



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:29 AM UTC

PDB ID : 4PLO / pdb_00004plo
Title : Crystal Structure of chicken Netrin-1 (LN-LE3) in complex with mouse DCC (FN4-5)
Authors : Xu, K.; Nikolov, D.B.
Deposited on : 2014-05-18
Resolution : 2.90 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:

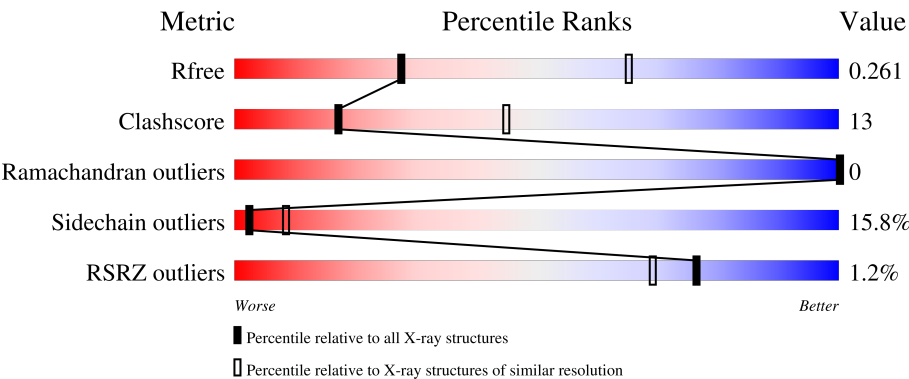
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	B	206	%63%28%•7%
2	A	432	%56%33%5%5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4868 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 Netrin receptor DCC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	192	Total	C	N	O	S	0	0	0
			1498	939	259	294	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	719	GLY	-	expression tag	UNP P70211
B	720	ALA	-	expression tag	UNP P70211
B	923	SER	-	expression tag	UNP P70211
B	924	GLY	-	expression tag	UNP P70211

- Molecule 2 is a protein called Netrin-1.

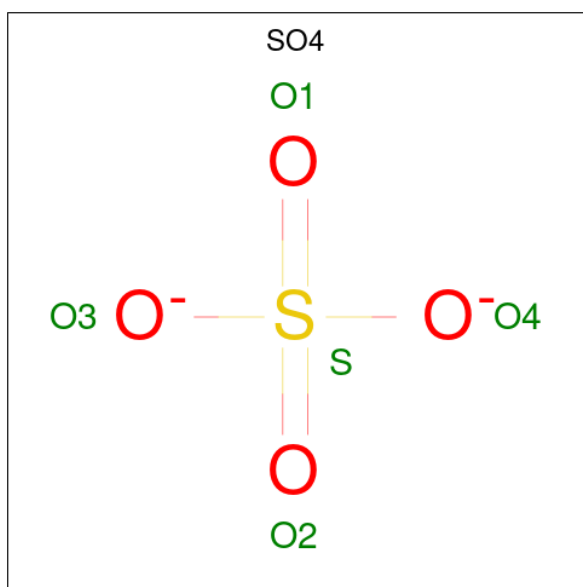
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	412	Total	C	N	O	S	0	0	0
			3230	1987	601	604	38			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O S	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

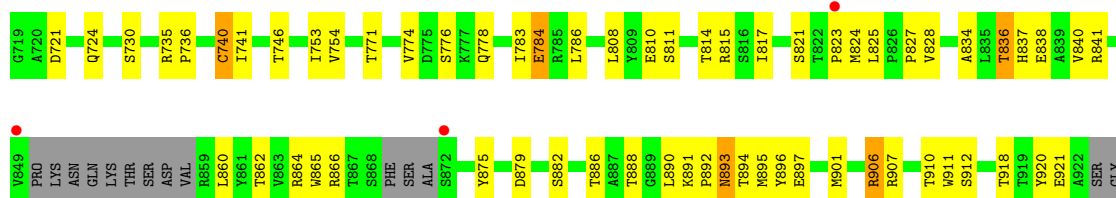
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	16	Total	O	0	0
			16	16		
6	A	56	Total	O	0	0
			56	56		

3 Residue-property plots

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.

