



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:40 AM UTC

PDB ID : 5CZX / pdb_00005czx
Title : Crystal structure of Notch3 NRR in complex with 20358 Fab
Authors : Hu, T.; Fryer, C.; Chopra, R.; Clark, K.
Deposited on : 2015-08-01
Resolution : 2.10 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

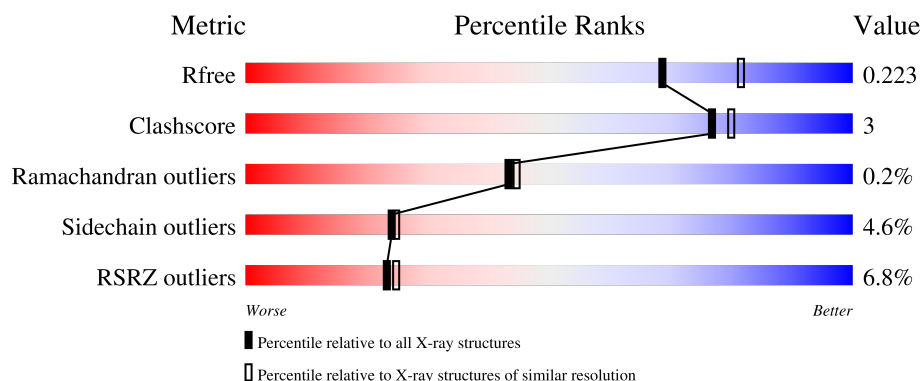
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	271	19% 76% 7% • 16%
1	B	271	8% 72% 11% • 16%
2	C	226	2% 88% 6% 5%
2	H	226	0% 88% 7% 5%
3	D	214	2% 86% 14%

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Mol	Chain	Length	Quality of chain
3	L	214	% 89% 10%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10929 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	227	Total	C	N	O	S	0	0	0
			1752	1076	320	334	22			
1	B	227	Total	C	N	O	S	0	0	0
			1752	1076	320	334	22			

There are 16 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
B	1641	GLY	-	expression tag	UNP Q9UM47
B	1642	SER	-	expression tag	UNP Q9UM47
B	1643	HIS	-	expression tag	UNP Q9UM47
B	1644	HIS	-	expression tag	UNP Q9UM47
B	1645	HIS	-	expression tag	UNP Q9UM47
B	1646	HIS	-	expression tag	UNP Q9UM47
B	1647	HIS	-	expression tag	UNP Q9UM47
B	1648	HIS	-	expression tag	UNP Q9UM47

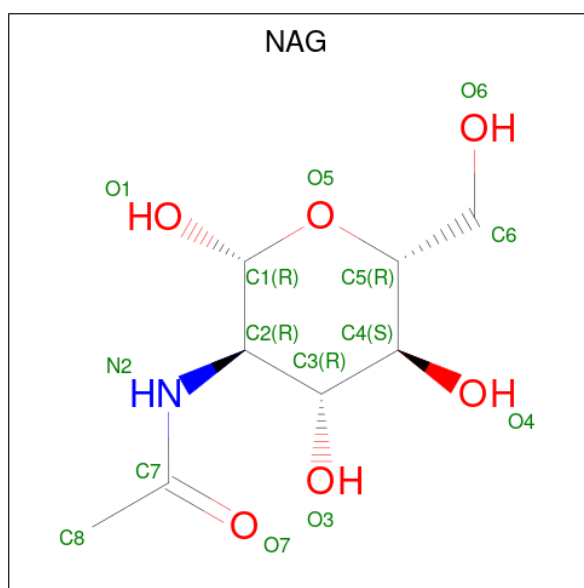
- Molecule 2 is a protein called 20358 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	214	Total	C	N	O	S	0	0	0
			1610	1018	269	316	7			
2	H	215	Total	C	N	O	S	0	0	0
			1614	1020	270	317	7			

- Molecule 3 is a protein called 20358 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	213	Total	C	N	O	S	0	0	0
			1637	1025	273	334	5			
3	L	213	Total	C	N	O	S	0	0	0
			1637	1025	273	334	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Ca	0	0
			3	3		
5	B	3	Total	Ca	0	0
			3	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Cl	0	0
			1	1		
7	H	1	Total	Cl	0	0
			1	1		

