



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:24 PM GMT

PDB ID : 4GW4
Title : Crystal structure of 3BNC60 Fab with P61A mutation
Authors : Diskin, R.; Fu, B.Z.; Bjorkman, P.J.
Deposited on : 2012-08-31
Resolution : 2.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

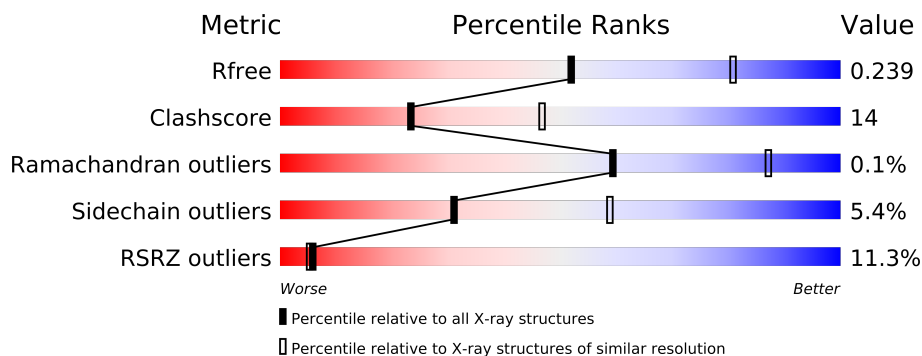
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.65 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}	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	206	
1	L	206	
2	A	229	
2	H	229	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12825 atoms, of which 6198 are hydrogens and 0 are deuterium.

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.

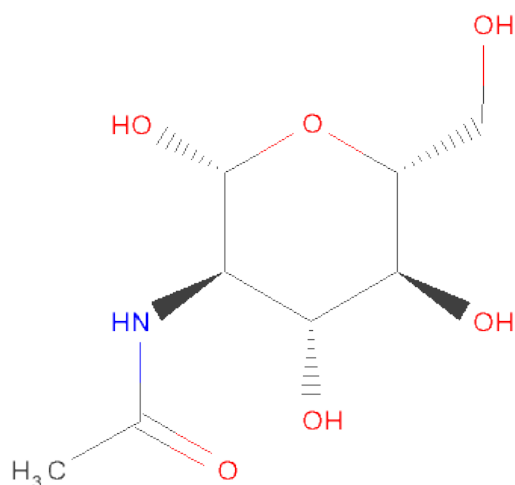
- Molecule 1 is a protein called 3BNC60 Fab Light-chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	198	Total	C	H	N	O	S	0	0	0
			3075	978	1519	269	305	4			
1	B	199	Total	C	H	N	O	S	0	0	0
			3090	982	1526	271	307	4			

- Molecule 2 is a protein called 3BNC60 Fab Heavy-chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	213	Total	C	H	N	O	S	0	0	0
			3224	1043	1580	286	310	5			
2	A	212	Total	C	H	N	O	S	0	0	0
			3209	1038	1573	285	308	5			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

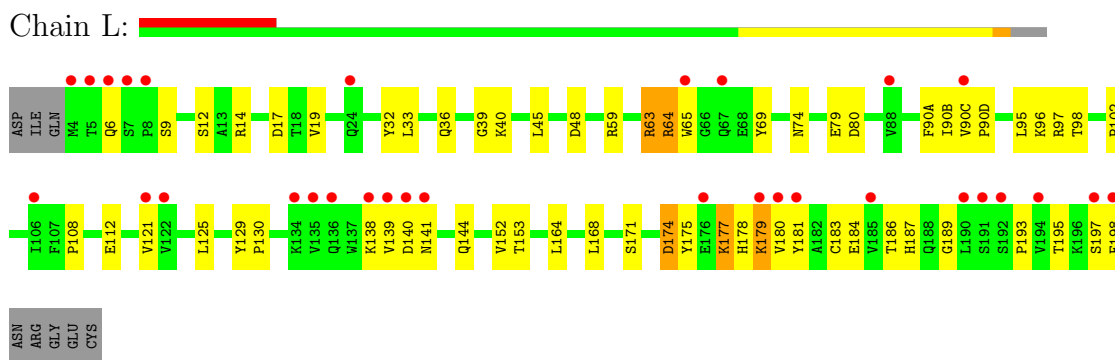
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	55	Total	O	0	0
			55	55		
4	H	36	Total	O	0	0
			36	36		
4	A	42	Total	O	0	0
			42	42		
4	B	66	Total	O	0	0
			66	66		