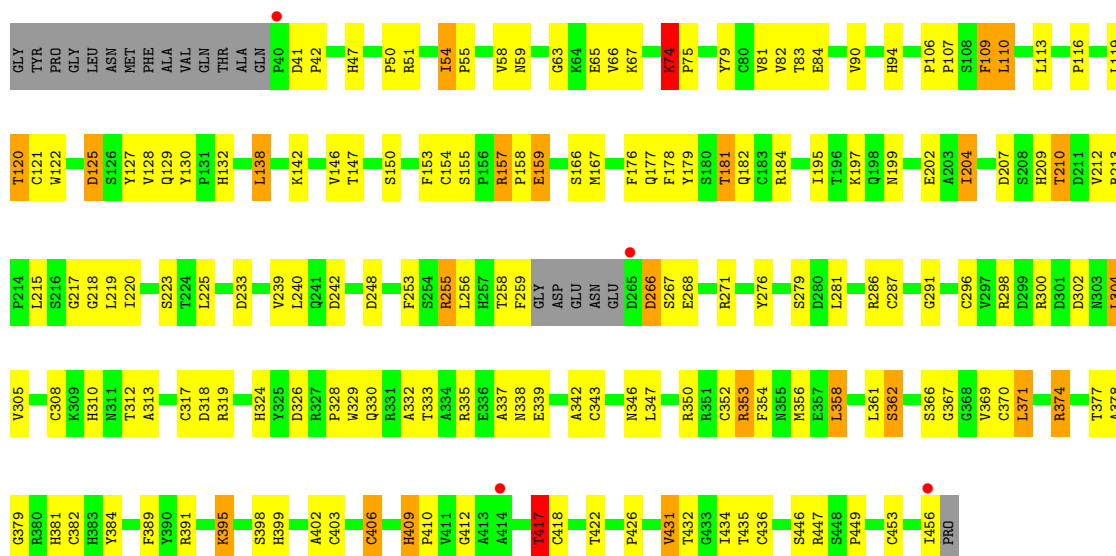
• Molecule 1: Netrin receptor DCC

Chain B: 



• Molecule 2: Netrin-1

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.48Å 72.94Å 285.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 2.90 48.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.75-2.90) 88.6 (48.75-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.224 , 0.288 (Not available) , 0.261	Depositor DCC
R_{free} test set	2000 reflections (8.76%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4868	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG, CA

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	0.52	0/1533	0.99	3/2092 (0.1%)
2	A	0.74	3/3310 (0.1%)	1.14	23/4479 (0.5%)
All	All	0.68	3/4843 (0.1%)	1.09	26/6571 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	109	PHE	C-O	-9.34	1.10	1.24
2	A	120	THR	C-O	-7.28	1.15	1.24
2	A	41	ASP	C-N	5.66	1.40	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	74	LYS	CA-C-N	-10.96	109.09	120.38
2	A	74	LYS	C-N-CA	-10.96	109.09	120.38
1	B	784	GLU	N-CA-C	8.47	123.80	113.38
2	A	435	THR	N-CA-C	-7.96	100.03	110.53
2	A	266	ASP	N-CA-C	7.25	121.84	112.92
2	A	395	LYS	CA-C-N	-6.98	113.31	120.85
2	A	395	LYS	C-N-CA	-6.98	113.31	120.85
2	A	155	SER	CA-C-N	-6.69	113.09	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	155	SER	C-N-CA	-6.69	113.09	119.85
1	B	721	ASP	N-CA-C	6.36	119.63	108.75
2	A	41	ASP	CA-C-N	-6.07	113.48	120.04
2	A	41	ASP	C-N-CA	-6.07	113.48	120.04
2	A	54	ILE	CA-C-N	-6.00	114.09	120.03
2	A	54	ILE	C-N-CA	-6.00	114.09	120.03
1	B	774	VAL	N-CA-C	5.65	115.42	108.53
2	A	435	THR	CA-C-N	-5.57	114.53	122.77
2	A	435	THR	C-N-CA	-5.57	114.53	122.77
2	A	417	THR	N-CA-C	5.43	117.37	108.52
2	A	308	CYS	CA-C-N	-5.42	114.48	123.37
2	A	308	CYS	C-N-CA	-5.42	114.48	123.37
2	A	116	PRO	CA-N-CD	-5.41	104.43	112.00
2	A	409	HIS	CA-C-N	5.18	125.48	119.47
2	A	409	HIS	C-N-CA	5.18	125.48	119.47
2	A	337	ALA	N-CA-C	-5.12	102.71	110.28
2	A	42	PRO	CA-N-CD	-5.02	104.97	112.00
2	A	138	LEU	N-CA-C	5.02	116.59	108.26