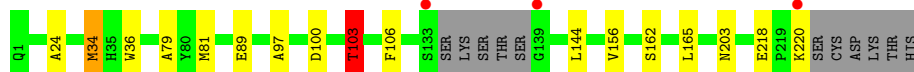
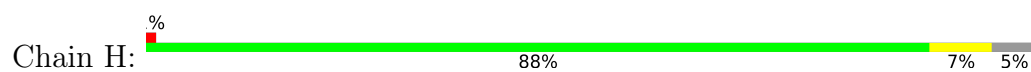
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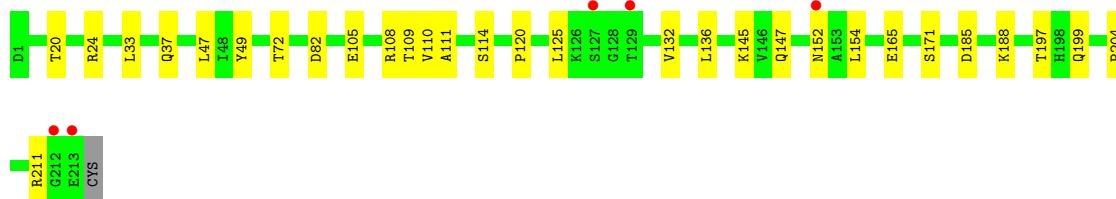
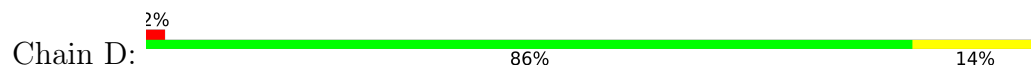
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	1	Total	Cl	0	0
			1	1		

- Molecule 8 is water.

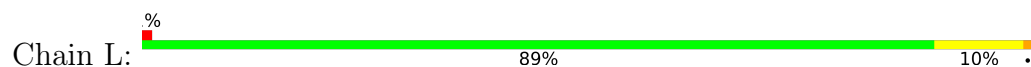
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	114	Total	O	0	0
			114	114		
8	B	121	Total	O	0	0
			121	121		
8	C	153	Total	O	0	0
			153	153		
8	D	154	Total	O	0	0
			154	154		
8	H	144	Total	O	0	0
			144	144		
8	L	164	Total	O	0	0
			164	164		



• Molecule 3: 20358 Fab light chain



• Molecule 3: 20358 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.34Å 123.86Å 150.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.10 29.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.99-2.10) 99.1 (29.99-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.190 , 0.226 (Not available) , 0.223	Depositor DCC
R_{free} test set	4809 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10929	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2160e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, NAG, CL, EDO

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	0.82	1/1790 (0.1%)	1.21	6/2427 (0.2%)
1	B	0.82	0/1790	1.20	3/2427 (0.1%)
2	C	0.80	0/1650	1.05	2/2249 (0.1%)
2	H	0.83	0/1654	1.06	2/2254 (0.1%)
3	D	0.82	0/1672	1.07	3/2270 (0.1%)
3	L	0.84	0/1672	1.08	1/2270 (0.0%)
All	All	0.82	1/10228 (0.0%)	1.12	17/13897 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1462	GLY	C-N	5.35	1.41	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1439	ASN	N-CA-C	8.12	123.22	113.16
2	H	103	THR	CB-CA-C	-7.65	94.00	110.45
2	C	103	THR	CB-CA-C	-6.38	96.74	110.45
1	B	1548	ASP	CA-CB-CG	5.86	118.45	112.60
1	B	1430	ALA	CA-C-N	5.58	132.21	121.54
1	B	1430	ALA	C-N-CA	5.58	132.21	121.54
1	A	1597	ASN	CA-C-N	5.45	128.60	120.87
1	A	1597	ASN	C-N-CA	5.45	128.60	120.87
2	H	100	ASP	CA-CB-CG	5.43	118.03	112.60
3	D	82	ASP	CA-CB-CG	5.41	118.01	112.60
3	D	114	SER	N-CA-C	-5.29	100.67	109.46
3	D	165	GLU	N-CA-C	-5.20	103.67	110.53
2	C	100	ASP	CA-CB-CG	5.17	117.77	112.60
3	L	114	SER	N-CA-C	-5.09	101.00	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1598	ASP	N-CA-C	5.04	117.75	110.28
1	A	1437	PHE	CA-C-N	5.04	131.51	122.38
1	A	1437	PHE	C-N-CA	5.04	131.51	122.38

