



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:19 PM UTC

PDB ID : 8B3K / pdb_00008b3k
Title : Crystal structure of human Plexin-B1 (20-535) in the unbound state
Authors : Cowan, R.; Hall, G.; Carr, M.
Deposited on : 2022-09-16
Resolution : 2.69 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

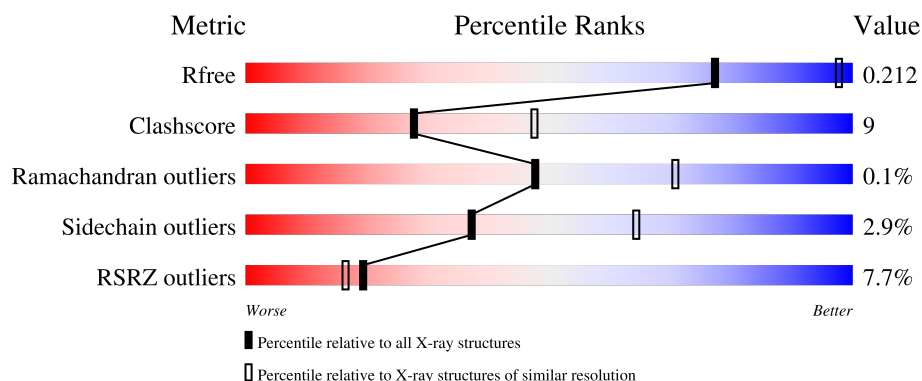
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	523	
1	B	523	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7722 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 Plexin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	492	Total	C	N	O	S	0	0	0
			3731	2343	651	715	22			
1	A	492	Total	C	N	O	S	0	1	0
			3739	2348	653	716	22			

There are 14 discrepancies between the modelled and reference sequences:

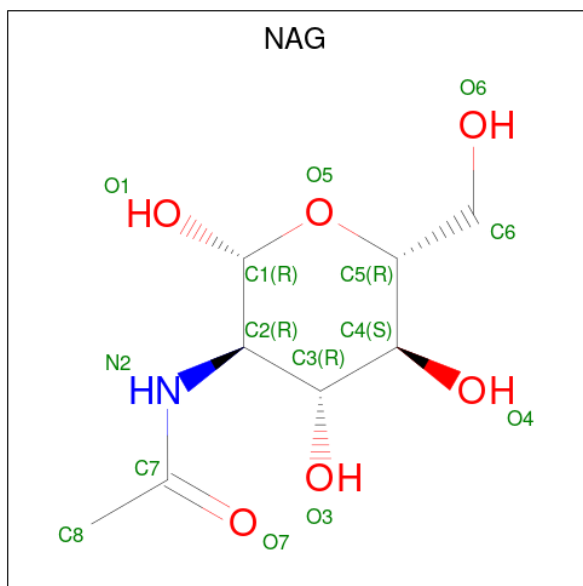
Chain	Residue	Modelled	Actual	Comment	Reference
B	536	LYS	-	expression tag	UNP O43157
B	537	HIS	-	expression tag	UNP O43157
B	538	HIS	-	expression tag	UNP O43157
B	539	HIS	-	expression tag	UNP O43157
B	540	HIS	-	expression tag	UNP O43157
B	541	HIS	-	expression tag	UNP O43157
B	542	HIS	-	expression tag	UNP O43157
A	536	LYS	-	expression tag	UNP O43157
A	537	HIS	-	expression tag	UNP O43157
A	538	HIS	-	expression tag	UNP O43157
A	539	HIS	-	expression tag	UNP O43157
A	540	HIS	-	expression tag	UNP O43157
A	541	HIS	-	expression tag	UNP O43157
A	542	HIS	-	expression tag	UNP O43157

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	7	Total	Cd	0	0
			7	7		
2	A	7	Total	Cd	0	0
			7	7		

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

C₈H₁₅NO₆).