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	63	GLY	Peptide
2	A	74	LYS	Peptide

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	B	1498	0	1462	26	0
2	A	3230	0	3054	92	0
3	A	42	0	39	0	0
4	A	25	0	0	3	0
5	A	1	0	0	0	0
6	A	56	0	0	7	0
6	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4868	0	4555	118	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 13.

All (118) 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)
2:A:166:SER:HB3	2:A:248:ASP:HB2	1.62	0.81
2:A:125:ASP:OD1	2:A:125:ASP:N	2.13	0.78
2:A:391:ARG:NH2	2:A:402:ALA:O	2.21	0.73
2:A:159:GLU:OE1	2:A:181:THR:OG1	2.06	0.71
2:A:158:PRO:HB3	2:A:276:TYR:HE1	1.55	0.71
1:B:837:HIS:HB2	1:B:892:PRO:HB3	1.72	0.70
2:A:199:ASN:ND2	2:A:202:GLU:OE2	2.24	0.69
2:A:110:LEU:HD13	2:A:122:TRP:HB3	1.75	0.68
1:B:834:ALA:HA	1:B:840:VAL:HG22	1.78	0.66
2:A:159:GLU:HA	2:A:210:THR:HG22	1.78	0.65
2:A:374:ARG:NH1	6:A:616:HOH:O	2.29	0.65
2:A:406:CYS:SG	2:A:418:CYS:N	2.70	0.65
1:B:906:ARG:O	1:B:907:ARG:NH1	2.30	0.64
2:A:350:ARG:NE	4:A:507:SO4:O2	2.31	0.63
2:A:352:CYS:SG	6:A:653:HOH:O	2.56	0.63
2:A:159:GLU:HG3	2:A:255:ARG:HB3	1.80	0.61
2:A:207:ASP:O	2:A:210:THR:OG1	2.15	0.61
2:A:379:GLY:HA2	2:A:382:CYS:H	1.66	0.61
1:B:740:CYS:SG	1:B:741:ILE:N	2.74	0.60
2:A:366:SER:OG	2:A:367:GLY:HA3	2.02	0.59
2:A:129:GLN:OE1	2:A:130:TYR:N	2.24	0.59
2:A:195:ILE:HD11	2:A:204:ILE:HG21	1.84	0.58
2:A:362:SER:OG	2:A:366:SER:O	2.12	0.58
2:A:395:LYS:HG2	2:A:399:HIS:ND1	2.17	0.58
2:A:298:ARG:HG2	2:A:302:ASP:OD1	2.03	0.58
2:A:347:LEU:O	6:A:616:HOH:O	2.16	0.58
2:A:389:PHE:HA	2:A:406:CYS:HB3	1.86	0.57
2:A:106:PRO:O	2:A:109:PHE:HB2	2.04	0.57
1:B:827:PRO:HD2	1:B:912:SER:HB3	1.87	0.57
2:A:333:THR:HG22	2:A:335:ARG:H	1.70	0.57
2:A:253:PHE:HB3	2:A:276:TYR:CZ	2.40	0.57
1:B:890:LEU:HD22	1:B:896:TYR:HE2	1.71	0.56
2:A:51:ARG:NH1	6:A:644:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:860:LEU:HD11	1:B:879:ASP:HB3	1.88	0.56
2:A:84:GLU:CD	2:A:213:ARG:HH22	2.15	0.55
