



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:11 PM BST

PDB ID : 6FG9
Title : Mouse SORCS2 ectodomain (sortilin related VPS10 domain containing receptor 2)
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Deposited on : 2018-01-10
Resolution : 4.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

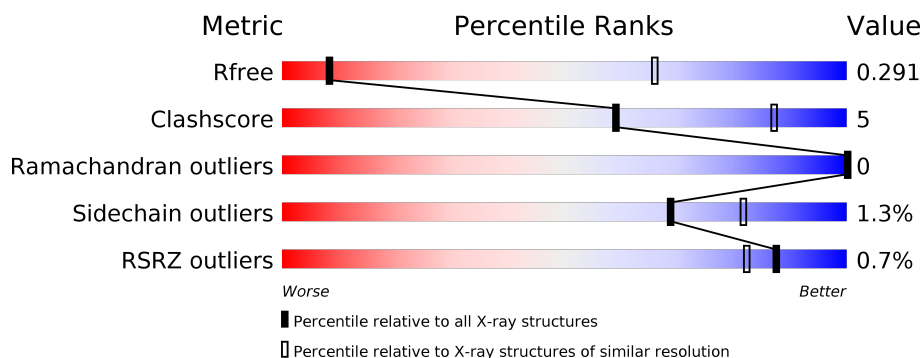
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 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	972	<div> <div></div> <div>81%13%6%</div> </div>
1	B	972	<div> <div></div> <div>82%12%6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1102	-	-	-	X
2	NAG	B	1104	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14712 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 VPS10 domain-containing receptor SorCS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	915	Total	C	N	O	S	0	0	0
			7269	4620	1239	1383	27			
1	B	918	Total	C	N	O	S	0	0	0
			7289	4633	1238	1391	27			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	GLY	-	cloning artifact	UNP Q9EPR5
A	252	THR	MET	conflict	UNP Q9EPR5
A	1078	ALA	-	expression tag	UNP Q9EPR5
A	1079	ALA	-	expression tag	UNP Q9EPR5
A	1080	ALA	-	expression tag	UNP Q9EPR5
A	1081	HIS	-	expression tag	UNP Q9EPR5
A	1082	HIS	-	expression tag	UNP Q9EPR5
A	1083	HIS	-	expression tag	UNP Q9EPR5
A	1084	HIS	-	expression tag	UNP Q9EPR5
A	1085	HIS	-	expression tag	UNP Q9EPR5
A	1086	HIS	-	expression tag	UNP Q9EPR5
B	115	GLY	-	cloning artifact	UNP Q9EPR5
B	252	THR	MET	conflict	UNP Q9EPR5
B	1078	ALA	-	expression tag	UNP Q9EPR5
B	1079	ALA	-	expression tag	UNP Q9EPR5
B	1080	ALA	-	expression tag	UNP Q9EPR5
B	1081	HIS	-	expression tag	UNP Q9EPR5
B	1082	HIS	-	expression tag	UNP Q9EPR5
B	1083	HIS	-	expression tag	UNP Q9EPR5
B	1084	HIS	-	expression tag	UNP Q9EPR5
B	1085	HIS	-	expression tag	UNP Q9EPR5
B	1086	HIS	-	expression tag	UNP Q9EPR5