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	1752	0	1625	5	0
1	B	1752	0	1625	16	0
2	C	1610	0	1569	6	0
2	H	1614	0	1572	9	0
3	D	1637	0	1592	14	0
3	L	1637	0	1592	12	0
4	A	14	0	13	1	0
4	B	14	0	13	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	12	0	18	0	0
6	B	8	0	12	0	0
6	C	4	0	6	0	0
6	D	8	0	12	1	0
6	H	4	0	6	0	0
6	L	4	0	6	0	0
7	C	1	0	0	0	0
7	H	1	0	0	0	0
7	L	1	0	0	0	0
8	A	114	0	0	0	0
8	B	121	0	0	1	0
8	C	153	0	0	1	0
8	D	154	0	0	0	0
8	H	144	0	0	0	0
8	L	164	0	0	0	0
All	All	10929	0	9661	58	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 3.

All (58) 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:B:1599:HIS:HD2	8:B:1884:HOH:O	1.71	0.72
3:D:108:ARG:HD2	3:D:171:SER:HB2	1.74	0.69
3:D:108:ARG:NH1	3:D:109:THR:O	2.28	0.67
2:H:162:SER:H	2:H:203:ASN:HD21	1.43	0.67
2:C:162:SER:H	2:C:203:ASN:HD21	1.41	0.66
2:H:24:ALA:HB2	2:H:34:MET:HE1	1.77	0.65
1:B:1459:HIS:HE1	1:B:1491:GLU:OE1	1.83	0.62
2:C:103:THR:HG21	3:D:49:TYR:HB2	1.82	0.62
3:L:110:VAL:HG21	3:L:199:GLN:HE21	1.64	0.61
3:L:110:VAL:HG21	3:L:199:GLN:NE2	2.16	0.60
3:D:110:VAL:HG21	3:D:199:GLN:NE2	2.17	0.59
1:B:1465:ARG:HA	1:B:1540:ARG:NH2	2.19	0.57
1:B:1512:VAL:HG21	1:B:1546:ARG:HD2	1.86	0.56
1:A:1528:SER:HB2	1:A:1545:PHE:HE2	1.69	0.56
3:L:61:ARG:NH2	3:L:81:GLU:OE2	2.40	0.54
3:D:108:ARG:HH12	3:D:111:ALA:HB2	1.72	0.53
2:C:36:TRP:CE2	2:C:81:MET:HB2	2.44	0.52
1:B:1577:VAL:HG13	1:B:1578:ILE:HG12	1.92	0.52
3:D:110:VAL:HG21	3:D:199:GLN:HE21	1.74	0.52
3:L:110:VAL:CG2	3:L:199:GLN:NE2	2.72	0.51
1:A:1528:SER:HB2	1:A:1545:PHE:CE2	2.47	0.50
1:B:1465:ARG:C	1:B:1540:ARG:NH2	2.70	0.49
3:D:185:ASP:HA	3:D:188:LYS:HD2	1.93	0.49
3:L:145:LYS:HB3	3:L:197:THR:HB	1.94	0.49
1:B:1465:ARG:O	1:B:1540:ARG:NH2	2.44	0.49
3:D:20:THR:HG23	3:D:72:THR:HG23	1.95	0.49
3:D:145:LYS:HB3	3:D:197:THR:HB	1.94	0.49
2:H:34:MET:HG2	2:H:79:ALA:HB2	1.96	0.48
1:B:1408:PRO:HG3	1:B:1434:TRP:CZ2	2.49	0.48
3:D:152:ASN:HD21	3:L:5:THR:HG23	1.79	0.47
1:B:1528:SER:HB2	1:B:1545:PHE:HE2	1.80	0.47
1:B:1465:ARG:CA	1:B:1540:ARG:NH2	2.79	0.46
1:B:1593:GLN:NE2	1:B:1598:ASP:HA	2.31	0.46
2:C:97:ALA:HB1	2:C:106:PHE:HB3	1.98	0.46
3:D:204:PRO:HD3	6:D:301:EDO:H21	1.98	0.46
2:H:103:THR:HG21	3:L:49:TYR:HB2	1.97	0.46
2:H:103:THR:HG23	3:L:50:ASP:OD2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1408:PRO:HG3	1:A:1434:TRP:CZ2	2.51	0.45
3:D:110:VAL:CG2	3:D:199:GLN:NE2	2.80	0.45
1:B:1528:SER:HB2	1:B:1545:PHE:CE2	2.51	0.44
1:B:1465:ARG:C	1:B:1540:ARG:HH21	2.26	0.44
3:L:83:PHE:CD2	3:L:106:ILE:HG12	2.53	0.43
1:A:1436:LEU:HB3	1:A:1443:ASP:OD2	2.18	0.43
1:B:1431:LEU:HB3	1:B:1432:GLN:H	1.54	0.43
3:L:120:PRO:HD3	3:L:132:VAL:HG22	2.01	0.43
3:D:37:GLN:HB2	3:D:47:LEU:HD11	2.01	0.42
2:H:97:ALA:HB1	2:H:106:PHE:HB3	2.01	0.42
2:H:81:MET:HE3	2:H:81:MET:HB3	1.94	0.42
2:C:216:ARG:NH2	8:C:403:HOH:O	2.53	0.42
2:C:81:MET:HE3	2:C:81:MET:HB3	1.94	0.42
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.55	0.42
3:D:120:PRO:HD3	3:D:132:VAL:HG22	2.03	0.41
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.01	0.41
1:B:1539:LEU:HD12	1:B:1543:LEU:HD11	2.03	0.41
3:L:83:PHE:CZ	3:L:106:ILE:HG23	2.55	0.41
1:B:1436:LEU:HB3	1:B:1443:ASP:OD2	2.21	0.41
1:A:1439:ASN:HA	4:A:1701:NAG:H82	2.03	0.41
2:H:34:MET:HG2	2:H:79:ALA:CB	2.51	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	221/271 (82%)	211 (96%)	9 (4%)	1 (0%)	24	22
1	B	221/271 (82%)	208 (94%)	11 (5%)	2 (1%)	14	10
2	C	210/226 (93%)	209 (100%)	1 (0%)	0	100	100
2	H	211/226 (93%)	210 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
3	L	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
All	All	1285/1422 (90%)	1248 (97%)	34 (3%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1393	GLN
1	B	1431	LEU
1	A	1390	ALA

