



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:53 PM GMT

PDB ID : 5BQC  
Title : Crystal structure of Norrin in complex with the cysteine-rich domain of Frizzled 4 and sucrose octasulfate  
Authors : Chang, T.-H.; Hsieh, F.-L.; Zebisch, M.; Harlos, K.; Jones, E.Y.  
Deposited on : 2015-05-28  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

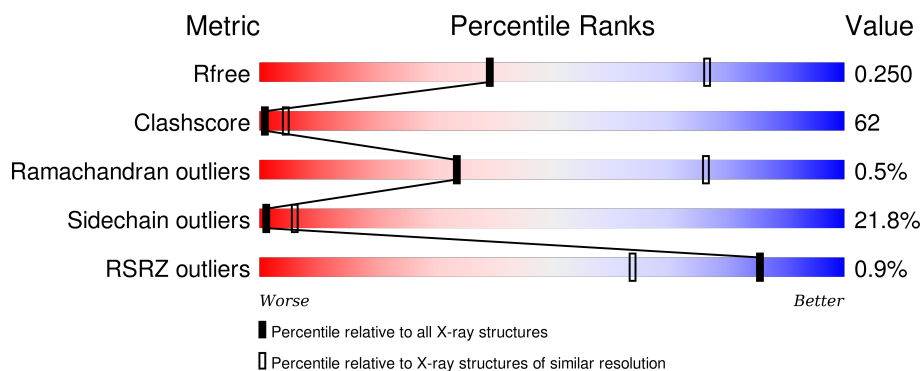
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	149	<div> <div></div> <div>26%</div> <div>46%</div> <div>12%</div> <div>17%</div> </div>
2	A	122	<div> <div></div> <div>32%</div> <div>34%</div> <div>16%</div> <div>18%</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
3	NAG	B	202	X	-	-	-
4	SCR	A	201	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1842 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 Frizzled-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	124	Total	C	N	O	S	0	0	0
			971	610	165	180	16			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	39	ASP	-	expression tag	UNP Q9ULV1
B	40	THR	-	expression tag	UNP Q9ULV1
B	41	GLY	-	expression tag	UNP Q9ULV1
B	180	GLY	-	expression tag	UNP Q9ULV1
B	181	THR	-	expression tag	UNP Q9ULV1
B	182	LEU	-	expression tag	UNP Q9ULV1
B	183	GLU	-	expression tag	UNP Q9ULV1
B	184	VAL	-	expression tag	UNP Q9ULV1
B	185	LEU	-	expression tag	UNP Q9ULV1
B	186	PHE	-	expression tag	UNP Q9ULV1
B	187	GLN	-	expression tag	UNP Q9ULV1

- Molecule 2 is a protein called Norrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	100	Total	C	N	O	S	0	0	0
			788	480	154	140	14			

There are 13 discrepancies between the modelled and reference sequences:

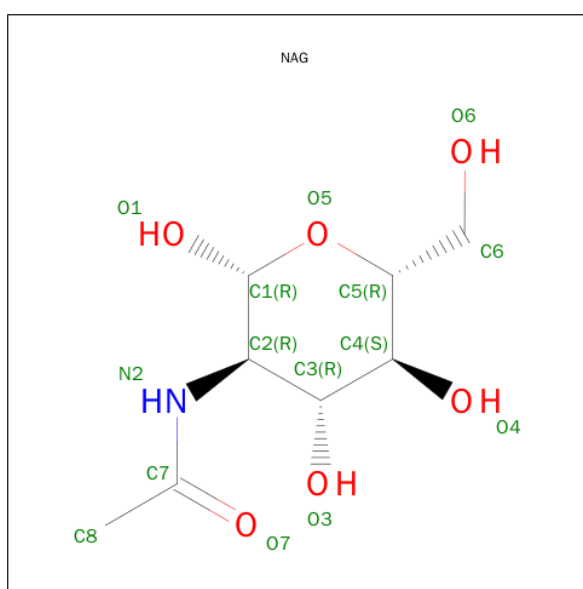
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q00604
A	23	PRO	-	expression tag	UNP Q00604
A	24	GLY	-	expression tag	UNP Q00604
A	134	GLY	-	expression tag	UNP Q00604
A	135	THR	-	expression tag	UNP Q00604