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

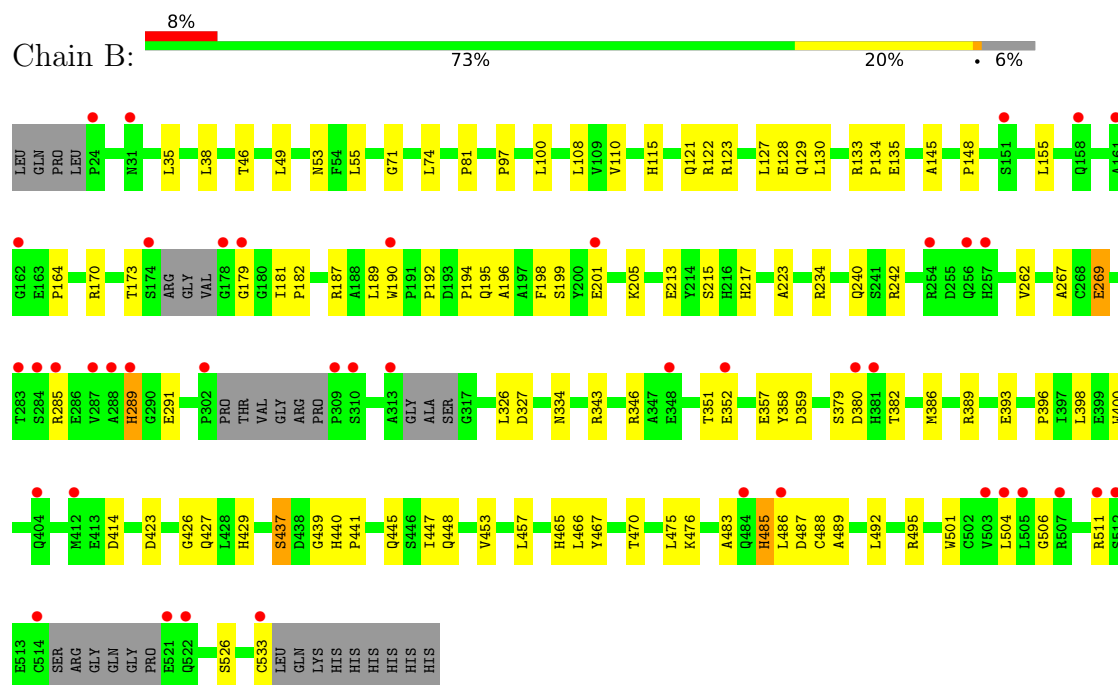
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	106	Total	O	0	0
			106	106		
4	A	104	Total	O	0	0
			104	104		

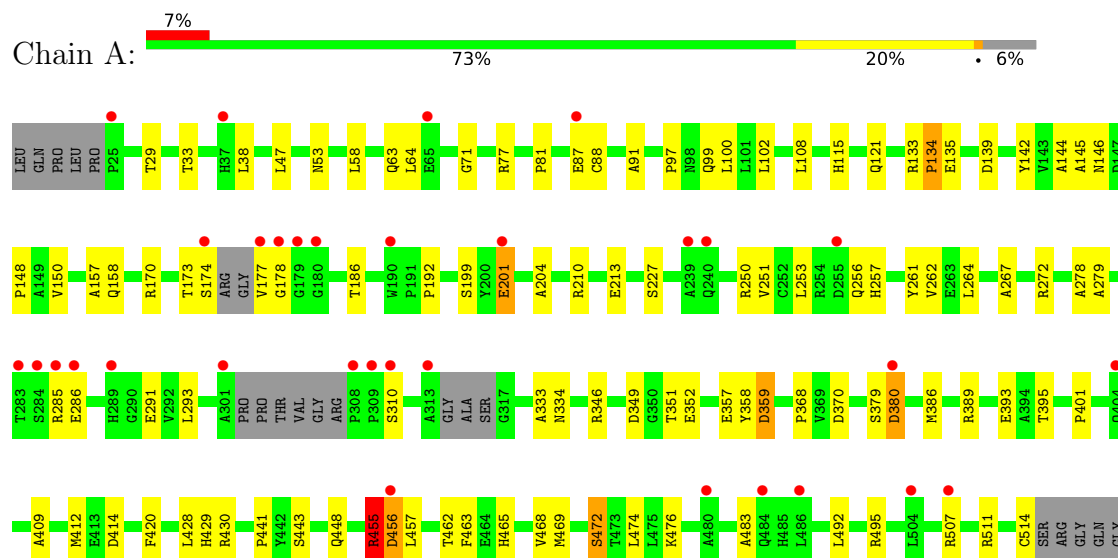
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Plexin-B1