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	189/228 (83%)	180 (95%)	9 (5%)	23	23
1	B	189/228 (83%)	179 (95%)	10 (5%)	20	19
2	C	178/189 (94%)	171 (96%)	7 (4%)	28	31
2	H	178/189 (94%)	170 (96%)	8 (4%)	24	25
3	D	186/187 (100%)	178 (96%)	8 (4%)	26	27
3	L	186/187 (100%)	177 (95%)	9 (5%)	23	23
All	All	1106/1208 (92%)	1055 (95%)	51 (5%)	24	25

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1399	GLN
1	A	1426	ARG
1	A	1432	GLN
1	A	1463	ARG
1	A	1470	VAL
1	A	1524	LEU
1	A	1526	ARG

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Mol	Chain	Res	Type
1	A	1535	LEU
1	A	1597	ASN
1	B	1387	CYS
1	B	1426	ARG
1	B	1432	GLN
1	B	1452	LEU
1	B	1470	VAL
1	B	1507	LEU
1	B	1524	LEU
1	B	1535	LEU
1	B	1617	VAL
1	B	1619	ARG
2	C	30	ARG
2	C	62	GLN
2	C	103	THR
2	C	144	LEU
2	C	156	VAL
2	C	165	LEU
2	C	218	GLU
3	D	24	ARG
3	D	33	LEU
3	D	105	GLU
3	D	125	LEU
3	D	136	LEU
3	D	147	GLN
3	D	154	LEU
3	D	211	ARG
2	H	34	MET
2	H	89	GLU
2	H	103	THR
2	H	144	LEU
2	H	156	VAL
2	H	165	LEU
2	H	218	GLU
2	H	220	LYS
3	L	11	LEU
3	L	24	ARG
3	L	81	GLU
3	L	105	GLU
3	L	106	ILE
3	L	125	LEU
3	L	136	LEU