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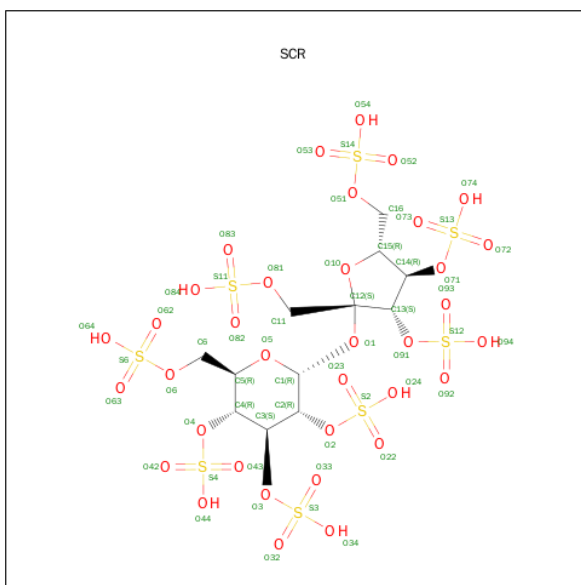
Chain	Residue	Modelled	Actual	Comment	Reference
A	136	GLU	-	expression tag	UNP Q00604
A	137	THR	-	expression tag	UNP Q00604
A	138	SER	-	expression tag	UNP Q00604
A	139	GLN	-	expression tag	UNP Q00604
A	140	VAL	-	expression tag	UNP Q00604
A	141	ALA	-	expression tag	UNP Q00604
A	142	PRO	-	expression tag	UNP Q00604
A	143	ALA	-	expression tag	UNP Q00604

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is SUCROSE OCTASULFATE (three-letter code: SCR) (formula:  $C_{12}H_{22}O_{35}S_8$ ).

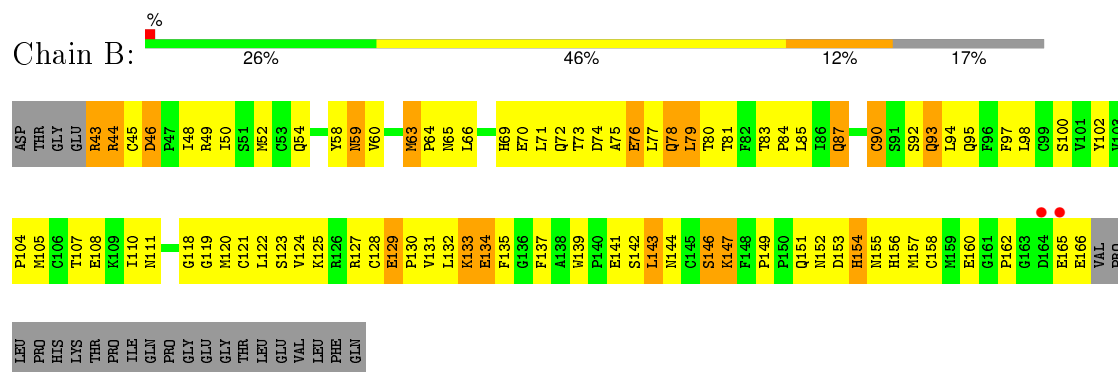


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			55	12	35	8		

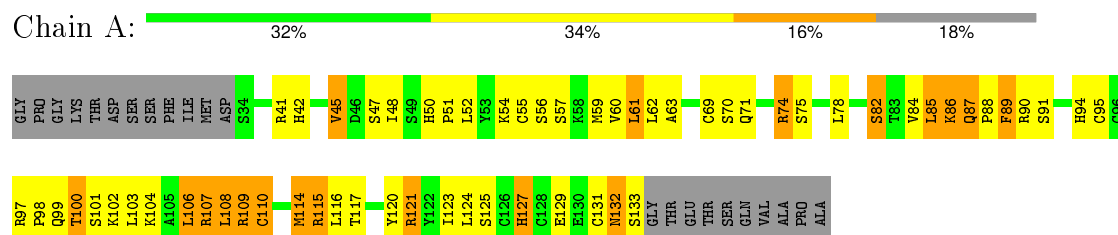
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Frizzled-4



