Full wwPDB X-ray Structure Validation Report (i)

Nov 28, 2016 – 02:49 PM EST

PDB ID	:	5CZV
Title	:	Crystal structure of Notch3 NRR in complex with 20350 Fab
Authors	:	Hu, T.; Fryer, C.; Chopra, R.; Clark, K.
Deposited on	:	2015-08-01
Resolution	:	3.19 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

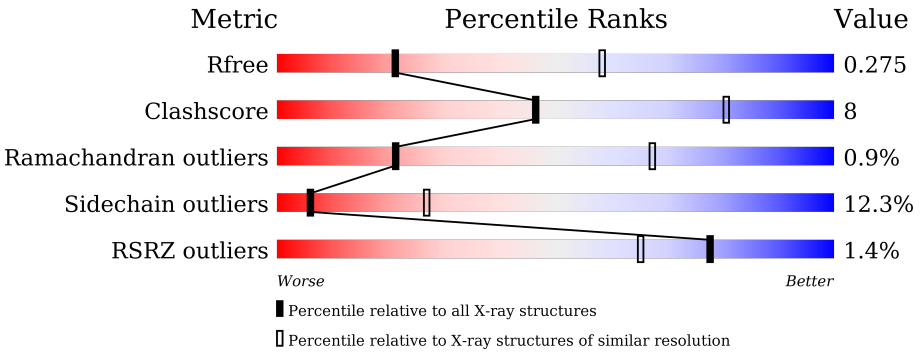
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 3.19 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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	271	% 67% 12% • 17%
2	H	223	3% 62% 26% • 8%
3	L	214	80% 16% ••

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4939 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 Neurogenic locus notch homolog protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1738	1067	315	335	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1641	GLY	-	expression tag	UNP Q9UM47
A	1642	SER	-	expression tag	UNP Q9UM47
A	1643	HIS	-	expression tag	UNP Q9UM47
A	1644	HIS	-	expression tag	UNP Q9UM47
A	1645	HIS	-	expression tag	UNP Q9UM47
A	1646	HIS	-	expression tag	UNP Q9UM47
A	1647	HIS	-	expression tag	UNP Q9UM47
A	1648	HIS	-	expression tag	UNP Q9UM47

- Molecule 2 is a protein called Fab 20350 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	206	Total	C	N	O	S	0	0	0
			1554	991	259	298	6			

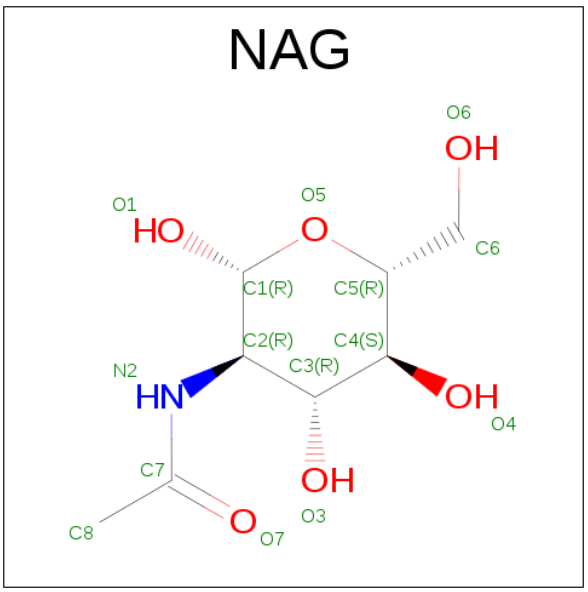
- Molecule 3 is a protein called Fab 20350 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1623	1020	270	327	6			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