2:A:129:GLN:HA	2:A:256:LEU:HD13	1.89	0.54
1:B:783:ILE:HG22	1:B:786:LEU:HD21	1.89	0.54
1:B:891:LYS:O	1:B:894:THR:OG1	2.21	0.54
2:A:369:VAL:N	6:A:653:HOH:O	2.40	0.53
1:B:910:THR:OG1	1:B:911:TRP:N	2.40	0.53
1:B:862:THR:HB	1:B:901:MET:HG2	1.90	0.53
2:A:109:PHE:CD2	2:A:120:THR:HB	2.44	0.52
2:A:74:LYS:HB2	2:A:75:PRO:HD2	1.91	0.52
2:A:378:ALA:HB3	2:A:384:TYR:CE1	2.44	0.52
2:A:317:CYS:O	2:A:329:TRP:NE1	2.42	0.52
2:A:417:THR:O	2:A:426:PRO:HD3	2.11	0.51
2:A:291:GLY:HA3	2:A:332:ALA:HB3	1.92	0.50
2:A:107:PRO:O	2:A:110:LEU:HB2	2.11	0.50
2:A:352:CYS:O	2:A:353:ARG:NE	2.45	0.49
2:A:431:VAL:HG22	2:A:453:CYS:SG	2.51	0.49
2:A:350:ARG:HH21	2:A:374:ARG:HH21	1.58	0.49
2:A:296:CYS:HB3	2:A:304:LEU:HD23	1.92	0.49
1:B:735:ARG:HD2	1:B:906:ARG:NH2	2.27	0.49
2:A:157:ARG:HD2	2:A:218:GLY:HA3	1.95	0.49
2:A:74:LYS:HB2	2:A:75:PRO:CD	2.42	0.49
2:A:431:VAL:HG12	2:A:432:THR:H	1.77	0.49
1:B:866:ARG:NH1	1:B:875:TYR:OH	2.46	0.49
1:B:864:ARG:HD3	1:B:911:TRP:CZ2	2.49	0.48
2:A:55:PRO:O	2:A:286:ARG:NH2	2.46	0.48
2:A:127:TYR:HB3	2:A:271:ARG:HD3	1.95	0.48
2:A:153:PHE:O	2:A:217:GLY:N	2.46	0.48
2:A:177:GLN:HG3	2:A:178:PHE:N	2.28	0.48
2:A:167:MET:HE1	2:A:242:ASP:OD1	2.14	0.48
2:A:212:VAL:O	2:A:215:LEU:HD23	2.14	0.48
2:A:286:ARG:HG2	2:A:286:ARG:HH21	1.79	0.47
2:A:330:GLN:HB2	2:A:338:ASN:HB2	1.96	0.47
2:A:313:ALA:HB3	2:A:319:ARG:HG3	1.96	0.47
2:A:154:CYS:SG	2:A:279:SER:HB3	2.54	0.47
1:B:821:SER:O	1:B:823:PRO:HD3	2.15	0.47
1:B:736:PRO:HA	1:B:741:ILE:HG12	1.97	0.47
2:A:94:HIS:ND1	4:A:504:SO4:O4	2.46	0.47
2:A:177:GLN:HG2	2:A:179:TYR:CZ	2.50	0.47
2:A:195:ILE:HG23	2:A:199:ASN:O	2.16	0.47
2:A:412:GLY:HA3	2:A:436:CYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:GLU:HG3	1:B:811:SER:H	1.79	0.46
2:A:84:GLU:OE1	2:A:213:ARG:NH2	2.48	0.46
2:A:142:LYS:HE3	2:A:287:CYS:SG	2.55	0.46
1:B:740:CYS:HB2	1:B:784:GLU:OE1	2.15	0.46
2:A:350:ARG:HH21	2:A:374:ARG:NH2	2.13	0.46
2:A:127:TYR:CD1	2:A:271:ARG:HB3	2.51	0.46
2:A:157:ARG:HG2	2:A:220:ILE:HD11	1.98	0.46