#### • Molecule 2: Norrin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.14Å 119.14Å 119.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.34 – 3.00 47.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.34-3.00) 100.0 (47.34-3.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.215 , 0.268 0.262 , 0.250	Depositor DCC
$R_{free}$ test set	483 reflections (4.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	111.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 72.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 10475 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	1842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NAG, SCR

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	0.37	0/995	0.54	0/1347
2	A	0.50	0/804	0.57	0/1078
All	All	0.43	0/1799	0.55	0/2425

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	59	ASN	Peptide

### 5.2 Too-close contacts [i](#)

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	971	0	933	129	0
2	A	788	0	779	88	4
3	B	28	0	26	3	0
4	A	55	0	22	27	4
All	All	1842	0	1760	225	4

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 62.

All (225) 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:107:ARG:HH11	4:A:201:SCR:H112	1.00	1.10
1:B:153:ASP:OD1	1:B:156:HIS:N	1.87	1.08
1:B:110:ILE:HB	2:A:59:MET:HE1	1.36	1.03
2:A:108:LEU:N	2:A:116:LEU:O	1.96	0.97
2:A:71:GLN:OE1	2:A:94:HIS:ND1	1.97	0.97
1:B:152:ASN:OD1	1:B:158:CYS:N	2.00	0.93
2:A:107:ARG:NH1	4:A:201:SCR:H112	1.81	0.93
1:B:165:GLU:CD	1:B:166:GLU:H	1.73	0.93
2:A:107:ARG:HD2	2:A:115:ARG:HD3	1.51	0.92
1:B:110:ILE:HB	2:A:59:MET:CE	2.00	0.91
1:B:90:CYS:SG	1:B:127:ARG:HB3	2.14	0.87
2:A:100:THR:HG23	2:A:124:LEU:HB2	1.54	0.86
2:A:107:ARG:HH11	4:A:201:SCR:C11	1.88	0.85
2:A:106:LEU:O	2:A:106:LEU:HD23	1.76	0.85
4:A:201:SCR:H161	4:A:201:SCR:H5	1.61	0.82
1:B:70:GLU:O	1:B:71:LEU:HD23	1.79	0.82
4:A:201:SCR:S14	4:A:201:SCR:H62	2.20	0.82
1:B:44:ARG:NH1	1:B:110:ILE:O	2.14	0.81
1:B:157:MET:HE2	2:A:60:VAL:HA	1.60	0.81
2:A:107:ARG:HG2	4:A:201:SCR:O64	1.81	0.79
2:A:61:LEU:O	2:A:62:LEU:HD23	1.83	0.78
2:A:88:PRO:HB2	2:A:89:PHE:CD1	2.19	0.78