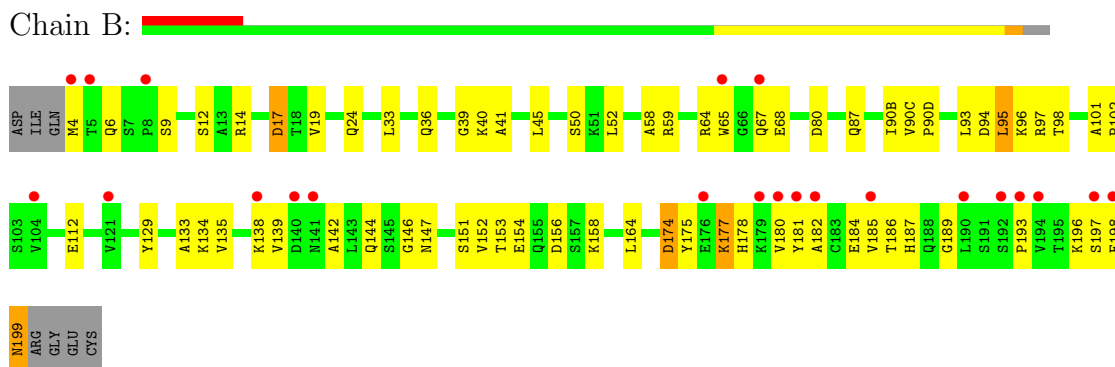
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