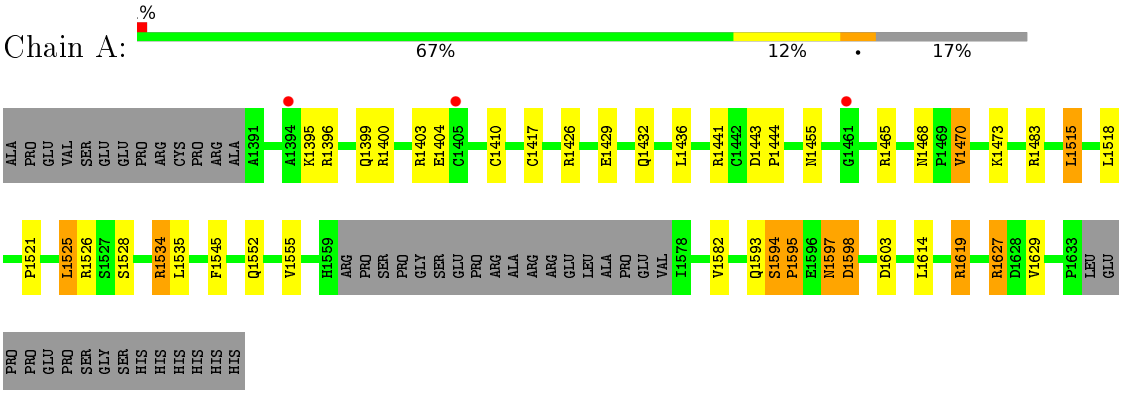
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	H	2	Total O 2 2	0	0
6	L	3	Total O 3 3	0	0

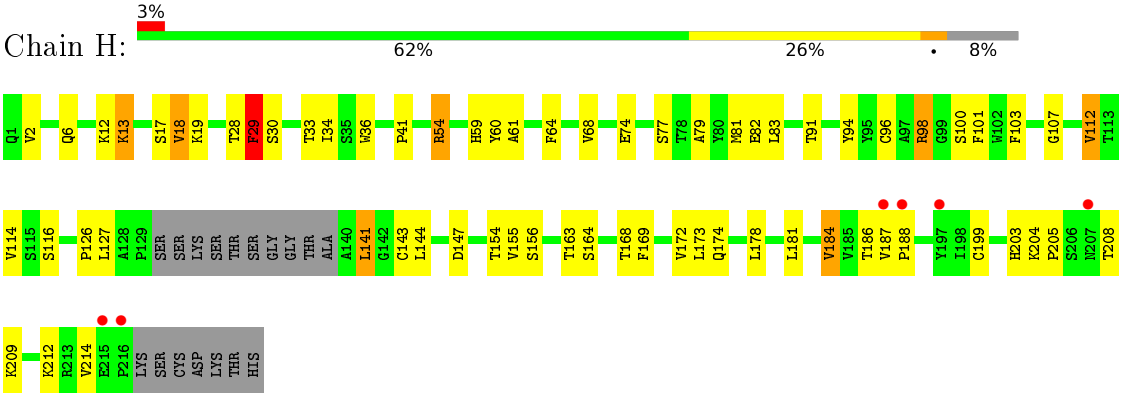
3 Residue-property plots (i)

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.

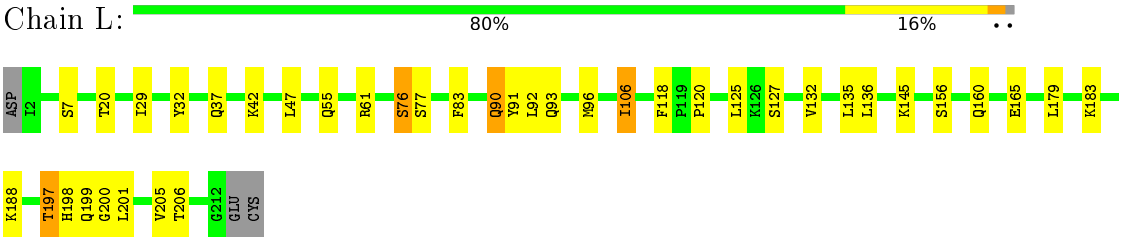
- Molecule 1: Neurogenic locus notch homolog protein 3