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

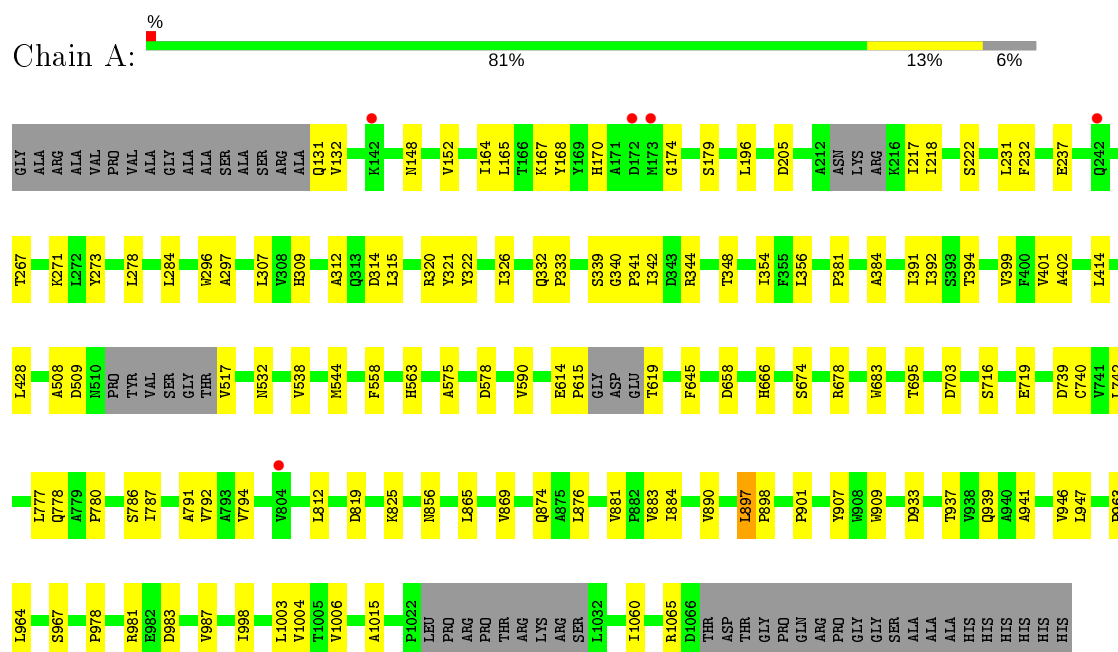


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	B	1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

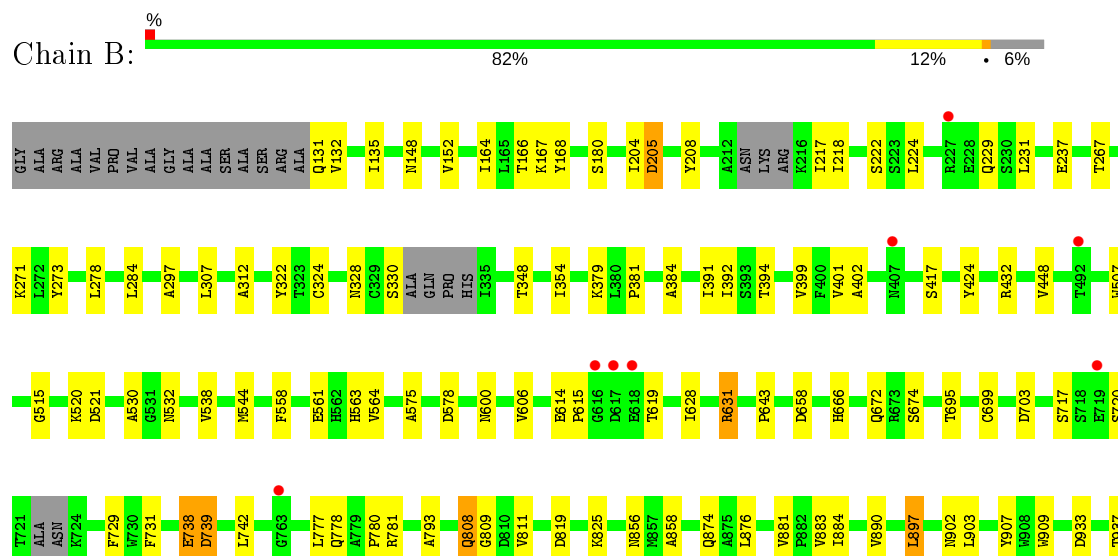
3 Residue-property plots [i](#)

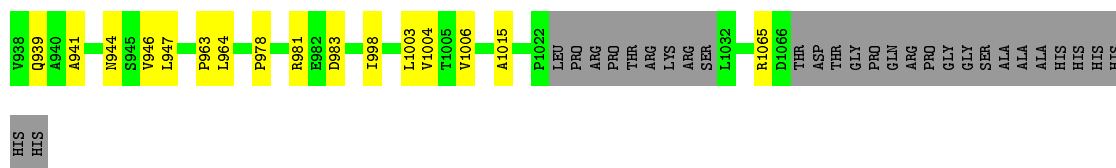
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: VPS10 domain-containing receptor SorCS2



- Molecule 1: VPS10 domain-containing receptor SorCS2





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	138.81Å 329.27Å 131.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 4.20 49.20 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.20-4.20) 99.8 (49.20-4.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.249 , 0.291 0.249 , 0.291	Depositor DCC
R_{free} test set	1163 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	164.8	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 99.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14712	wwPDB-VP
Average B, all atoms (Å ²)	196.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: 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	0.24	0/7433	0.45	0/10114
1	B	0.24	0/7453	0.45	0/10141
All	All	0.24	0/14886	0.45	0/20255

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	7269	0	7153	67	0
1	B	7289	0	7167	70	0
2	A	70	0	65	2	0
2	B	84	0	78	2	0
All	All	14712	0	14463	137	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 5.