• Molecule 1: Plexin-B1





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	266.69Å 266.69Å 108.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.67 – 2.69 66.67 – 2.69	Depositor EDS
% Data completeness (in resolution range)	69.7 (66.67-2.69) 63.7 (66.67-2.69)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.199 , 0.245 (Not available) , 0.212	Depositor DCC
R_{free} test set	1901 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7722	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.41% 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: CD, 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	0.58	4/3831 (0.1%)	0.84	8/5229 (0.2%)
1	B	0.54	2/3824 (0.1%)	0.76	4/5220 (0.1%)
All	All	0.56	6/7655 (0.1%)	0.80	12/10449 (0.1%)

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
1	A	0	2
1	B	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	GLU	CG-CD	6.89	1.69	1.52
1	B	352	GLU	CB-CG	6.33	1.71	1.52
1	B	352	GLU	CG-CD	6.17	1.67	1.52
1	A	201	GLU	CB-CG	5.53	1.69	1.52
1	A	87	GLU	CB-CG	5.33	1.68	1.52
1	A	87	GLU	CG-CD	5.16	1.65	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	GLU	CA-CB-CG	8.34	130.79	114.10
1	A	272	ARG	N-CA-C	-8.21	102.41	111.36
1	B	352	GLU	N-CA-C	-7.19	99.25	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	465	HIS	CA-CB-CG	6.45	120.25	113.80
1	B	485	HIS	CB-CA-C	6.45	120.39	109.75
1	A	349	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	380	ASP	CA-CB-CG	5.74	118.33	112.60
1	A	401	PRO	N-CA-C	5.64	122.15	113.75
1	A	395	THR	CB-CA-C	5.47	116.58	108.87
1	A	455	ARG	N-CA-C	-5.31	105.50	111.28
1	B	352	GLU	CB-CG-CD	5.11	121.29	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	389	ARG	Sidechain
1	A	455	ARG	Sidechain
1	B	234	ARG	Sidechain

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	3739	0	3577	63	2
1	B	3731	0	3571	70	1
2	A	7	0	0	0	0
2	B	7	0	0	0	0
3	A	14	0	13	1	0
3	B	14	0	13	1	0
4	A	104	0	0	2	0
4	B	106	0	0	11	0
All	All	7722	0	7174	132	2

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 9.

