1/1
4	NAG	M	301	-	-	2/6/23/26	0/1/1/1
4	NAG	B	701	-	-	4/6/23/26	0/1/1/1
4	NAG	A	702	-	-	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(^{o})	Ideal(^{o})
4	C	702	NAG	C2-N2-C7	4.38	129.15	122.90

There are no chirality outliers.

All (23) 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	C	702	NAG	O5-C5-C6-O6
4	D	701	NAG	O5-C5-C6-O6
4	M	301	NAG	O5-C5-C6-O6
4	B	702	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	D	701	NAG	C4-C5-C6-O6
4	B	701	NAG	C8-C7-N2-C2
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	C	702	NAG	C4-C5-C6-O6
4	B	702	NAG	C4-C5-C6-O6
4	A	701	NAG	O5-C5-C6-O6
4	A	701	NAG	C4-C5-C6-O6
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	D	701	NAG	2	0
4	C	702	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	561/627 (89%)	-0.07	5 (0%)	84	75	15, 64, 126, 188	14 (2%)
1	B	530/627 (84%)	-0.08	8 (1%)	73	61	18, 64, 122, 187	16 (3%)
1	C	539/627 (85%)	0.05	7 (1%)	77	65	16, 69, 139, 209	8 (1%)
1	D	509/627 (81%)	-0.02	8 (1%)	72	59	14, 75, 142, 227	8 (1%)
2	H	182/221 (82%)	0.05	5 (2%)	54	39	15, 42, 144, 194	0
2	I	198/221 (89%)	-0.00	5 (2%)	57	43	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%)	0.05	5 (2%)	53	37	17, 41, 149, 187	0
3	L	185/216 (85%)	0.15	10 (5%)	25	14	19, 57, 145, 209	0
3	M	203/216 (93%)	0.27	13 (6%)	19	11	22, 62, 156, 215	0
3	N	184/216 (85%)	0.16	7 (3%)	40	26	15, 56, 144, 194	0
3	O	200/216 (92%)	0.32	20 (10%)	7	4	18, 65, 165, 221	0
All	All	3646/4256 (85%)	0.03	96 (2%)	56	40	14, 62, 143, 227	46 (1%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	135	THR	7.9
3	O	119	VAL	5.8
3	O	123	PRO	5.5
3	M	136	LEU	5.3
3	L	134	ALA	4.9
2	I	185	SER	4.9
1	A	235	ALA	4.9
3	L	111	GLY	4.6
1	D	193	PRO	4.4
1	C	208	CYS	3.8
3	M	121	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	O	205	THR	3.7
1	C	270	SER	3.7
3	L	136	LEU	3.7
3	O	163	VAL	3.6
1	C	200	PHE	3.5
1	A	257	PRO	3.5
1	D	245	VAL	3.4
3	O	156	SER	3.4
3	N	159	VAL	3.3
3	N	121	LEU	3.3
1	C	202	PRO	3.3
3	N	120	THR	3.2
3	M	137	VAL	3.2
1	B	112	LEU	3.1
3	M	120	THR	3.0
3	O	149	THR	3.0
1	C	252	GLN	3.0
3	M	123	PRO	3.0
1	D	160	ASN	2.9
3	O	162	GLY	2.9
2	K	185	SER	2.9
2	H	130	ALA	2.9
1	B	79	PRO	2.9
3	N	119	VAL	2.9
3	L	123	PRO	2.8
3	L	199	VAL	2.8
2	I	145	CYS	2.7
3	M	156	SER	2.7
2	H	185	SER	2.7
3	O	161	ALA	2.7
1	A	269	ALA	2.7
3	O	139	LEU	2.7
2	J	185	SER	2.6
2	J	125	SER	2.6
3	O	197	CYS	2.6
2	J	212	VAL	2.5
3	M	113	PRO	2.5
2	K	178	SER	2.5
2	I	146	LEU	2.5
1	C	207	CYS	2.4
3	O	118	SER	2.4
3	N	148	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	568	SER	2.4
3	N	147	ALA	2.4
2	H	129	LEU	2.4
1	D	215	GLY	2.4
2	I	189	VAL	2.4
3	L	185	THR	2.4
3	O	117	PRO	2.4
2	K	124	PRO	2.4
3	O	147	ALA	2.4
3	L	149	THR	2.4
3	M	207	GLU	2.3
3	O	198	GLN	2.3
3	L	184	LEU	2.3
3	O	185	THR	2.3
3	O	194	SER	2.3
2	H	128	PRO	2.3
3	O	148	VAL	2.2
1	A	577	ALA	2.2
3	L	116	ALA	2.2
3	M	140	ILE	2.2
3	M	182	LEU	2.2
1	D	185	THR	2.2
3	L	148	VAL	2.2
1	B	55	LEU	2.2
1	B	250	THR	2.2
3	M	183	SER	2.2
1	D	170	VAL	2.1
2	K	177	SER	2.1
1	D	79	PRO	2.1
3	O	165	THR	2.1
3	M	124	PRO	2.1
1	D	305	GLY	2.1
2	H	149	ASP	2.1
1	A	203	ASN	2.1
1	B	247	ASN	2.1
1	B	558	ALA	2.1
3	O	164	GLU	2.1
2	I	142	ALA	2.0
1	B	562	ASP	2.0
3	N	122	PHE	2.0
1	B	565	HIS	2.0
2	K	203	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	O	199	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	M	301	14/15	0.75	0.31	85,94,103,106	0
4	NAG	C	702	14/15	0.78	0.26	26,46,57,59	0
4	NAG	C	703	14/15	0.81	0.23	37,58,70,87	0
4	NAG	B	701	14/15	0.88	0.18	29,44,51,51	0
4	NAG	B	702	14/15	0.89	0.26	54,59,85,91	0
4	NAG	D	702	14/15	0.90	0.22	30,37,49,53	0
4	NAG	A	702	14/15	0.90	0.21	21,34,53,71	0
4	NAG	D	703	14/15	0.91	0.17	23,45,56,68	0
4	NAG	D	701	14/15	0.92	0.21	30,47,62,64	0
4	NAG	C	701	14/15	0.92	0.20	25,47,67,71	0
4	NAG	A	701	14/15	0.93	0.22	35,45,54,56	0

6.5 Other polymers (i)

There are no such residues in this entry.