All (137) 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:781:ARG:HB2	1:B:808:GLN:HB3	1.67	0.77
1:B:205:ASP:N	1:B:205:ASP:OD2	2.19	0.76
1:A:898:PRO:HG2	1:A:901:PRO:HG3	1.68	0.75
1:B:780:PRO:HD3	1:B:856:ASN:HD22	1.52	0.74
1:B:964:LEU:HB2	1:B:1015:ALA:HB3	1.69	0.73
1:B:217:ILE:HG21	1:B:237:GLU:HG2	1.71	0.73
1:A:964:LEU:HB2	1:A:1015:ALA:HB3	1.70	0.72
1:A:217:ILE:HG21	1:A:237:GLU:HG2	1.73	0.71
1:A:876:LEU:HD22	1:A:947:LEU:HB3	1.74	0.69
1:B:674:SER:HB3	1:B:695:THR:HB	1.75	0.69
1:B:963:PRO:HB2	1:B:1065:ARG:HB3	1.76	0.68
1:B:394:THR:HG22	1:B:399:VAL:HG13	1.76	0.67
1:B:448:VAL:HA	1:B:521:ASP:OD2	1.93	0.67
1:A:674:SER:HB3	1:A:695:THR:HB	1.75	0.67
1:A:297:ALA:HB2	1:A:307:LEU:HB2	1.78	0.66
1:A:963:PRO:HB2	1:A:1065:ARG:HB3	1.78	0.66
1:B:811:VAL:HG11	1:B:856:ASN:HD21	1.61	0.66
1:B:544:MET:HB2	1:B:558:PHE:HB2	1.78	0.65
1:A:394:THR:HG22	1:A:399:VAL:HG13	1.80	0.63
1:B:563:HIS:NE2	1:B:578:ASP:OD2	2.31	0.63
1:A:267:THR:HB	1:A:271:LYS:HB2	1.80	0.63
1:B:324:CYS:SG	1:B:330:SER:N	2.67	0.63
1:B:218:ILE:HG21	1:B:278:LEU:HD11	1.81	0.62
1:B:778:GLN:HG2	1:B:809:GLY:HA3	1.80	0.62
1:B:876:LEU:HD22	1:B:947:LEU:HB3	1.80	0.62
1:B:777:LEU:HG	1:B:858:ALA:HB2	1.81	0.62
1:A:544:MET:HB2	1:A:558:PHE:HB2	1.80	0.62
1:B:793:ALA:HB3	1:B:944:ASN:HB2	1.82	0.62
1:B:267:THR:HB	1:B:271:LYS:HB2	1.84	0.59
1:B:297:ALA:HB2	1:B:307:LEU:HB2	1.83	0.59
2:A:1103:NAG:H83	2:A:1103:NAG:H3	1.85	0.58
1:A:218:ILE:HG21	1:A:278:LEU:HD11	1.84	0.58
1:A:381:PRO:HB2	1:A:384:ALA:HB3	1.85	0.58
1:B:381:PRO:HB2	1:B:384:ALA:HB3	1.86	0.58
1:B:520:LYS:HE3	1:B:564:VAL:HB	1.86	0.58
1:B:379:LYS:HE2	1:B:738:GLU:OE2	2.04	0.58
1:A:332:GLN:N	1:A:333:PRO:HD2	2.19	0.57
1:B:811:VAL:HG11	1:B:856:ASN:ND2	2.18	0.57
1:B:148:ASN:HB2	1:B:168:TYR:HA	1.86	0.57
1:A:874:GLN:HB2	1:A:897:LEU:HD13	1.86	0.57
1:A:563:HIS:NE2	1:A:578:ASP:OD2	2.38	0.56
1:A:740:CYS:O	1:A:778:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ALA:HB2	1:A:517:VAL:HG12	1.89	0.55
1:A:978:PRO:HA	1:A:981:ARG:HE	1.72	0.55
1:B:883:VAL:HG11	1:B:1004:VAL:HG11	1.89	0.55
2:A:1104:NAG:H3	2:A:1104:NAG:H83	1.88	0.54
1:A:881:VAL:HG23	1:A:1006:VAL:HG11	1.88	0.54