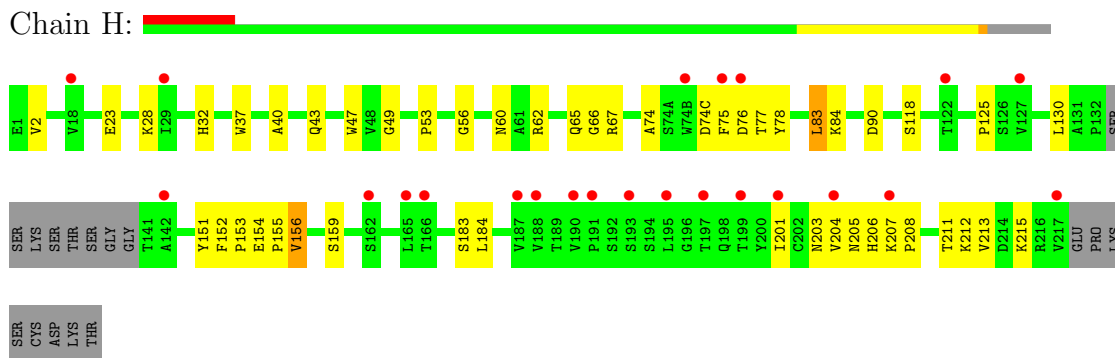
- Molecule 1: 3BNC60 Fab Light-chain



- Molecule 1: 3BNC60 Fab Light-chain

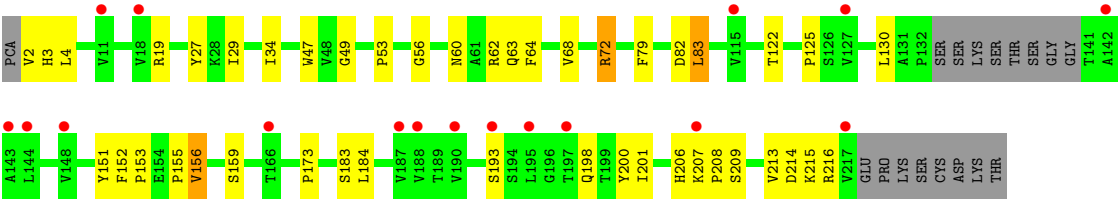


- Molecule 2: 3BNC60 Fab Heavy-chain



- Molecule 2: 3BNC60 Fab Heavy-chain

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.57Å 154.88Å 74.24Å 90.00° 109.75° 90.00°	Depositor
Resolution (Å)	39.35 – 2.65 39.69 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.35-2.65) 92.9 (39.69-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_966)	Depositor
R, R_{free}	0.213 , 0.256 0.194 , 0.239	Depositor DCC
R_{free} test set	1853 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39070 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12825	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCA, 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	B	0.56	0/1598	0.70	0/2171
1	L	0.54	0/1590	0.72	0/2160
2	A	0.49	0/1684	0.62	0/2299
2	H	0.49	0/1685	0.64	0/2302
All	All	0.52	0/6557	0.67	0/8932