2:A:70:SER:OG	2:A:71:GLN:NE2	2.17	0.78
1:B:165:GLU:CD	1:B:166:GLU:N	2.37	0.77
2:A:107:ARG:CD	2:A:115:ARG:HD3	2.15	0.76
1:B:141:GLU:OE2	1:B:144:ASN:ND2	2.18	0.75
2:A:108:LEU:O	2:A:116:LEU:N	2.19	0.75
1:B:65:ASN:HB2	1:B:69:HIS:HB2	1.69	0.74
2:A:109:ARG:NH1	2:A:115:ARG:HH21	1.85	0.74
2:A:103:LEU:HD23	2:A:104:LYS:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:OD1	1:B:146:SER:OG	2.06	0.73
1:B:121:CYS:SG	1:B:122:LEU:N	2.61	0.73
2:A:85:LEU:HD22	2:A:86:LYS:O	1.88	0.73
2:A:109:ARG:HH12	2:A:115:ARG:HH21	1.34	0.73
1:B:70:GLU:C	1:B:71:LEU:HD23	2.10	0.72
1:B:121:CYS:O	1:B:125:LYS:N	2.21	0.72
2:A:41:ARG:HD2	2:A:123:ILE:O	1.90	0.71
2:A:132:ASN:ND2	2:A:132:ASN:O	2.22	0.71
1:B:142:SER:OG	1:B:143:LEU:HD23	1.91	0.71
4:A:201:SCR:C5	4:A:201:SCR:H161	2.21	0.70
4:A:201:SCR:O63	4:A:201:SCR:O53	2.10	0.70
1:B:93:GLN:OE1	1:B:162:PRO:HD2	1.91	0.70
1:B:45:CYS:C	1:B:46:ASP:OD1	2.31	0.70
1:B:132:LEU:O	1:B:134:GLU:O	2.10	0.69
2:A:99:GLN:HB3	2:A:125:SER:OG	1.93	0.69
2:A:127:HIS:NE2	2:A:129:GLU:OE2	2.25	0.68
1:B:153:ASP:OD2	1:B:155:ASN:HB2	1.92	0.68
4:A:201:SCR:O53	4:A:201:SCR:H62	1.93	0.68
1:B:44:ARG:NH1	1:B:111:ASN:HA	2.09	0.68
1:B:65:ASN:ND2	1:B:102:TYR:O	2.27	0.67
1:B:45:CYS:HB3	1:B:60:VAL:CG1	2.25	0.67
1:B:151:GLN:O	1:B:156:HIS:CD2	2.48	0.67
4:A:201:SCR:C16	4:A:201:SCR:H5	2.24	0.67
1:B:65:ASN:CB	1:B:69:HIS:HB2	2.25	0.66
2:A:106:LEU:C	2:A:106:LEU:HD23	2.15	0.66
1:B:90:CYS:SG	1:B:127:ARG:C	2.74	0.66
1:B:130:PRO:O	1:B:133:LYS:HB2	1.96	0.66
1:B:59:ASN:CB	1:B:60:VAL:HG23	2.27	0.64
4:A:201:SCR:H161	4:A:201:SCR:O1	1.98	0.63
2:A:107:ARG:NH1	4:A:201:SCR:H1	2.14	0.63
2:A:103:LEU:HD23	2:A:104:LYS:H	1.64	0.62
2:A:88:PRO:HB2	2:A:89:PHE:CE1	2.34	0.61
2:A:109:ARG:HH12	2:A:115:ARG:NH2	1.98	0.61
4:A:201:SCR:H14	4:A:201:SCR:O92	2.01	0.60
2:A:100:THR:CG2	2:A:124:LEU:HB2	2.31	0.60
2:A:75:SER:CB	2:A:91:SER:HB3	2.32	0.60
1:B:157:MET:CE	2:A:60:VAL:HA	2.31	0.59
2:A:100:THR:HG22	2:A:125:SER:OG	2.03	0.58
2:A:87:GLN:N	2:A:88:PRO:HD3	2.18	0.58
2:A:132:ASN:HD22	2:A:132:ASN:C	2.06	0.58
2:A:85:LEU:CD2	2:A:87:GLN:HB2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:201:SCR:H15	4:A:201:SCR:O54	2.03	0.58