1:A:777:LEU:HD21	1:A:812:LEU:HD11	1.90	0.54
1:A:348:THR:HG22	1:A:354:ILE:HG23	1.90	0.54
1:B:606:VAL:HG22	1:B:628:ILE:HG22	1.89	0.54
1:B:204:ILE:HG21	1:B:224:LEU:HB3	1.89	0.53
1:A:148:ASN:HB2	1:A:168:TYR:HA	1.89	0.53
1:A:320:ARG:HG2	1:A:340:GLY:O	2.07	0.53
1:B:166:THR:OG1	1:B:180:SER:OG	2.22	0.53
1:B:515:GLY:C	1:B:561:GLU:OE2	2.48	0.52
1:A:884:ILE:HD13	1:A:890:VAL:HG22	1.91	0.52
1:B:884:ILE:HD13	1:B:890:VAL:HG22	1.92	0.52
1:A:340:GLY:N	1:A:341:PRO:HD3	2.25	0.52
1:A:794:VAL:HB	1:A:869:VAL:HG22	1.92	0.52
1:B:902:ASN:OD1	2:B:1106:NAG:N2	2.44	0.51
1:B:819:ASP:OD2	1:B:825:LYS:NZ	2.23	0.51
1:A:222:SER:HA	1:A:231:LEU:HD23	1.93	0.51
1:B:348:THR:HG22	1:B:354:ILE:HG23	1.92	0.50
1:A:152:VAL:HG13	1:A:164:ILE:HG12	1.93	0.50
1:A:987:VAL:HG21	1:B:729:PHE:HB2	1.94	0.50
1:A:883:VAL:HG11	1:A:1004:VAL:HG11	1.94	0.50
1:B:152:VAL:HG13	1:B:164:ILE:HG12	1.93	0.49
1:A:998:ILE:HD11	1:A:1003:LEU:HD11	1.93	0.49
1:B:532:ASN:ND2	1:B:538:VAL:HG22	2.27	0.49
1:A:909:TRP:HB2	1:A:937:THR:HB	1.94	0.49
1:A:339:SER:C	1:A:341:PRO:HD3	2.33	0.49
1:B:998:ILE:HD11	1:B:1003:LEU:HD11	1.94	0.49
1:B:978:PRO:HA	1:B:981:ARG:HE	1.77	0.49
1:A:392:ILE:HD11	1:A:402:ALA:HB2	1.95	0.48
1:A:819:ASP:OD2	1:A:825:LYS:NZ	2.23	0.48
1:B:392:ILE:HD11	1:B:402:ALA:HB2	1.95	0.48
1:A:792:VAL:HG21	1:B:946:VAL:HG11	1.95	0.48
1:B:563:HIS:O	1:B:575:ALA:HA	2.14	0.48
1:A:716:SER:OG	1:A:719:GLU:OE1	2.32	0.48
1:B:907:TYR:HB2	1:B:939:GLN:HB3	1.96	0.48
1:B:881:VAL:HG23	1:B:1006:VAL:HG11	1.95	0.48
1:A:658:ASP:OD2	1:A:666:HIS:NE2	2.47	0.48
1:A:309:HIS:HB3	1:A:321:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:TRP:HZ3	1:A:326:ILE:HD11	1.79	0.47
1:B:312:ALA:HB3	1:B:322:TYR:CE2	2.50	0.47
1:A:273:TYR:CZ	1:A:284:LEU:HD13	2.51	0.46
1:B:222:SER:HA	1:B:231:LEU:HD23	1.97	0.46
1:A:532:ASN:ND2	1:A:538:VAL:HG22	2.31	0.46
1:B:874:GLN:HB2	1:B:897:LEU:HD13	1.98	0.46
1:A:312:ALA:HB3	1:A:322:TYR:CE2	2.50	0.46
1:B:600:ASN:OD1	2:B:1103:NAG:N2	2.48	0.46
1:A:780:PRO:HD3	1:A:856:ASN:HD22	1.81	0.46
1:B:909:TRP:HB2	1:B:937:THR:HB	1.98	0.46
1:B:273:TYR:CZ	1:B:284:LEU:HD13	2.52	0.45
1:B:312:ALA:HB3	1:B:322:TYR:HE2	1.81	0.45
1:B:739:ASP:HA	1:B:809:GLY:HA2	1.98	0.45