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1564	1526	0	62	0
1	L	1556	1519	0	57	0
2	A	1636	1573	0	30	0
2	H	1644	1580	0	36	0
3	B	14	0	13	4	0
3	L	14	0	13	5	0
4	A	42	0	0	2	0
4	B	66	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	36	0	0	8	0
4	L	55	0	0	7	0
All	All	6627	6198	26	183	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (183) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:97:ARG:NH1	1:B:98:THR:O	2.03	0.92
1:B:52:LEU:O	4:B:439:HOH:O	1.86	0.92
1:L:63:ARG:HD2	3:L:301:NAG:H81	1.54	0.89
1:L:97:ARG:NH1	1:L:98:THR:O	2.05	0.87
1:L:63:ARG:NH1	3:L:301:NAG:O7	2.10	0.85
1:B:101:ALA:O	4:B:426:HOH:O	1.94	0.83
1:B:90(C):VAL:HG11	1:B:90(D):PRO:HD2	1.59	0.82
1:L:59:ARG:NH1	1:L:80:ASP:OD2	2.13	0.81
2:A:215:LYS:NZ	1:B:112:GLU:OE1	2.13	0.81
1:B:156:ASP:OD1	1:B:158:LYS:HG2	1.83	0.77
1:B:199:ASN:OD1	4:B:457:HOH:O	2.03	0.76
1:L:40:LYS:N	4:L:446:HOH:O	2.20	0.74
1:B:50:SER:O	4:B:461:HOH:O	2.06	0.74
2:H:118:SER:O	4:H:321:HOH:O	2.06	0.73
3:B:301:NAG:O6	4:B:432:HOH:O	2.07	0.73
2:A:56:GLY:O	4:A:306:HOH:O	2.05	0.72
1:B:6:GLN:HB2	1:B:90(C):VAL:HG13	1.70	0.72
1:L:174:ASP:HA	1:L:177:LYS:HE3	1.72	0.72
2:A:193:SER:OG	4:A:330:HOH:O	2.08	0.71
1:B:154:GLU:OE1	4:B:448:HOH:O	2.08	0.71
1:L:59:ARG:HH12	1:L:80:ASP:CG	1.95	0.70
1:B:90(C):VAL:HG11	1:B:90(D):PRO:CD	2.21	0.70
2:H:65:GLN:OE1	4:H:329:HOH:O	2.10	0.69
2:H:76:ASP:O	4:H:324:HOH:O	2.08	0.69
2:H:151:TYR:CE2	2:H:156:VAL:CG1	2.77	0.68
1:B:41:ALA:O	4:B:403:HOH:O	2.10	0.67
1:B:93:LEU:O	4:B:410:HOH:O	2.12	0.66
1:L:139:VAL:HG23	1:L:180:VAL:O	1.95	0.66
1:L:6:GLN:HB2	1:L:90(C):VAL:HG11	1.78	0.66
1:B:24:GLN:OE1	4:B:431:HOH:O	2.14	0.65
1:B:59:ARG:NH1	1:B:80:ASP:OD2	2.30	0.65
2:A:206:HIS:CE1	2:A:208:PRO:HG2	2.33	0.63
1:L:90(C):VAL:CG1	1:L:90(D):PRO:HD2	2.29	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:65:TRP:HB2	3:B:301:NAG:H83	1.82	0.62
1:B:58:ALA:O	4:B:416:HOH:O	2.16	0.62
1:B:65:TRP:CB	3:B:301:NAG:H83	2.30	0.62
2:A:173:PRO:HG2	1:B:151:SER:OG	2.01	0.60
3:L:301:NAG:O6	4:L:452:HOH:O	2.17	0.60
1:L:39:GLY:C	4:L:446:HOH:O	2.39	0.60
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.84	0.59
1:L:178:HIS:O	1:L:179:LYS:HB2	2.04	0.58
2:A:151:TYR:CE2	2:A:156:VAL:CG1	2.87	0.58
1:L:65:TRP:CD1	3:L:301:NAG:H83	2.39	0.58
1:L:174:ASP:HA	1:L:177:LYS:CE	2.34	0.58
1:L:108:PRO:HB3	1:L:198:PHE:CE2	2.39	0.58
1:L:108:PRO:HB3	1:L:198:PHE:CD2	2.38	0.58
1:B:199:ASN:OD1	1:B:199:ASN:C	2.41	0.57
1:L:36:GLN:HB2	1:L:45:LEU:HD11	1.85	0.57
1:B:39:GLY:C	1:B:40:LYS:HD2	2.25	0.57
1:L:39:GLY:CA	4:L:446:HOH:O	2.52	0.57
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.40	0.57
1:L:90(C):VAL:HG13	1:L:90(D):PRO:HD2	1.86	0.57
2:H:151:TYR:CZ	2:H:156:VAL:HG12	2.40	0.57
2:H:23:GLU:OE2	2:H:77:THR:HG22	2.05	0.57
1:B:6:GLN:HB2	1:B:90(C):VAL:CG1	2.36	0.56
1:L:186:THR:HG23	1:L:193:PRO:HG3	1.86	0.56
2:H:56:GLY:O	4:H:317:HOH:O	2.18	0.55