1:B:125:LYS:HA	1:B:139:TRP:CZ3	2.38	0.58
1:B:73:THR:O	1:B:76:GLU:HB3	2.04	0.58
1:B:157:MET:HE2	2:A:60:VAL:CA	2.31	0.57
2:A:61:LEU:HG	2:A:62:LEU:N	2.17	0.57
2:A:107:ARG:NH1	4:A:201:SCR:O22	2.36	0.57
2:A:101:SER:HB2	2:A:121:ARG:HD2	1.87	0.57
1:B:45:CYS:HB3	1:B:60:VAL:HG11	1.87	0.57
1:B:45:CYS:CB	1:B:60:VAL:HG11	2.35	0.57
1:B:45:CYS:HB3	1:B:60:VAL:HG12	1.87	0.57
3:B:201:NAG:H3	3:B:201:NAG:H83	1.87	0.57
2:A:60:VAL:HG22	2:A:61:LEU:N	2.19	0.56
1:B:149:PRO:HB2	1:B:156:HIS:CD2	2.40	0.56
1:B:44:ARG:N	1:B:108:GLU:OE2	2.38	0.56
1:B:85:LEU:HD12	1:B:132:LEU:HD13	1.87	0.56
2:A:82:SER:HB2	2:A:84:VAL:O	2.05	0.56
1:B:122:LEU:HD12	1:B:165:GLU:HG3	1.88	0.56
2:A:107:ARG:NH1	4:A:201:SCR:O2	2.38	0.56
1:B:97:PHE:O	1:B:100:SER:HB3	2.06	0.56
1:B:93:GLN:OE1	1:B:162:PRO:CD	2.53	0.55
1:B:77:LEU:O	1:B:80:THR:OG1	2.18	0.55
2:A:75:SER:HB3	2:A:91:SER:HB3	1.89	0.54
1:B:46:ASP:N	1:B:46:ASP:OD1	2.39	0.54
1:B:157:MET:CE	2:A:60:VAL:CA	2.85	0.54
1:B:97:PHE:HE2	1:B:143:LEU:HD12	1.72	0.54
2:A:107:ARG:CZ	2:A:115:ARG:CZ	2.86	0.54
1:B:153:ASP:OD1	1:B:156:HIS:ND1	2.40	0.54
2:A:107:ARG:CD	2:A:115:ARG:CD	2.86	0.54
1:B:44:ARG:HH12	1:B:110:ILE:C	2.11	0.53
2:A:110:CYS:N	2:A:114:MET:O	2.36	0.53
1:B:66:LEU:HG	1:B:104:PRO:HG3	1.91	0.53
1:B:94:LEU:CD1	1:B:98:LEU:HD11	2.38	0.53
1:B:125:LYS:HA	1:B:139:TRP:CH2	2.44	0.53
1:B:75:ALA:O	1:B:79:LEU:HD23	2.09	0.53
1:B:144:ASN:OD1	3:B:201:NAG:H82	2.08	0.52
1:B:144:ASN:O	1:B:147:LYS:HD3	2.08	0.52
1:B:63:MET:HG3	1:B:64:PRO:HA	1.90	0.52
2:A:107:ARG:NH1	2:A:115:ARG:CZ	2.73	0.52
1:B:70:GLU:HA	1:B:70:GLU:OE1	2.10	0.52
1:B:48:ILE:HD13	1:B:59:ASN:O	2.10	0.52
1:B:129:GLU:N	1:B:130:PRO:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:LEU:HD22	2:A:87:GLN:HB2	1.91	0.52
4:A:201:SCR:C5	4:A:201:SCR:C16	2.85	0.52
1:B:90:CYS:SG	1:B:127:ARG:CB	2.95	0.52
1:B:132:LEU:O	1:B:137:PHE:HB2	2.09	0.51
2:A:107:ARG:HH11	4:A:201:SCR:H1	1.74	0.51
1:B:83:THR:HG22	1:B:84:PRO:HD3	1.93	0.51
1:B:59:ASN:HB3	1:B:60:VAL:HG23	1.92	0.51
1:B:94:LEU:HG	1:B:98:LEU:HD11	1.93	0.51
1:B:83:THR:O	1:B:87:GLN:NE2	2.44	0.51
2:A:56:SER:O	2:A:108:LEU:HD13	2.11	0.51