1:A:563:HIS:O	1:A:575:ALA:HA	2.17	0.45
1:A:170:HIS:ND1	1:A:174:GLY:HA3	2.31	0.44
1:A:742:LEU:HD21	1:A:777:LEU:HA	1.99	0.44
1:A:787:ILE:HB	1:A:791:ALA:CB	2.48	0.44
1:B:391:ILE:HD13	1:B:401:VAL:HG23	1.99	0.44
1:A:645:PHE:HB3	1:A:683:TRP:HB3	1.99	0.43
1:A:941:ALA:HB2	1:A:946:VAL:HG22	1.99	0.43
1:B:717:SER:O	1:B:720:SER:OG	2.34	0.43
1:B:530:ALA:HB2	1:B:544:MET:SD	2.58	0.43
1:A:590:VAL:O	1:A:678:ARG:NH2	2.51	0.42
1:B:417:SER:HB3	1:B:424:TYR:CE2	2.54	0.42
1:B:614:GLU:HG3	1:B:615:PRO:HD2	2.01	0.42
1:A:391:ILE:HD13	1:A:401:VAL:HG23	2.01	0.42
1:A:414:LEU:HB3	1:A:428:LEU:HB3	2.02	0.42
1:A:967:SER:HB3	1:A:1060:ILE:HG23	2.00	0.42
1:A:787:ILE:HB	1:A:791:ALA:HB2	2.02	0.42
1:B:167:LYS:HD2	1:B:205:ASP:HB3	2.02	0.42
1:B:521:ASP:N	1:B:521:ASP:OD1	2.53	0.42
1:B:658:ASP:OD2	1:B:666:HIS:NE2	2.52	0.42
1:A:342:ILE:HG22	1:A:344:ARG:N	2.34	0.42
1:B:628:ILE:O	1:B:631:ARG:HB2	2.20	0.42
1:B:781:ARG:HG3	1:B:808:GLN:NE2	2.35	0.42
1:A:196:LEU:HD13	1:A:232:PHE:CE2	2.55	0.41
1:A:658:ASP:N	1:A:658:ASP:OD1	2.53	0.41
1:A:131:GLN:HG3	1:A:132:VAL:HG13	2.01	0.41
1:A:614:GLU:HG3	1:A:615:PRO:HD2	2.02	0.41
1:B:672:GLN:HG3	1:B:699:CYS:SG	2.59	0.41
1:A:907:TYR:HB2	1:A:939:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:HD13	1:B:229:GLN:HE21	1.85	0.41
1:A:786:SER:HA	1:A:865:LEU:HD22	2.03	0.41
1:B:131:GLN:HG3	1:B:132:VAL:HG13	2.02	0.41
1:B:941:ALA:HB2	1:B:946:VAL:HG22	2.01	0.41
1:B:432:ARG:HB3	1:B:507:TRP:CH2	2.56	0.41
1:A:165:LEU:HD11	1:A:179:SER:HB2	2.02	0.41
1:B:135:ILE:HG13	1:B:643:PRO:HG2	2.03	0.41
1:A:314:ASP:OD1	1:A:315:LEU:N	2.53	0.41
1:A:167:LYS:HD2	1:A:205:ASP:CG	2.41	0.40
1:A:332:GLN:N	1:A:333:PRO:CD	2.84	0.40
1:A:342:ILE:HD11	1:A:356:LEU:HD11	2.03	0.40
1:B:152:VAL:HG22	1:B:164:ILE:HG23	2.03	0.40
1:B:658:ASP:N	1:B:658:ASP:OD1	2.53	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	905/972 (93%)	817 (90%)	88 (10%)	0	100	100
1	B	908/972 (93%)	828 (91%)	80 (9%)	0	100	100
All	All	1813/1944 (93%)	1645 (91%)	168 (9%)	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	A	822/862 (95%)	815 (99%)	7 (1%)	78	87
1	B	825/862 (96%)	810 (98%)	15 (2%)	59	76
All	All	1647/1724 (96%)	1625 (99%)	22 (1%)	69	82