All (132) 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:285:ARG:HH22	1:B:289:HIS:CE1	2.01	0.78
1:B:327:ASP:OD2	4:B:701:HOH:O	2.04	0.75
1:A:250:ARG:HG2	1:A:250:ARG:HH11	1.51	0.75
1:B:380:ASP:OD2	4:B:702:HOH:O	2.08	0.72
1:A:262:VAL:HG22	1:A:386:MET:HE3	1.71	0.71
1:A:359:ASP:OD2	4:A:701:HOH:O	2.10	0.70
1:B:115:HIS:ND1	4:B:703:HOH:O	2.14	0.67
1:A:77:ARG:HG2	1:A:146:ASN:HD22	1.61	0.66
1:A:150:VAL:HG21	1:A:173:THR:HG22	1.79	0.64
1:A:139:ASP:HA	1:A:142:TYR:CE2	2.34	0.62
1:A:99:GLN:HG2	1:A:144:ALA:HB1	1.81	0.62
1:B:398:LEU:HD13	1:B:400:TRP:NE1	2.15	0.61
1:B:155:LEU:HD21	1:B:223:ALA:HB2	1.83	0.60
1:B:445:GLN:NE2	4:B:706:HOH:O	2.30	0.60
1:B:343:ARG:NH2	4:B:707:HOH:O	2.32	0.60
1:A:77:ARG:HG2	1:A:146:ASN:ND2	2.18	0.59
1:A:177:VAL:HG12	1:A:178:GLY:H	1.66	0.59
1:B:195:GLN:HG2	4:B:746:HOH:O	2.03	0.58
1:B:201:GLU:H	1:B:201:GLU:CD	2.12	0.58
1:B:164:PRO:HB2	1:B:189:LEU:HB2	1.85	0.58
1:B:483:ALA:C	1:B:485:HIS:H	2.10	0.58
1:A:409:ALA:HB3	1:A:420:PHE:HB2	1.85	0.57
1:B:398:LEU:HD13	1:B:400:TRP:CE2	2.39	0.57
1:B:467:TYR:CE1	1:B:476:LYS:HD2	2.39	0.57
1:B:504:LEU:C	1:B:506:GLY:H	2.13	0.56
1:A:448:GLN:HE22	1:A:472:SER:HB2	1.69	0.56
1:A:278:ALA:HB2	1:A:455:ARG:HG2	1.87	0.56
1:A:210:ARG:HD2	1:A:213:GLU:CD	2.30	0.56
1:A:334:ASN:HD22	3:A:608:NAG:H83	1.72	0.55
1:A:279:ALA:HB1	1:A:293:LEU:HD11	1.87	0.55
1:A:58:LEU:HD23	1:A:64:LEU:HA	1.88	0.55
1:B:504:LEU:O	1:B:506:GLY:N	2.34	0.54
1:B:55:LEU:HD11	1:B:110:VAL:HG11	1.90	0.54
1:B:53:ASN:HB3	1:B:71:GLY:O	2.08	0.54
1:B:196:ALA:O	1:B:199:SER:OG	2.23	0.54
1:A:88:CYS:SG	1:A:91:ALA:HB2	2.49	0.53
1:A:77:ARG:O	1:A:177:VAL:HA	2.09	0.53
1:A:448:GLN:NE2	1:A:472:SER:HB2	2.24	0.53
1:A:514:CYS:HB3	1:A:522:GLN:HE21	1.74	0.52
1:B:346:ARG:HA	1:B:351:THR:O	2.10	0.52
1:B:334:ASN:HD22	3:B:608:NAG:H83	1.73	0.52
1:A:38:LEU:HD11	1:A:47:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:VAL:HA	1:B:386:MET:O	2.09	0.52
1:B:285:ARG:O	1:B:285:ARG:HD3	2.10	0.51
1:B:393:GLU:HG2	4:B:753:HOH:O	2.11	0.51
1:A:455:ARG:C	1:A:457:LEU:H	2.18	0.50
1:B:35:LEU:HD22	1:B:49:LEU:HD22	1.92	0.50
1:B:483:ALA:C	1:B:485:HIS:N	2.68	0.50
1:A:250:ARG:HG2	1:A:250:ARG:NH1	2.23	0.50
1:B:170:ARG:HH12	1:B:173:THR:HG22	1.77	0.50
1:A:483:ALA:HB2	1:A:507:ARG:HH22	1.76	0.50
1:B:414:ASP:OD2	1:B:511:ARG:NH1	2.44	0.49
1:B:495:ARG:NH1	1:B:526:SER:O	2.45	0.49
1:B:437:SER:HB2	1:B:439:GLY:H	1.77	0.49
1:B:291:GLU:HB2	1:B:326:LEU:HD12	1.94	0.49
1:B:379:SER:HB3	1:B:382:THR:HG23	1.94	0.49
1:B:467:TYR:HE1	1:B:476:LYS:HD2	1.78	0.49
1:B:357:GLU:HG3	1:B:358:TYR:N	2.28	0.49
1:B:426:GLY:HA2	1:B:453:VAL:HG23	1.95	0.48
1:B:492:LEU:HA	1:B:526:SER:HB2	1.94	0.48
1:B:145:ALA:HA	1:B:170:ARG:NH2	2.28	0.48
1:A:133:ARG:O	1:A:134:PRO:C	2.56	0.48
1:A:145:ALA:HA	1:A:170:ARG:NH2	2.29	0.48
1:A:429:HIS:HB3	1:A:441:PRO:HB3	1.95	0.48
1:B:122:ARG:HD3	1:B:127:LEU:O	2.13	0.47
1:A:357:GLU:HG3	1:A:358:TYR:N	2.29	0.47
1:B:192:PRO:O	1:B:194:PRO:HD3	2.14	0.47