1:B:59:ASN:HB2	1:B:60:VAL:HG23	1.92	0.50
2:A:100:THR:HG22	2:A:125:SER:CB	2.41	0.50
2:A:107:ARG:NH1	4:A:201:SCR:S2	2.84	0.50
1:B:141:GLU:CD	1:B:144:ASN:HD22	2.13	0.50
1:B:78:GLN:O	1:B:81:THR:HG23	2.11	0.50
2:A:45:VAL:HG12	2:A:61:LEU:HD12	1.94	0.50
2:A:109:ARG:NH2	2:A:115:ARG:NE	2.60	0.49
2:A:75:SER:HA	2:A:91:SER:HA	1.93	0.49
3:B:202:NAG:O3	3:B:202:NAG:O7	2.29	0.49
1:B:121:CYS:O	1:B:124:VAL:HB	2.12	0.49
2:A:89:PHE:CD1	2:A:89:PHE:N	2.80	0.49
1:B:118:GLY:O	1:B:121:CYS:N	2.45	0.49
2:A:101:SER:CB	2:A:121:ARG:HD2	2.42	0.49
2:A:97:ARG:HB3	2:A:98:PRO:HD2	1.93	0.49
1:B:110:ILE:CB	2:A:59:MET:HE1	2.25	0.49
1:B:97:PHE:HB2	1:B:120:MET:HE3	1.95	0.49
1:B:122:LEU:O	1:B:123:SER:C	2.51	0.48
1:B:85:LEU:CD1	1:B:132:LEU:HD13	2.43	0.48
1:B:149:PRO:HB2	1:B:156:HIS:HD2	1.76	0.48
1:B:52:MET:O	1:B:95:GLN:NE2	2.47	0.48
1:B:63:MET:CE	1:B:72:GLN:HA	2.43	0.48
1:B:110:ILE:CB	2:A:59:MET:CE	2.85	0.48
1:B:44:ARG:NH1	1:B:107:THR:O	2.46	0.48
1:B:58:TYR:CE2	1:B:105:MET:HA	2.48	0.47
2:A:109:ARG:HA	2:A:115:ARG:HG2	1.96	0.47
1:B:48:ILE:N	1:B:48:ILE:HD12	2.28	0.47
1:B:122:LEU:O	1:B:125:LYS:N	2.48	0.47
1:B:118:GLY:O	1:B:119:GLY:C	2.51	0.47
2:A:85:LEU:C	2:A:86:LYS:HG3	2.36	0.47
1:B:153:ASP:CG	1:B:156:HIS:CE1	2.87	0.47
2:A:97:ARG:HB3	2:A:98:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:107:ARG:HA	2:A:116:LEU:O	2.15	0.46
1:B:59:ASN:HB3	1:B:60:VAL:CG2	2.45	0.46
2:A:52:LEU:HD12	2:A:52:LEU:O	2.16	0.46
1:B:135:PHE:HB2	1:B:137:PHE:HD2	1.80	0.46
2:A:100:THR:O	2:A:124:LEU:N	2.46	0.46
1:B:154:HIS:ND1	1:B:154:HIS:N	2.60	0.46
1:B:76:GLU:O	1:B:80:THR:HG23	2.15	0.46
1:B:144:ASN:O	1:B:147:LYS:HG2	2.16	0.45
1:B:85:LEU:HD12	1:B:132:LEU:CD1	2.46	0.45
2:A:88:PRO:CB	2:A:89:PHE:CE1	2.98	0.45
4:A:201:SCR:O5	4:A:201:SCR:H161	2.16	0.45
1:B:160:GLU:OE1	2:A:102:LYS:NZ	2.49	0.45
1:B:44:ARG:CZ	1:B:111:ASN:HA	2.47	0.45
2:A:110:CYS:SG	2:A:116:LEU:CD1	3.05	0.44
1:B:130:PRO:HA	1:B:133:LYS:HD3	1.98	0.44
1:B:45:CYS:N	1:B:108:GLU:OE2	2.44	0.44
1:B:69:HIS:CE1	1:B:75:ALA:HA	2.53	0.44
2:A:107:ARG:NE	4:A:201:SCR:O82	2.51	0.44
2:A:71:GLN:HB2	2:A:94:HIS:ND1	2.33	0.44
1:B:129:GLU:N	1:B:130:PRO:CD	2.81	0.44
2:A:60:VAL:CG2	2:A:61:LEU:N	2.80	0.44