2:A:395:LYS:HB3	2:A:399:HIS:HB3	1.97	0.45
2:A:158:PRO:HB3	2:A:276:TYR:CE1	2.44	0.45
1:B:890:LEU:HD22	1:B:896:TYR:CE2	2.52	0.45
2:A:296:CYS:HB3	2:A:304:LEU:CD2	2.47	0.45
2:A:177:GLN:HG3	2:A:178:PHE:H	1.82	0.44
2:A:350:ARG:HD3	2:A:374:ARG:NH2	2.32	0.44
2:A:197:LYS:NZ	6:A:650:HOH:O	2.33	0.44
2:A:253:PHE:HB3	2:A:276:TYR:CE1	2.53	0.44
2:A:153:PHE:CE2	2:A:158:PRO:HD3	2.53	0.44
1:B:836:THR:C	1:B:920:TYR:HB2	2.43	0.44
2:A:310:HIS:O	2:A:339:GLU:HB2	2.18	0.44
2:A:350:ARG:NH2	2:A:374:ARG:HE	2.16	0.44
1:B:893:ASN:O	1:B:893:ASN:ND2	2.42	0.43
1:B:730:SER:HB2	1:B:746:THR:OG1	2.18	0.43
2:A:209:HIS:ND1	4:A:505:SO4:O1	2.49	0.43
2:A:128:VAL:O	2:A:132:HIS:HB2	2.19	0.43
2:A:358:LEU:O	2:A:362:SER:OG	2.38	0.42
1:B:735:ARG:HA	1:B:736:PRO:HD2	1.93	0.42
1:B:865:TRP:HA	1:B:897:GLU:O	2.19	0.42
2:A:50:PRO:HB3	2:A:310:HIS:CD2	2.55	0.42
2:A:339:GLU:OE1	2:A:339:GLU:N	2.40	0.42
2:A:346:ASN:ND2	6:A:641:HOH:O	2.16	0.41
2:A:409:HIS:HA	2:A:410:PRO:HD2	1.81	0.41
2:A:371:LEU:HD12	2:A:371:LEU:HA	1.71	0.41
2:A:434:ILE:HD13	2:A:434:ILE:HA	1.82	0.41
2:A:447:ARG:O	2:A:449:PRO:HD3	2.21	0.41
2:A:324:HIS:CD2	2:A:342:ALA:HB2	2.56	0.41
2:A:298:ARG:NH2	2:A:304:LEU:HD12	2.36	0.40
2:A:326:ASP:OD1	2:A:367:GLY:HA3	2.21	0.40
2:A:370:CYS:SG	2:A:381:HIS:HA	2.60	0.40
2:A:58:VAL:HG12	2:A:59:ASN:N	2.36	0.40
2:A:79:TYR:CZ	2:A:94:HIS:HB2	2.56	0.40
2:A:184:ARG:HH11	2:A:184:ARG:HD3	1.75	0.40
2:A:328:PRO:HG3	2:A:354:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:ARG:HD2	1:B:875:TYR:CD1	2.55	0.40
2:A:389:PHE:CA	2:A:406:CYS:HB3	2.51	0.40
1:B:895:MET:HA	1:B:918:THR:HA	2.02	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	B	186/206 (90%)	184 (99%)	2 (1%)	0	100	100
2	A	408/432 (94%)	388 (95%)	20 (5%)	0	100	100
All	All	594/638 (93%)	572 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	B	169/181 (93%)	146 (86%)	23 (14%)	3	12
2	A	361/378 (96%)	300 (83%)	61 (17%)	2	7
All	All	530/559 (95%)	446 (84%)	84 (16%)	2	8