1:B:129:GLN:HB3	4:B:759:HOH:O	2.13	0.47
1:B:457:LEU:HD11	1:B:466:LEU:HD21	1.97	0.47
1:A:492:LEU:HD23	1:A:532:GLY:HA2	1.97	0.47
1:A:285:ARG:H	1:A:412:MET:HE2	1.78	0.47
1:B:429:HIS:HB3	1:B:441:PRO:HB3	1.97	0.46
1:B:213:GLU:OE1	1:B:242:ARG:NH2	2.47	0.46
1:B:285:ARG:HD3	1:B:285:ARG:C	2.40	0.46
1:A:346:ARG:HA	1:A:351:THR:O	2.16	0.46
1:B:504:LEU:H	1:B:504:LEU:HD12	1.80	0.46
1:A:201:GLU:OE2	1:A:257:HIS:NE2	2.49	0.46
1:B:46:THR:HG21	1:A:352:GLU:HG3	1.98	0.46
1:A:157:ALA:CB	1:A:253:LEU:HD22	2.46	0.46
1:A:174:SER:O	1:A:177:VAL:HG21	2.16	0.46
1:B:447:ILE:HG23	1:B:475:LEU:HD22	1.98	0.45
1:A:469:MET:HG3	1:A:474:LEU:HB2	1.98	0.45
1:B:389:ARG:HD3	4:B:744:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLN:H	1:A:256:GLN:CD	2.23	0.45
1:B:81:PRO:HB3	1:B:115:HIS:HB3	1.98	0.45
1:B:97:PRO:HG2	1:B:148:PRO:HB3	1.98	0.45
1:A:63:GLN:NE2	4:A:703:HOH:O	2.26	0.45
1:A:210:ARG:HD2	1:A:213:GLU:OE1	2.17	0.44
1:A:455:ARG:O	1:A:457:LEU:N	2.38	0.44
1:B:448:GLN:OE1	1:B:470:THR:OG1	2.19	0.44
1:B:187:ARG:HD3	1:B:198:PHE:O	2.18	0.44
1:A:227:SER:HB3	1:A:250:ARG:HD2	2.00	0.44
1:A:264:LEU:HD11	1:A:333:ALA:HB2	2.00	0.44
1:A:430:ARG:HD2	1:A:443:SER:HB3	2.00	0.44
1:B:215:SER:O	1:B:217:HIS:ND1	2.51	0.43
1:B:179:GLY:HA2	4:B:741:HOH:O	2.17	0.43
1:B:379:SER:CB	1:B:382:THR:HG23	2.47	0.43
1:B:55:LEU:HB3	1:B:127:LEU:HD21	2.01	0.43
1:A:455:ARG:C	1:A:457:LEU:N	2.76	0.43
1:B:486:LEU:HD23	1:B:486:LEU:HA	1.87	0.43
1:A:428:LEU:HD22	1:A:468:VAL:HG21	2.00	0.43
1:B:100:LEU:HA	1:B:100:LEU:HD12	1.68	0.42
1:B:217:HIS:HB3	4:B:795:HOH:O	2.17	0.42
1:A:81:PRO:HB3	1:A:115:HIS:HB3	2.01	0.42
1:B:267:ALA:HB3	1:B:393:GLU:HG3	2.01	0.42
1:A:514:CYS:HB3	1:A:522:GLN:NE2	2.33	0.42
1:A:108:LEU:O	1:A:121:GLN:HA	2.19	0.42
1:B:488:CYS:HA	1:B:501:TRP:CE3	2.54	0.42
1:B:133:ARG:O	1:B:134:PRO:C	2.61	0.42
1:A:465:HIS:CD2	1:A:476:LYS:HE2	2.55	0.42
1:B:181:ILE:HA	1:B:182:PRO:HD3	1.82	0.42
1:B:423:ASP:OD2	1:B:427:GLN:HB2	2.19	0.42
1:B:121:GLN:O	1:B:130:LEU:HD12	2.20	0.42
1:B:488:CYS:O	1:B:489:ALA:C	2.63	0.42
1:A:97:PRO:HG2	1:A:148:PRO:HB3	2.02	0.41
1:A:53:ASN:HB3	1:A:71:GLY:O	2.20	0.41
1:A:186:THR:HB	1:A:204:ALA:HB1	2.03	0.41
1:A:414:ASP:OD2	1:A:511:ARG:HD2	2.20	0.41
1:A:267:ALA:HB3	1:A:393:GLU:HG2	2.01	0.41
1:B:108:LEU:O	1:B:121:GLN:HA	2.20	0.41
1:B:504:LEU:C	1:B:506:GLY:N	2.76	0.41
1:A:29:THR:HG23	1:A:472:SER:O	2.21	0.41
1:A:100:LEU:HG	1:A:102:LEU:HD12	2.02	0.41
1:A:368:PRO:HB2	1:A:370:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLU:HG3	1:B:396:PRO:HD2	2.04	0.40
1:A:251:VAL:HG12	1:A:261:TYR:HA	2.02	0.40
1:A:462:THR:O	1:A:463:PHE:HB2	2.22	0.40
1:A:186:THR:HG21	1:A:256:GLN:HA	2.03	0.40
1:A:495:ARG:HD3	1:A:526:SER:O	2.21	0.40
1:B:487:ASP:OD2	1:B:489:ALA:HB3	2.21	0.40
1:A:285:ARG:NH1	1:A:286:GLU:OE1	2.55	0.40
1:A:357:GLU:HG3	1:A:358:TYR:H	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:HIS:CE1	1:A:380:ASP:OD1[15_555]	2.10	0.10
1:B:135:GLU:OE2	1:A:135:GLU:OE2[8_555]	2.19	0.01