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	509	ASP
1	A	619	THR
1	A	703	ASP
1	A	739	ASP
1	A	897	LEU
1	A	933	ASP
1	A	983	ASP
1	B	205	ASP
1	B	208	TYR
1	B	328	ASN
1	B	619	THR
1	B	631	ARG
1	B	703	ASP
1	B	731	PHE
1	B	738	GLU
1	B	739	ASP
1	B	742	LEU
1	B	808	GLN
1	B	897	LEU
1	B	903	LEU
1	B	933	ASP
1	B	983	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	778	GLN
1	B	856	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1105	1	14,14,15	0.40	0	17,19,21	0.63	1 (5%)
2	NAG	A	1103	1	14,14,15	0.52	0	17,19,21	1.28	2 (11%)
2	NAG	A	1104	1	14,14,15	0.44	0	17,19,21	1.25	1 (5%)
2	NAG	B	1101	1	14,14,15	0.26	0	17,19,21	0.41	0
2	NAG	B	1106	1	14,14,15	0.39	0	17,19,21	0.56	0
2	NAG	B	1102	1	14,14,15	0.21	0	17,19,21	0.49	0
2	NAG	A	1102	1	14,14,15	0.30	0	17,19,21	0.56	0
2	NAG	B	1103	1	14,14,15	0.38	0	17,19,21	0.53	0
2	NAG	A	1105	1	14,14,15	0.30	0	17,19,21	0.42	0
2	NAG	A	1101	1	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	B	1104	1	14,14,15	0.30	0	17,19,21	0.60	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1105	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1103	1	-	5/6/23/26	0/1/1/1
2	NAG	A	1104	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1101	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1106	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1102	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1102	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1103	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1105	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1101	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1104	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1104	NAG	C2-N2-C7	4.35	129.10	122.90
2	A	1103	NAG	C2-N2-C7	4.24	128.94	122.90
2	B	1105	NAG	C1-O5-C5	2.17	115.13	112.19
2	A	1103	NAG	C1-C2-N2	2.15	114.16	110.49
2	B	1104	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1102	NAG	O5-C5-C6-O6
2	A	1103	NAG	O5-C5-C6-O6
2	B	1106	NAG	O5-C5-C6-O6
2	A	1101	NAG	O5-C5-C6-O6
2	B	1106	NAG	C4-C5-C6-O6
2	A	1103	NAG	C4-C5-C6-O6
2	B	1102	NAG	C4-C5-C6-O6
2	B	1104	NAG	C4-C5-C6-O6
2	A	1101	NAG	C4-C5-C6-O6
2	A	1103	NAG	C8-C7-N2-C2
2	A	1103	NAG	O7-C7-N2-C2
2	A	1104	NAG	C8-C7-N2-C2
2	A	1104	NAG	O7-C7-N2-C2
2	B	1104	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	B	1104	NAG	O7-C7-N2-C2
2	B	1104	NAG	O5-C5-C6-O6
2	B	1103	NAG	O5-C5-C6-O6
2	A	1102	NAG	C4-C5-C6-O6
2	A	1102	NAG	O5-C5-C6-O6
2	B	1106	NAG	C3-C2-N2-C7
2	A	1102	NAG	C3-C2-N2-C7
2	B	1103	NAG	C3-C2-N2-C7
2	B	1103	NAG	C4-C5-C6-O6
2	A	1103	NAG	C3-C2-N2-C7
2	A	1104	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1103	NAG	1	0
2	A	1104	NAG	1	0
2	B	1106	NAG	1	0
2	B	1103	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 [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	A	915/972 (94%)	-0.24	5 (0%) 91 86	127, 208, 257, 344	0
1	B	918/972 (94%)	-0.36	8 (0%) 84 77	111, 183, 246, 320	0
All	All	1833/1944 (94%)	-0.30	13 (0%) 87 82	111, 194, 254, 344	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	MET	4.1
1	A	172	ASP	3.9
1	B	618	GLU	3.9
1	B	616	GLY	3.4
1	B	407	ASN	3.0
1	B	763	GLY	2.9
1	B	719	GLU	2.8
1	B	227	ARG	2.5
1	B	617	ASP	2.5
1	B	492	THR	2.4
1	A	804	VAL	2.2
1	A	142	LYS	2.1
1	A	242	GLN	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 monosaccharides 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(\AA^2)	Q<0.9
2	NAG	A	1105	14/15	0.63	0.30	194,259,287,310	0
2	NAG	B	1105	14/15	0.68	0.35	191,222,240,250	0
2	NAG	A	1102	14/15	0.71	0.58	208,240,260,263	0
2	NAG	B	1102	14/15	0.72	0.21	201,228,252,255	0
2	NAG	A	1101	14/15	0.77	0.40	200,249,261,262	0
2	NAG	B	1104	14/15	0.77	0.52	169,219,239,252	0
2	NAG	A	1103	14/15	0.79	0.26	204,217,247,276	0
2	NAG	B	1106	14/15	0.80	0.48	189,235,259,266	0
2	NAG	B	1103	14/15	0.83	0.40	201,224,244,253	0
2	NAG	B	1101	14/15	0.85	0.19	188,207,229,240	0
2	NAG	A	1104	14/15	0.94	0.16	178,204,226,231	0

6.5 Other polymers [i](#)

There are no such residues in this entry.