- Molecule 2: Fab 20350 heavy chain



- Molecule 3: Fab 20350 light chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	91.92Å 104.35Å 92.85Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	29.62 – 3.19 29.62 – 3.19	Depositor EDS
% Data completeness (in resolution range)	85.9 (29.62-3.19) 85.9 (29.62-3.19)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.204 , 0.257 0.222 , 0.275	Depositor DCC
R_{free} test set	566 reflections (4.88%)	DCC
Wilson B-factor (Å^2)	48.7	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4939	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.88% 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: CA, 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	0.53	0/1777	0.75	0/2411
2	H	0.48	0/1597	0.76	0/2178
3	L	0.50	0/1658	0.73	0/2250
All	All	0.51	0/5032	0.75	0/6839

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	1738	0	1607	25	0
2	H	1554	0	1514	40	0
3	L	1623	0	1577	14	0
4	A	3	0	0	0	0
5	A	14	0	13	0	0
6	A	2	0	0	0	0
6	H	2	0	0	0	0
6	L	3	0	0	0	0
All	All	4939	0	4711	73	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 8.

All (73) 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:A:1515:LEU:HD12	1:A:1629:VAL:HG12	1.27	1.13
2:H:91:THR:HG22	2:H:114:VAL:H	1.31	0.95
1:A:1594:SER:HB3	1:A:1595:PRO:HA	1.54	0.87
2:H:12:LYS:HG3	2:H:18:VAL:HG13	1.59	0.82
1:A:1521:PRO:O	1:A:1525:LEU:HG	1.83	0.79
1:A:1515:LEU:CD1	1:A:1629:VAL:HG12	2.10	0.79
1:A:1444:PRO:HB3	2:H:59:HIS:HB2	1.63	0.78
1:A:1515:LEU:HD12	1:A:1629:VAL:CG1	2.11	0.75
1:A:1597:ASN:H	1:A:1597:ASN:HD22	1.33	0.73
1:A:1525:LEU:HD23	1:A:1555:VAL:HG11	1.69	0.73
2:H:68:VAL:HG12	2:H:83:LEU:HD13	1.71	0.71
2:H:91:THR:HG22	2:H:114:VAL:N	2.06	0.69
1:A:1619:ARG:HG3	1:A:1619:ARG:O	1.93	0.69
1:A:1594:SER:HB3	1:A:1595:PRO:CA	2.26	0.65
2:H:13:LYS:HG3	2:H:116:SER:HA	1.81	0.62
3:L:90:GLN:HG2	3:L:92:LEU:H	1.66	0.60
3:L:201:LEU:HD13	3:L:205:VAL:HG22	1.83	0.60
3:L:125:LEU:HD22	3:L:183:LYS:HG3	1.83	0.60
2:H:30:SER:O	2:H:54:ARG:HD3	2.01	0.60
1:A:1396:ARG:HD3	1:A:1410:CYS:O	2.02	0.60
1:A:1534:ARG:HH21	1:A:1534:ARG:CG	2.15	0.60
2:H:19:LYS:HZ3	2:H:82:GLU:HB2	1.66	0.59
2:H:34:ILE:HG21	2:H:79:ALA:CB	2.33	0.58
2:H:12:LYS:HE3	2:H:18:VAL:HG12	1.86	0.58
2:H:94:TYR:HE1	2:H:112:VAL:HG22	1.69	0.58
1:A:1597:ASN:ND2	1:A:1597:ASN:H	2.02	0.56
2:H:168:THR:HG23	2:H:181:LEU:HD21	1.86	0.56
1:A:1518:LEU:HD11	1:A:1627:ARG:HD3	1.87	0.56