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	483/523 (92%)	460 (95%)	22 (5%)	1 (0%)	43	65
1	B	469/523 (90%)	436 (93%)	33 (7%)	0	100	100
All	All	952/1046 (91%)	896 (94%)	55 (6%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	ASP

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	397/422 (94%)	386 (97%)	11 (3%)	38	65
1	B	397/422 (94%)	384 (97%)	13 (3%)	33	60
All	All	794/844 (94%)	770 (97%)	24 (3%)	37	63

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	LEU
1	B	74	LEU
1	B	123	ARG
1	B	128	GLU
1	B	190	TRP
1	B	205	LYS
1	B	240	GLN
1	B	269	GLU
1	B	289	HIS
1	B	359	ASP
1	B	437	SER
1	B	440	HIS
1	B	533	CYS
1	A	33	THR
1	A	134	PRO
1	A	158[A]	GLN
1	A	158[B]	GLN
1	A	192	PRO
1	A	199	SER
1	A	291	GLU
1	A	310	SER
1	A	359	ASP
1	A	379	SER
1	A	472	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	37	HIS
1	B	57	GLN
1	B	289	HIS
1	B	381	HIS
1	B	416	HIS
1	B	440	HIS
1	B	449	GLN
1	B	471	GLN
1	A	366	GLN
1	A	449	GLN
1	A	484	GLN
1	A	494	HIS
1	A	522	GLN