1:B:33:LEU:HD23	1:B:33:LEU:C	2.27	0.55
2:A:184:LEU:HD12	2:A:184:LEU:C	2.27	0.55
2:H:154:GLU:HG3	4:H:325:HOH:O	2.07	0.54
2:A:207:LYS:N	2:A:208:PRO:HD2	2.22	0.54
2:A:47:TRP:CZ2	2:A:49:GLY:HA2	2.42	0.54
1:B:135:VAL:HG12	1:B:185:VAL:HG13	1.90	0.54
2:H:43:GLN:HG2	4:H:323:HOH:O	2.07	0.54
1:L:184:GLU:HB2	1:L:195:THR:HG23	1.90	0.54
1:L:181:TYR:HB2	1:L:198:PHE:CE1	2.43	0.53
2:A:122:THR:CG2	2:A:209:SER:OG	2.57	0.53
1:B:97:ARG:NE	4:B:411:HOH:O	2.41	0.53
1:B:59:ARG:HH12	1:B:80:ASP:CG	2.11	0.53
1:L:184:GLU:CB	1:L:195:THR:HG23	2.39	0.53
2:A:64:PHE:HB3	2:A:68:VAL:CG2	2.39	0.52
1:L:102:PRO:HD3	1:L:187:HIS:CD2	2.44	0.52
1:B:181:TYR:O	1:B:197:SER:HA	2.09	0.52
1:L:175:TYR:HA	1:L:181:TYR:HH	1.74	0.52
1:L:90(D):PRO:HG2	4:L:426:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:171:SER:OG	1:L:174:ASP:OD2	2.27	0.52
1:B:139:VAL:HG23	1:B:180:VAL:O	2.08	0.52
1:B:138:LYS:NZ	1:B:184:GLU:OE1	2.42	0.52
1:B:178:HIS:NE2	4:B:441:HOH:O	2.33	0.52
1:L:90(A):PHE:C	1:L:90(B):ILE:HD12	2.31	0.52
1:L:64:ARG:CD	1:L:69:TYR:HE2	2.23	0.51
1:L:121:VAL:CG1	1:L:168:LEU:HD23	2.40	0.51
2:A:122:THR:HG23	2:A:209:SER:OG	2.10	0.51
2:A:201:ILE:CG2	2:A:214:ASP:OD1	2.59	0.51
1:B:146:GLY:O	1:B:147:ASN:OD1	2.29	0.51
2:A:201:ILE:HD12	2:A:216:ARG:HA	1.93	0.50
2:H:152:PHE:CD1	2:H:153:PRO:CA	2.94	0.50
2:H:40:ALA:HB3	2:H:43:GLN:HG3	1.92	0.50
1:L:97:ARG:NH2	4:L:419:HOH:O	2.43	0.50
1:L:187:HIS:CD2	1:L:189:GLY:H	2.30	0.50
2:A:198:GLN:HG2	2:A:200:TYR:CE1	2.47	0.50
2:H:32:HIS:O	2:H:53:PRO:HG2	2.12	0.49
1:L:65:TRP:CG	3:L:301:NAG:H83	2.47	0.49
1:L:181:TYR:CB	1:L:198:PHE:CE1	2.96	0.49
2:A:53:PRO:O	2:A:72:ARG:HD2	2.13	0.49
2:H:152:PHE:CG	2:H:153:PRO:HA	2.48	0.49
1:L:183:CYS:O	1:L:195:THR:HA	2.12	0.49
2:A:3:HIS:CD2	2:A:4:LEU:H	2.31	0.49
1:L:6:GLN:HB2	1:L:90(C):VAL:CG1	2.43	0.49
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.45	0.49
1:B:180:VAL:HA	1:B:198:PHE:O	2.13	0.49
2:H:152:PHE:CE1	2:H:153:PRO:HB3	2.48	0.49
2:H:74:ALA:HB1	2:H:78:TYR:CE2	2.49	0.48
1:B:133:ALA:C	1:B:134:LYS:HD2	2.34	0.48
1:L:152:VAL:HG12	1:L:153:THR:O	2.13	0.48
1:L:112:GLU:CD	2:H:215:LYS:HZ3	2.16	0.48
1:B:14:ARG:O	1:B:17:ASP:HB2	2.14	0.48
1:L:140:ASP:OD1	1:L:180:VAL:HG21	2.14	0.48
1:B:175:TYR:HA	1:B:181:TYR:HH	1.78	0.48
1:L:14:ARG:NH2	1:L:96:LYS:NZ	2.61	0.47
2:H:153:PRO:O	2:H:206:HIS:NE2	2.47	0.47
2:A:125:PRO:HB3	2:A:151:TYR:HB3	1.96	0.47
2:H:152:PHE:CD1	2:H:153:PRO:HA	2.49	0.47
1:B:90(D):PRO:O	4:B:445:HOH:O	2.21	0.47
2:H:151:TYR:CE2	2:H:156:VAL:HG11	2.50	0.47
1:B:174:ASP:HA	1:B:177:LYS:HE2	1.97	0.46
1:L:90(B):ILE:HD11	2:H:37:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:186:THR:HG23	1:B:193:PRO:HG3	1.97	0.46
1:L:181:TYR:O	1:L:197:SER:HA	2.15	0.46
2:A:153:PRO:O	2:A:206:HIS:HE1	1.99	0.46
1:L:180:VAL:HA	1:L:198:PHE:O	2.16	0.46
1:L:90(C):VAL:HG12	4:L:426:HOH:O	2.16	0.46
1:L:97:ARG:HG3	1:L:97:ARG:HH11	1.81	0.46
1:L:129:TYR:CG	1:L:130:PRO:HA	2.51	0.46