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Mol	Chain	Res	Type
3	L	154	LEU
3	L	211	ARG

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

Mol	Chain	Res	Type
1	A	1393	GLN
1	A	1399	GLN
1	A	1406	ASN
1	A	1432	GLN
1	A	1455	ASN
1	B	1459	HIS
1	B	1593	GLN
1	B	1597	ASN
1	B	1599	HIS
2	C	39	GLN
2	C	203	ASN
3	D	38	GLN
3	D	53	ASN
3	D	152	ASN
3	D	160	GLN
3	D	199	GLN
2	H	39	GLN
2	H	203	ASN
3	L	38	GLN
3	L	53	ASN
3	L	137	ASN
3	L	199	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	$\# Z > 2$
6	EDO	D	302	-	3,3,3	0.66	0	2,2,2	0.32	0
6	EDO	C	302	-	3,3,3	0.66	0	2,2,2	0.20	0
6	EDO	H	302	-	3,3,3	0.54	0	2,2,2	0.28	0
6	EDO	A	1707	-	3,3,3	0.58	0	2,2,2	0.17	0
6	EDO	L	302	-	3,3,3	0.56	0	2,2,2	0.47	0
6	EDO	A	1705	-	3,3,3	0.36	0	2,2,2	0.46	0
4	NAG	B	1701	1	14,14,15	0.27	0	17,19,21	0.67	1 (5%)
6	EDO	B	1705	-	3,3,3	0.52	0	2,2,2	0.33	0
4	NAG	A	1701	1	14,14,15	0.39	0	17,19,21	1.55	2 (11%)
6	EDO	D	301	-	3,3,3	0.44	0	2,2,2	0.22	0
6	EDO	B	1706	-	3,3,3	0.45	0	2,2,2	0.53	0
6	EDO	A	1706	-	3,3,3	0.51	0	2,2,2	0.42	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
6	EDO	D	302	-	-	0/1/1/1	-
6	EDO	C	302	-	-	0/1/1/1	-
6	EDO	H	302	-	-	0/1/1/1	-
6	EDO	A	1707	-	-	1/1/1/1	-
6	EDO	L	302	-	-	0/1/1/1	-
6	EDO	A	1705	-	-	0/1/1/1	-
4	NAG	B	1701	1	-	0/6/23/26	0/1/1/1
6	EDO	B	1705	-	-	0/1/1/1	-
4	NAG	A	1701	1	-	0/6/23/26	0/1/1/1
6	EDO	D	301	-	-	0/1/1/1	-
6	EDO	B	1706	-	-	0/1/1/1	-
6	EDO	A	1706	-	-	0/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1701	NAG	C1-O5-C5	4.90	118.76	112.19
4	A	1701	NAG	O5-C1-C2	3.73	117.06	111.29
4	B	1701	NAG	C1-O5-C5	2.25	115.20	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1707	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1701	NAG	1	0
6	D	301	EDO	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, 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	A	227/271 (83%)	0.93	51 (22%) 2 2	20, 43, 89, 123	0
1	B	227/271 (83%)	0.51	23 (10%) 12 13	19, 38, 85, 119	0
2	C	214/226 (94%)	-0.16	4 (1%) 66 69	18, 29, 54, 96	0
2	H	215/226 (95%)	-0.15	3 (1%) 73 75	19, 29, 53, 81	0
3	D	213/214 (99%)	0.14	5 (2%) 61 64	19, 32, 59, 97	0
3	L	213/214 (99%)	-0.19	3 (1%) 73 75	17, 27, 48, 64	0
All	All	1309/1422 (92%)	0.19	89 (6%) 23 25	17, 32, 68, 123	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1390	ALA	7.0
1	B	1390	ALA	6.8
1	A	1391	ALA	6.4
1	B	1391	ALA	6.0
1	B	1394	ALA	6.0
1	A	1387	CYS	5.8
1	A	1388	PRO	4.6
1	B	1393	GLN	4.4