3:L:145:LYS:HB3	3:L:197:THR:OG1	2.05	0.56
2:H:6:GLN:HE22	2:H:96:CYS:H	1.55	0.55
3:L:91:TYR:HA	3:L:96:MET:SD	2.47	0.54
2:H:184:VAL:HG11	3:L:135:LEU:HD22	1.89	0.54
2:H:94:TYR:CE1	2:H:112:VAL:HG22	2.43	0.53
2:H:174:GLN:HA	3:L:160:GLN:HE22	1.73	0.53
2:H:147:ASP:HB3	2:H:178:LEU:HD13	1.91	0.53
1:A:1528:SER:HB2	1:A:1545:PHE:HE2	1.73	0.53
2:H:6:GLN:HE21	2:H:107:GLY:HA3	1.74	0.53
2:H:2:VAL:HB	2:H:98:ARG:HH12	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:LEU:HB3	3:L:118:PHE:CD1	2.43	0.52
2:H:29:PHE:CE1	2:H:74:GLU:HA	2.45	0.52
1:A:1598:ASP:HB2	2:H:101:PHE:HD2	1.75	0.51
2:H:12:LYS:HG3	2:H:18:VAL:CG1	2.35	0.51
1:A:1528:SER:HB2	1:A:1545:PHE:CE2	2.47	0.50
1:A:1429:GLU:OE1	3:L:93:GLN:HG2	2.12	0.50
1:A:1468:ASN:OD1	1:A:1470:VAL:HG23	2.12	0.49
2:H:68:VAL:CG1	2:H:83:LEU:HD13	2.41	0.49
2:H:91:THR:CG2	2:H:114:VAL:H	2.13	0.49
2:H:169:PHE:O	2:H:181:LEU:HG	2.12	0.49
1:A:1534:ARG:HG3	1:A:1534:ARG:HH21	1.78	0.48
2:H:29:PHE:CZ	2:H:74:GLU:HA	2.48	0.48
2:H:6:GLN:NE2	2:H:96:CYS:H	2.11	0.48
3:L:198:HIS:CD2	3:L:200:GLY:H	2.33	0.46
2:H:28:THR:C	2:H:30:SER:H	2.19	0.46
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.51	0.46
3:L:29:ILE:O	3:L:32:TYR:HD1	1.99	0.45
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.97	0.44
2:H:60:TYR:CD1	2:H:68:VAL:HG23	2.53	0.44
3:L:120:PRO:HD3	3:L:132:VAL:HG22	2.00	0.44
1:A:1468:ASN:OD1	1:A:1470:VAL:CG2	2.66	0.43
1:A:1555:VAL:HG23	1:A:1582:VAL:HG22	2.00	0.43
3:L:83:PHE:CE2	3:L:106:ILE:HA	2.53	0.43
2:H:29:PHE:CZ	2:H:77:SER:HA	2.54	0.42
2:H:126:PRO:HG3	2:H:212:LYS:HD2	2.01	0.42
1:A:1436:LEU:HB3	1:A:1443:ASP:OD2	2.19	0.42
1:A:1400:ARG:HH21	1:A:1627:ARG:NH1	2.18	0.42
2:H:12:LYS:O	2:H:114:VAL:HA	2.20	0.42
2:H:141:LEU:HB2	2:H:214:VAL:HG11	2.02	0.41
1:A:1455:ASN:HD21	1:A:1614:LEU:HD21	1.85	0.41
2:H:203:HIS:CD2	2:H:205:PRO:HD2	2.55	0.41
2:H:64:PHE:HB3	2:H:68:VAL:HG13	2.02	0.41
2:H:61:ALA:HB3	2:H:64:PHE:HD2	1.86	0.41
2:H:64:PHE:O	2:H:68:VAL:HG22	2.22	0.40
2:H:187:VAL:HB	2:H:188:PRO:HD2	2.03	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	A	221/271 (82%)	214 (97%)	5 (2%)	2 (1%)	21 67
2	H	202/223 (91%)	190 (94%)	9 (4%)	3 (2%)	13 55
3	L	209/214 (98%)	202 (97%)	6 (3%)	1 (0%)	34 78
All	All	632/708 (89%)	606 (96%)	20 (3%)	6 (1%)	21 67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	29	PHE
2	H	41	PRO
1	A	1594	SER
1	A	1595	PRO
3	L	76	SER
2	H	155	VAL