1:B:87:GLN:HB2	1:B:90(B):ILE:HD13	1.98	0.46
1:B:65:TRP:HB2	3:B:301:NAG:C8	2.45	0.45
2:H:204:VAL:HG11	2:H:205:ASN:N	2.30	0.45
1:B:182:ALA:HA	1:B:196:LYS:O	2.15	0.45
1:B:36:GLN:HB2	1:B:45:LEU:HD11	1.97	0.45
2:H:211:THR:O	2:H:212:LYS:HG3	2.16	0.45
1:B:65:TRP:N	1:B:68:GLU:O	2.45	0.45
2:A:62:ARG:HG3	2:A:63:GLN:N	2.31	0.45
1:L:178:HIS:O	1:L:179:LYS:CB	2.64	0.45
1:B:67:GLN:HB2	4:B:452:HOH:O	2.17	0.45
1:B:187:HIS:CD2	1:B:189:GLY:H	2.34	0.45
1:B:102:PRO:HD3	1:B:187:HIS:CD2	2.53	0.44
2:A:152:PHE:CD1	2:A:153:PRO:CA	3.01	0.44
2:H:207:LYS:N	2:H:208:PRO:HD2	2.31	0.44
1:B:4:MET:HA	1:B:24:GLN:O	2.18	0.44
1:L:138:LYS:HE3	1:L:141:ASN:HA	2.00	0.44
1:B:68:GLU:HB3	4:B:431:HOH:O	2.17	0.43
2:A:64:PHE:HB3	2:A:68:VAL:HG23	1.99	0.43
1:B:198:PHE:CD1	1:B:198:PHE:C	2.92	0.43
1:L:33:LEU:C	1:L:33:LEU:HD23	2.38	0.43
1:L:59:ARG:HB2	1:L:74:ASN:O	2.18	0.43
2:A:151:TYR:CZ	2:A:156:VAL:HG12	2.54	0.43
1:L:152:VAL:CG2	1:L:164:LEU:HD12	2.49	0.43
2:A:27:TYR:CE2	2:A:29:ILE:HA	2.53	0.43
1:B:24:GLN:NE2	1:B:68:GLU:OE1	2.46	0.43
1:B:138:LYS:HA	1:B:142:ALA:O	2.18	0.43
1:B:146:GLY:C	1:B:147:ASN:OD1	2.57	0.43
2:H:74(C):ASP:O	2:H:75:PHE:HB2	2.18	0.43
1:L:64:ARG:HD2	1:L:69:TYR:HE2	1.84	0.42
2:H:62:ARG:NH2	4:H:322:HOH:O	2.52	0.42
2:H:66:GLY:O	2:H:84:LYS:HE2	2.19	0.42
2:H:152:PHE:HA	2:H:153:PRO:HA	1.83	0.42
1:B:90(C):VAL:HG11	1:B:90(D):PRO:N	2.34	0.42
1:B:134:LYS:O	1:B:185:VAL:HA	2.20	0.42
1:L:59:ARG:NH2	1:L:79:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:152:PHE:CD1	2:H:153:PRO:N	2.87	0.42
1:B:152:VAL:HG12	1:B:153:THR:O	2.20	0.42
2:H:184:LEU:HD12	2:H:184:LEU:C	2.39	0.42
2:H:62:ARG:CZ	4:H:322:HOH:O	2.67	0.41
1:B:95:LEU:HD12	1:B:95:LEU:HA	1.79	0.41
2:H:151:TYR:CZ	2:H:156:VAL:CG1	3.03	0.41
1:B:96:LYS:HA	1:B:129:TYR:OH	2.20	0.41
2:A:34:ILE:HG13	2:A:79:PHE:CE2	2.56	0.41
2:A:152:PHE:CD1	2:A:153:PRO:HA	2.55	0.41
2:A:152:PHE:CG	2:A:153:PRO:HA	2.56	0.41
1:B:139:VAL:CG1	1:B:144:GLN:HE22	2.32	0.41
2:A:201:ILE:CD1	2:A:216:ARG:HG3	2.51	0.41
1:L:32:TYR:CZ	1:L:48:ASP:HB2	2.55	0.41
1:B:65:TRP:O	1:B:68:GLU:HG3	2.21	0.41
1:L:121:VAL:HG12	1:L:168:LEU:HD23	2.03	0.41
2:A:19:ARG:HB2	2:A:82:ASP:OD1	2.20	0.41
1:L:125:LEU:N	1:L:125:LEU:HD12	2.36	0.41
1:B:164:LEU:C	1:B:164:LEU:HD23	2.41	0.40
2:A:68:VAL:HG22	2:A:83:LEU:HD23	2.03	0.40
1:B:152:VAL:CG2	1:B:164:LEU:HD12	2.51	0.40
2:H:83:LEU:HD23	2:H:83:LEU:HA	1.92	0.40
1:L:139:VAL:CG1	1:L:144:GLN:HE22	2.34	0.40
2:H:201:ILE:O	2:H:203:ASN:ND2	2.54	0.40
1:B:94:ASP:OD1	1:B:94:ASP:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	197/206 (96%)	184 (93%)	13 (7%)	0	100	100
1	L	196/206 (95%)	182 (93%)	13 (7%)	1 (0%)	38	68
2	A	208/229 (91%)	198 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	209/229 (91%)	198 (95%)	11 (5%)	0	100	100
All	All	810/870 (93%)	762 (94%)	47 (6%)	1 (0%)	59	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	179	LYS