1:B:43:ARG:HB3	1:B:43:ARG:CZ	2.47	0.44
1:B:125:LYS:HG3	1:B:139:TRP:CZ3	2.51	0.44
1:B:128:CYS:C	1:B:130:PRO:HD2	2.38	0.44
1:B:119:GLY:HA2	1:B:165:GLU:HB3	2.00	0.43
1:B:131:VAL:HG12	1:B:135:PHE:HE1	1.83	0.43
2:A:103:LEU:CD2	2:A:104:LYS:O	2.66	0.43
1:B:95:GLN:HA	1:B:98:LEU:HD12	2.01	0.43
1:B:85:LEU:HD23	1:B:85:LEU:O	2.19	0.43
1:B:58:TYR:CD2	1:B:105:MET:HA	2.53	0.43
2:A:107:ARG:NH1	4:A:201:SCR:C1	2.82	0.43
1:B:90:CYS:O	1:B:127:ARG:HD3	2.19	0.43
2:A:48:ILE:C	2:A:48:ILE:HD12	2.39	0.43
1:B:44:ARG:HH21	1:B:44:ARG:HG3	1.83	0.43
1:B:45:CYS:HB2	1:B:60:VAL:HG11	2.00	0.43
1:B:143:LEU:CD2	1:B:143:LEU:N	2.81	0.43
1:B:66:LEU:HG	1:B:104:PRO:CG	2.48	0.43
1:B:45:CYS:SG	1:B:107:THR:N	2.92	0.43
1:B:65:ASN:HD21	1:B:102:TYR:HA	1.84	0.43
1:B:79:LEU:O	1:B:80:THR:C	2.57	0.43
1:B:97:PHE:HE2	1:B:143:LEU:CD1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:O	1:B:97:PHE:HB3	2.19	0.42
2:A:42:HIS:O	2:A:63:ALA:HA	2.19	0.42
2:A:85:LEU:O	2:A:87:GLN:HG3	2.19	0.42
2:A:132:ASN:O	2:A:133:SER:OG	2.33	0.42
1:B:153:ASP:OD2	1:B:156:HIS:CE1	2.73	0.42
1:B:130:PRO:O	1:B:133:LYS:N	2.52	0.42
2:A:107:ARG:CZ	4:A:201:SCR:H1	2.50	0.42
1:B:50:ILE:HG23	1:B:76:GLU:OE2	2.20	0.42
1:B:94:LEU:O	1:B:98:LEU:HD12	2.20	0.42
4:A:201:SCR:H1	4:A:201:SCR:H112	1.81	0.42
1:B:132:LEU:C	1:B:134:GLU:O	2.57	0.42
1:B:73:THR:HG23	1:B:74:ASP:N	2.35	0.41
1:B:97:PHE:HD1	1:B:120:MET:CE	2.33	0.41
2:A:69:CYS:SG	2:A:95:CYS:O	2.78	0.41
4:A:201:SCR:O1	4:A:201:SCR:S2	2.78	0.41
1:B:90:CYS:SG	1:B:128:CYS:N	2.92	0.41
4:A:201:SCR:O24	4:A:201:SCR:H3	2.21	0.41
1:B:125:LYS:HB2	1:B:139:TRP:CH2	2.56	0.41
1:B:65:ASN:HB3	1:B:69:HIS:N	2.35	0.41
2:A:78:LEU:HB2	2:A:87:GLN:O	2.20	0.41
1:B:153:ASP:CG	1:B:156:HIS:ND1	2.74	0.40
1:B:63:MET:HE2	1:B:72:GLN:N	2.36	0.40
1:B:110:ILE:HG13	1:B:111:ASN:H	1.86	0.40
2:A:60:VAL:HG21	2:A:120:TYR:OH	2.19	0.40
1:B:63:MET:CG	1:B:64:PRO:HA	2.51	0.40
2:A:107:ARG:NE	2:A:115:ARG:CD	2.84	0.40
2:A:74:ARG:O	2:A:91:SER:HB2	2.21	0.40
2:A:50:HIS:ND1	2:A:51:PRO:HD2	2.36	0.40
4:A:201:SCR:O51	4:A:201:SCR:C6	2.70	0.40
1:B:132:LEU:HD12	1:B:132:LEU:HA	1.87	0.40
1:B:83:THR:N	1:B:84:PRO:CD	2.85	0.40