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	188/228 (82%)	164 (87%)	24 (13%)	5 25
2	H	171/186 (92%)	146 (85%)	25 (15%)	4 19
3	L	184/189 (97%)	166 (90%)	18 (10%)	10 38
All	All	543/603 (90%)	476 (88%)	67 (12%)	6 27

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1395	LYS
1	A	1399	GLN
1	A	1403	ARG
1	A	1404	GLU
1	A	1417	CYS
1	A	1426	ARG
1	A	1432	GLN
1	A	1441	ARG
1	A	1465	ARG
1	A	1470	VAL
1	A	1473	LYS
1	A	1483	ARG
1	A	1515	LEU
1	A	1525	LEU
1	A	1526	ARG
1	A	1534	ARG
1	A	1535	LEU
1	A	1552	GLN
1	A	1593	GLN
1	A	1597	ASN
1	A	1598	ASP
1	A	1603	ASP
1	A	1619	ARG
1	A	1627	ARG
2	H	13	LYS
2	H	17	SER
2	H	18	VAL
2	H	29	PHE
2	H	33	THR
2	H	54	ARG
2	H	98	ARG
2	H	100	SER
2	H	103	PHE
2	H	112	VAL
2	H	141	LEU
2	H	143	CYS
2	H	144	LEU
2	H	154	THR
2	H	156	SER
2	H	163	THR
2	H	164	SER
2	H	172	VAL

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Mol	Chain	Res	Type
2	H	173	LEU
2	H	184	VAL
2	H	186	THR
2	H	199	CYS
2	H	204	LYS
2	H	208	THR
2	H	209	LYS
3	L	7	SER
3	L	20	THR
3	L	42	LYS
3	L	55	GLN
3	L	61	ARG
3	L	76	SER
3	L	77	SER
3	L	90	GLN
3	L	106	ILE
3	L	127	SER
3	L	136	LEU
3	L	156	SER
3	L	165	GLU
3	L	179	LEU
3	L	188	LYS
3	L	197	THR
3	L	199	GLN
3	L	206	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1455	ASN
1	A	1459	HIS
1	A	1597	ASN
2	H	6	GLN
2	H	195	GLN
2	H	202	ASN
3	L	55	GLN
3	L	160	GLN
3	L	198	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	5004	1	14,14,15	0.32	0	15,19,21	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	5004	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	225/271 (83%)	-0.27	3 (1%) 79 67	26, 49, 96, 136	0
2	H	206/223 (92%)	-0.07	6 (2%) 55 41	39, 78, 116, 137	0
3	L	211/214 (98%)	-0.23	0 100 100	25, 63, 135, 157	0
All	All	642/708 (90%)	-0.20	9 (1%) 78 65	25, 63, 122, 157	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1461	GLY	6.8
1	A	1405	CYS	3.1
2	H	215	GLU	2.9
2	H	216	PRO	2.8
2	H	187	VAL	2.5
2	H	188	PRO	2.5
1	A	1394	ALA	2.4
2	H	207	ASN	2.4
2	H	197	TYR	2.2

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

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

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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	CA	A	5003	1/1	0.99	0.07	-1.57	40,40,40,40	0
4	CA	A	5001	1/1	0.95	0.05	-1.73	61,61,61,61	0
4	CA	A	5002	1/1	0.92	0.07	-2.57	55,55,55,55	0
5	NAG	A	5004	14/15	0.58	0.29	-	110,113,115,115	0

6.5 Other polymers

There are no such residues in this entry.