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	B	175/182 (96%)	166 (95%)	9 (5%)	33	62
1	L	174/182 (96%)	165 (95%)	9 (5%)	32	61
2	A	180/194 (93%)	170 (94%)	10 (6%)	30	56
2	H	180/194 (93%)	170 (94%)	10 (6%)	30	56
All	All	709/752 (94%)	671 (95%)	38 (5%)	31	59

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

Mol	Chain	Res	Type
1	L	9	SER
1	L	12	SER
1	L	17	ASP
1	L	19	VAL
1	L	63	ARG
1	L	64	ARG
1	L	95	LEU
1	L	174	ASP
1	L	177	LYS
2	H	2	VAL
2	H	28	LYS
2	H	60	ASN
2	H	83	LEU
2	H	130	LEU

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Mol	Chain	Res	Type
2	H	155	PRO
2	H	156	VAL
2	H	159	SER
2	H	183	SER
2	H	213	VAL
2	A	2	VAL
2	A	60	ASN
2	A	72	ARG
2	A	83	LEU
2	A	130	LEU
2	A	155	PRO
2	A	156	VAL
2	A	159	SER
2	A	183	SER
2	A	213	VAL
1	B	9	SER
1	B	12	SER
1	B	17	ASP
1	B	19	VAL
1	B	64	ARG
1	B	95	LEU
1	B	174	ASP
1	B	177	LYS
1	B	199	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	24	GLN
1	L	36	GLN
1	L	77	GLN
1	L	149	GLN
1	L	178	HIS
1	L	187	HIS
2	H	3	HIS
2	H	43	GLN
2	H	59	ASN
2	H	60	ASN
2	H	65	GLN
2	H	170	HIS
2	H	177	GLN

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Mol	Chain	Res	Type
2	H	203	ASN
2	A	3	HIS
2	A	59	ASN
2	A	60	ASN
2	A	177	GLN
2	A	203	ASN
1	B	24	GLN
1	B	187	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	PCA	H	1	2	8,8,9	6.70	3 (37%)	8,10,12	5.42	4 (50%)

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
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	O-C	17.79	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CD-N	5.78	1.46	1.34
2	H	1	PCA	CA-C	2.46	1.52	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	CA-N-CD	-14.47	103.06	114.37
2	H	1	PCA	OE-CD-CG	-3.04	121.92	126.70
2	H	1	PCA	CB-CA-N	2.43	110.72	103.72
2	H	1	PCA	C-CA-N	2.01	111.17	110.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
3	NAG	B	301	1	12,14,15	0.70	1 (8%)	15,19,21	1.21	1 (6%)
3	NAG	L	301	1	12,14,15	0.70	0	15,19,21	1.44	2 (13%)