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	724	GLN
1	B	740	CYS
1	B	753	ILE
1	B	754	VAL
1	B	771	THR
1	B	776	SER
1	B	778	GLN
1	B	808	LEU
1	B	814	THR
1	B	815	ARG
1	B	817	ILE
1	B	824	MET
1	B	825	LEU
1	B	828	VAL
1	B	836	THR
1	B	838	GLU
1	B	841	ARG
1	B	882	SER
1	B	886	THR
1	B	888	THR
1	B	893	ASN
1	B	906	ARG
1	B	921	GLU
2	A	47	HIS
2	A	54	ILE
2	A	65	GLU
2	A	66	VAL
2	A	67	LYS
2	A	74	LYS
2	A	81	VAL
2	A	82	VAL
2	A	83	THR
2	A	90	VAL
2	A	110	LEU
2	A	113	LEU
2	A	119	LEU
2	A	121	CYS
2	A	125	ASP
2	A	138	LEU
2	A	146	VAL
2	A	147	THR
2	A	150	SER
2	A	157	ARG

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Mol	Chain	Res	Type
2	A	159	GLU
2	A	176	PHE
2	A	181	THR
2	A	182	GLN
2	A	204	ILE
2	A	210	THR
2	A	219	LEU
2	A	223	SER
2	A	225	LEU
2	A	233	ASP
2	A	239	VAL
2	A	240	LEU
2	A	255	ARG
2	A	258	THR
2	A	259	PHE
2	A	266	ASP
2	A	267	SER
2	A	268	GLU
2	A	281	LEU
2	A	300	ARG
2	A	304	LEU
2	A	305	VAL
2	A	312	THR
2	A	318	ASP
2	A	343	CYS
2	A	353	ARG
2	A	356	MET
2	A	358	LEU
2	A	361	LEU
2	A	362	SER
2	A	371	LEU
2	A	374	ARG
2	A	377	THR
2	A	398	SER
2	A	403	CYS
2	A	406	CYS
2	A	417	THR
2	A	422	THR
2	A	431	VAL
2	A	446	SER
2	A	456	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	728	GLN
1	B	733	HIS
1	B	801	ASN
1	B	916	HIS
2	A	182	GLN
2	A	282	GLN
2	A	330	GLN
2	A	344	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
3	NAG	A	502	2	14,14,15	1.30	2 (14%)	17,19,21	2.56	6 (35%)
4	SO4	A	507	-	4,4,4	0.25	0	6,6,6	0.15	0
3	NAG	A	503	2	14,14,15	0.79	1 (7%)	17,19,21	0.80	0
3	NAG	A	501	2	14,14,15	0.50	0	17,19,21	0.58	0
4	SO4	A	508	-	4,4,4	0.26	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	504	-	4,4,4	0.28	0	6,6,6	0.20	0
4	SO4	A	505	-	4,4,4	0.25	0	6,6,6	0.32	0
4	SO4	A	506	-	4,4,4	0.32	0	6,6,6	0.33	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
3	NAG	A	503	2	-	3/6/23/26	0/1/1/1
3	NAG	A	502	2	-	4/6/23/26	0/1/1/1
3	NAG	A	501	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAG	C2-N2	-2.94	1.41	1.46
3	A	502	NAG	C1-C2	2.87	1.56	1.52
3	A	503	NAG	O5-C1	2.37	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAG	C2-N2-C7	-5.28	115.82	122.90
3	A	502	NAG	C4-C3-C2	4.47	117.58	111.02
3	A	502	NAG	O5-C5-C6	4.22	115.87	107.66
3	A	502	NAG	C1-O5-C5	4.04	117.60	112.19
3	A	502	NAG	C1-C2-N2	-3.52	104.89	110.43
3	A	502	NAG	O3-C3-C2	-2.23	104.78	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	NAG	C1-C2-N2-C7
3	A	502	NAG	C8-C7-N2-C2
3	A	502	NAG	O7-C7-N2-C2
3	A	503	NAG	O5-C5-C6-O6
3	A	503	NAG	C4-C5-C6-O6
3	A	502	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	502	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	507	SO4	1	0
4	A	504	SO4	1	0
4	A	505	SO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	192/206 (93%)	-0.03	3 (1%) 70 62	14, 54, 88, 103	0
2	A	412/432 (95%)	-0.24	4 (0%) 79 73	9, 30, 72, 90	0
All	All	604/638 (94%)	-0.17	7 (1%) 76 69	9, 37, 79, 103	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	849	VAL	4.1
2	A	265	ASP	2.7
2	A	40	PRO	2.7
2	A	414	ALA	2.6
2	A	456	ILE	2.1
1	B	872	SER	2.1
1	B	823	PRO	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
3	NAG	A	502	14/15	0.43	0.20	32,47,62,70	0
3	NAG	A	503	14/15	0.61	0.15	46,58,68,73	0
4	SO4	A	508	5/5	0.75	0.10	70,80,89,91	0
4	SO4	A	507	5/5	0.88	0.06	66,70,78,80	0
3	NAG	A	501	14/15	0.90	0.07	38,40,46,50	0
4	SO4	A	504	5/5	0.93	0.07	52,60,60,68	0
4	SO4	A	505	5/5	0.95	0.09	34,35,45,49	0
5	CA	A	509	1/1	0.96	0.08	15,15,15,15	0
4	SO4	A	506	5/5	0.97	0.07	16,16,21,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.