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 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 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	B	608	1	14,14,15	0.41	0	17,19,21	0.73	0
3	NAG	A	608	1	14,14,15	0.32	0	17,19,21	0.47	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	B	608	1	-	4/6/23/26	0/1/1/1
3	NAG	A	608	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	608	NAG	O5-C5-C6-O6
3	B	608	NAG	O5-C5-C6-O6
3	A	608	NAG	C4-C5-C6-O6
3	B	608	NAG	C4-C5-C6-O6
3	B	608	NAG	C8-C7-N2-C2
3	B	608	NAG	O7-C7-N2-C2
3	A	608	NAG	C8-C7-N2-C2
3	A	608	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	608	NAG	1	0
3	A	608	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	492/523 (94%)	0.27	34 (6%)	23 19	21, 43, 70, 98	1 (0%)
1	B	492/523 (94%)	0.43	42 (8%)	16 14	30, 45, 79, 108	0
All	All	984/1046 (94%)	0.35	76 (7%)	19 16	21, 44, 75, 108	1 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	PRO	8.4
1	A	309	PRO	6.1
1	B	507	ARG	5.4
1	B	289	HIS	5.1
1	A	456	ASP	5.1
1	B	302	PRO	5.0
1	A	174	SER	4.9
1	B	521	GLU	4.7
1	A	289	HIS	4.6
1	B	24	PRO	4.4
1	B	178	GLY	4.1
1	B	504	LEU	4.0
1	A	521	GLU	4.0
1	A	301	ALA	4.0
1	A	504	LEU	4.0
1	B	288	ALA	4.0
1	B	313	ALA	4.0
1	A	177	VAL	4.0
1	B	256	GLN	3.9
1	B	505	LEU	3.8
1	B	352	GLU	3.8
1	B	381	HIS	3.6
1	A	25	PRO	3.6
1	A	313	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	404	GLN	3.5
1	B	179	GLY	3.5
1	B	162	GLY	3.4
1	B	310	SER	3.3
1	B	309	PRO	3.3
1	B	486	LEU	3.3
1	A	87	GLU	3.3
1	B	285	ARG	3.2
1	A	37	HIS	3.1
1	A	284	SER	3.1
1	A	239	ALA	3.0
1	B	287	VAL	3.0
1	B	190	TRP	3.0
1	A	310	SER	2.9
1	B	522	GLN	2.9
1	A	380	ASP	2.9
1	B	503	VAL	2.9
1	A	179	GLY	2.9
1	B	348	GLU	2.8
1	A	190	TRP	2.8
1	A	507	ARG	2.8
1	A	285	ARG	2.7
1	A	283	THR	2.6
1	A	522	GLN	2.6
1	B	514	CYS	2.6
1	B	533	CYS	2.6
1	B	158	GLN	2.6
1	B	511	ARG	2.6
1	A	286	GLU	2.5
1	A	178	GLY	2.5
1	B	484	GLN	2.5
1	B	174	SER	2.5
1	B	512	SER	2.5
1	B	412	MET	2.5
1	B	257	HIS	2.4
1	B	161	ALA	2.4
1	B	31	ASN	2.3
1	B	254	ARG	2.3
1	A	255	ASP	2.3
1	B	201	GLU	2.3
1	A	486	LEU	2.3
1	A	201	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	151	SER	2.2
1	B	283	THR	2.2
1	A	240	GLN	2.2
1	A	180	GLY	2.2
1	B	380	ASP	2.2
1	B	284	SER	2.2
1	A	484	GLN	2.1
1	A	404	GLN	2.0
1	A	65	GLU	2.0
1	A	480	ALA	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(Å ²)	Q<0.9
2	CD	A	605	1/1	0.83	0.15	155,155,155,155	0
2	CD	B	605	1/1	0.87	0.13	139,139,139,139	0
3	NAG	A	608	14/15	0.90	0.12	48,52,56,59	0
3	NAG	B	608	14/15	0.92	0.11	43,48,64,71	0
2	CD	A	606	1/1	0.92	0.11	142,142,142,142	0
2	CD	B	604	1/1	0.97	0.07	74,74,74,74	0
2	CD	A	601	1/1	0.97	0.09	78,78,78,78	0
2	CD	A	604	1/1	0.98	0.04	70,70,70,70	0
2	CD	A	602	1/1	0.99	0.06	53,53,53,53	0
2	CD	A	603	1/1	0.99	0.06	71,71,71,71	0
2	CD	B	601	1/1	0.99	0.07	71,71,71,71	0
2	CD	B	602	1/1	0.99	0.07	62,62,62,62	0
2	CD	B	606	1/1	0.99	0.07	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	A	607	1/1	0.99	0.04	81,81,81,81	0
2	CD	B	607	1/1	0.99	0.07	54,54,54,54	0
2	CD	B	603	1/1	0.99	0.07	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.