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
3	NAG	B	301	1	-	0/6/23/26	0/1/1/1
3	NAG	L	301	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NAG	O5-C5	-2.16	1.41	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	301	NAG	O5-C5-C6	3.93	111.11	106.98
3	B	301	NAG	O5-C5-C6	3.45	110.60	106.98
3	L	301	NAG	C3-C2-N2	-2.74	107.59	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	199/206 (96%)	0.52	22 (11%) 6 5	22, 62, 134, 187	0
1	L	198/206 (96%)	0.77	31 (15%) 3 3	24, 62, 127, 192	0
2	A	212/229 (92%)	0.51	17 (8%) 12 12	22, 64, 128, 145	0
2	H	213/229 (93%)	0.66	23 (10%) 6 6	21, 70, 128, 148	0
All	All	822/870 (94%)	0.61	93 (11%) 6 5	21, 65, 130, 192	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	190	VAL	7.6
1	L	4	MET	7.1
2	A	190	VAL	7.1
1	L	179	LYS	6.3
2	A	195	LEU	6.1
1	L	5	THR	5.9
2	H	197	THR	5.4
1	B	180	VAL	5.4
1	L	67	GLN	4.8
1	B	194	VAL	4.7
1	L	185	VAL	4.6
1	B	4	MET	4.5
1	L	194	VAL	4.4
2	H	142	ALA	4.3
2	H	193	SER	4.3
1	L	138	LYS	4.2
2	H	199	THR	4.1
2	A	188	VAL	4.0
2	H	188	VAL	4.0
2	A	217	VAL	3.9
2	H	195	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	L	106	ILE	3.9
1	L	8	PRO	3.9
2	H	127	VAL	3.7
2	H	201	ILE	3.5
1	L	7	SER	3.5
1	L	192	SER	3.4
2	H	166	THR	3.4
1	B	5	THR	3.3
2	A	197	THR	3.3
1	B	185	VAL	3.3
1	B	198	PHE	3.3
1	L	140	ASP	3.3
2	H	217	VAL	3.2
1	B	8	PRO	3.2
2	H	18	VAL	3.1
1	L	197	SER	3.1
2	A	193	SER	3.1
1	L	180	VAL	3.1
1	L	65	TRP	3.1
1	B	192	SER	3.0
1	B	182	ALA	3.0
1	B	140	ASP	3.0
1	L	191	SER	2.9
2	A	11	VAL	2.9
1	L	135	VAL	2.9
2	A	127	VAL	2.9
2	H	207	LYS	2.8
2	A	207	LYS	2.8
1	B	65	TRP	2.8
1	L	24	GLN	2.8
1	L	198	PHE	2.8
1	L	181	TYR	2.7
1	B	179	LYS	2.7
1	L	139	VAL	2.7
1	B	121	VAL	2.7
1	B	138	LYS	2.6
1	B	181	TYR	2.6
2	A	143	ALA	2.6
1	B	104	VAL	2.6
2	H	75	PHE	2.6
2	H	191	PRO	2.6
1	L	176	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	121	VAL	2.5
1	L	6	GLN	2.5
2	H	187	VAL	2.5
2	A	187	VAL	2.5
1	L	141	ASN	2.5
1	B	141	ASN	2.4
2	H	122	THR	2.4
1	B	197	SER	2.4
2	A	18	VAL	2.4
2	H	165	LEU	2.4
1	L	190	LEU	2.3
2	H	29	ILE	2.3
2	A	148	VAL	2.3
1	L	136	GLN	2.2
2	H	74(B)	TRP	2.2
1	B	176	GLU	2.2
1	L	122	VAL	2.2
2	H	204	VAL	2.2
2	A	142	ALA	2.2
1	B	67	GLN	2.2
2	H	76	ASP	2.2
2	H	162	SER	2.2
2	A	166	THR	2.1
1	L	134	LYS	2.1
1	L	90(C)	VAL	2.1
2	A	144	LEU	2.1
1	L	88	VAL	2.1
1	B	193	PRO	2.1
1	B	190	LEU	2.1
2	A	115	VAL	2.0

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PCA	H	1	8/9	0.28	-	87,111,130,144	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	L	301	14/15	0.22	-	26,64,79,84	0
3	NAG	B	301	14/15	0.15	-	49,79,95,104	0

6.5 Other polymers

There are no such residues in this entry.