2	H	133	SER	4.3
1	B	1431	LEU	4.2
1	B	1388	PRO	4.2
1	A	1577	VAL	4.1
1	A	1392	CYS	4.1
1	B	1577	VAL	4.0
1	A	1431	LEU	3.8
1	B	1389	ARG	3.8
1	A	1421	VAL	3.6
1	B	1395	LYS	3.6
1	A	1559	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	133	SER	3.5
1	A	1578	ILE	3.4
1	B	1597	ASN	3.4
1	B	1392	CYS	3.3
1	A	1389	ARG	3.3
3	L	129	THR	3.3
1	A	1406	ASN	3.3
1	B	1434	TRP	3.2
1	B	1387	CYS	3.2
1	A	1395	LYS	3.2
1	B	1399	GLN	3.2
2	H	220	LYS	3.1
2	C	220	LYS	3.1
1	A	1408	PRO	3.1
1	A	1438	ASN	3.1
1	A	1410	CYS	3.1
3	D	127	SER	3.1
1	A	1434	TRP	3.0
1	A	1633	PRO	3.0
1	B	1396	ARG	2.9
1	A	1409	GLY	2.9
1	A	1417	CYS	2.9
1	A	1581	VAL	2.8
1	A	1420	SER	2.8
1	A	1524	LEU	2.8
2	C	1	GLN	2.7
1	A	1414	GLY	2.7
1	A	1396	ARG	2.7
3	D	129	THR	2.7
1	A	1397	GLY	2.7
1	A	1394	ALA	2.7
1	A	1519	LEU	2.7
1	A	1403	ARG	2.6
1	B	1462	GLY	2.6
1	A	1407	SER	2.6
1	B	1578	ILE	2.5
1	A	1422	GLY	2.5
1	A	1430	ALA	2.5
1	A	1393	GLN	2.5
1	A	1551	GLY	2.5
3	L	127	SER	2.5
1	A	1520	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1411	GLY	2.4
3	D	152	ASN	2.4
1	A	1516	THR	2.4
3	L	81	GLU	2.4
1	A	1405	CYS	2.4
1	A	1412	TRP	2.4
1	A	1556	PHE	2.3
1	B	1559	HIS	2.3
1	B	1402	ASP	2.2
1	B	1436	LEU	2.2
2	H	139	GLY	2.2
1	A	1402	ASP	2.2
1	A	1514	VAL	2.2
1	A	1555	VAL	2.2
1	A	1629	VAL	2.1
1	A	1627	ARG	2.1
1	B	1405	CYS	2.1
1	A	1518	LEU	2.1
3	D	213	GLU	2.1
2	C	65	GLN	2.1
1	B	1550	HIS	2.1
3	D	212	GLY	2.1
1	A	1441	ARG	2.1
1	A	1558	TYR	2.0
1	A	1579	GLY	2.0
1	A	1419	LEU	2.0
1	B	1403	ARG	2.0
1	A	1461	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	1701	14/15	0.68	0.18	78,88,92,93	0
4	NAG	A	1701	14/15	0.74	0.18	61,66,70,72	0
6	EDO	H	302	4/4	0.85	0.17	51,52,52,53	0
7	CL	L	301	1/1	0.86	0.14	58,58,58,58	0
6	EDO	D	301	4/4	0.89	0.13	37,41,44,46	0
6	EDO	A	1705	4/4	0.93	0.09	29,30,30,35	0
7	CL	C	301	1/1	0.94	0.16	42,42,42,42	0
7	CL	H	301	1/1	0.94	0.21	35,35,35,35	0
6	EDO	A	1707	4/4	0.94	0.09	29,32,34,39	0
6	EDO	B	1706	4/4	0.95	0.09	27,29,33,35	0
6	EDO	C	302	4/4	0.95	0.10	33,35,37,40	0
6	EDO	B	1705	4/4	0.95	0.08	29,33,37,40	0
6	EDO	D	302	4/4	0.95	0.10	27,28,31,32	0
5	CA	B	1703	1/1	0.96	0.05	42,42,42,42	0
5	CA	A	1702	1/1	0.96	0.09	71,71,71,71	0
5	CA	B	1702	1/1	0.96	0.05	71,71,71,71	0
6	EDO	A	1706	4/4	0.97	0.05	27,27,29,29	0
6	EDO	L	302	4/4	0.98	0.04	23,23,25,28	0
5	CA	A	1704	1/1	0.99	0.02	24,24,24,24	0
5	CA	A	1703	1/1	0.99	0.02	36,36,36,36	0
5	CA	B	1704	1/1	1.00	0.01	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.