All (4) 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)
2:A:107:ARG:NH1	4:A:201:SCR:O51[10 _ 444]	1.75	0.45
2:A:107:ARG:NH1	4:A:201:SCR:C15[10 _ 444]	1.97	0.23
2:A:115:ARG:NH2	4:A:201:SCR:O73[10 _ 444]	2.05	0.15
2:A:107:ARG:CZ	4:A:201:SCR:C16[10 _ 444]	2.14	0.06

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	122/149 (82%)	111 (91%)	11 (9%)	0	100	100
2	A	98/122 (80%)	93 (95%)	4 (4%)	1 (1%)	19	61
All	All	220/271 (81%)	204 (93%)	15 (7%)	1 (0%)	34	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	87	GLN

### 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	B	113/135 (84%)	93 (82%)	20 (18%)	2	11
2	A	93/110 (84%)	68 (73%)	25 (27%)	0	3
All	All	206/245 (84%)	161 (78%)	45 (22%)	1	6

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	ARG
1	B	44	ARG
1	B	46	ASP
1	B	49	ARG
1	B	54	GLN

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Mol	Chain	Res	Type
1	B	63	MET
1	B	76	GLU
1	B	78	GLN
1	B	79	LEU
1	B	87	GLN
1	B	90	CYS
1	B	92	SER
1	B	93	GLN
1	B	129	GLU
1	B	133	LYS
1	B	134	GLU
1	B	143	LEU
1	B	146	SER
1	B	147	LYS
1	B	154	HIS
2	A	45	VAL
2	A	47	SER
2	A	54	LYS
2	A	55	CYS
2	A	57	SER
2	A	61	LEU
2	A	74	ARG
2	A	82	SER
2	A	85	LEU
2	A	86	LYS
2	A	89	PHE
2	A	90	ARG
2	A	100	THR
2	A	106	LEU
2	A	107	ARG
2	A	108	LEU
2	A	109	ARG
2	A	110	CYS
2	A	114	MET
2	A	115	ARG
2	A	117	THR
2	A	121	ARG
2	A	127	HIS
2	A	131	CYS
2	A	132	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	GLN
1	B	95	GLN
2	A	71	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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$
4	SCR	A	201	1,2	55,56,56	1.36	2 (3%)	79,92,92	1.58	15 (18%)
3	NAG	B	201	1	14,14,15	0.69	0	15,19,21	1.36	2 (13%)
3	NAG	B	202	1	14,14,15	0.64	0	15,19,21	0.78	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
4	SCR	A	201	1,2	-	1/49/88/88	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	201	1	-	0/6/23/26	0/1/1/1
3	NAG	B	202	1	1/1/5/7	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	SCR	O3-C3	-2.62	1.40	1.46
4	A	201	SCR	O43-S4	2.09	1.53	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	SCR	C3-C4-C5	-3.63	102.67	110.58
4	A	201	SCR	C4-C3-C2	-3.37	103.05	110.48
4	A	201	SCR	O5-C1-O1	-3.20	99.18	110.01
4	A	201	SCR	O1-C12-O10	-2.65	101.94	110.49
3	B	201	NAG	O7-C7-C8	-2.62	117.25	122.07
4	A	201	SCR	C11-C12-C13	-2.57	109.04	115.27
4	A	201	SCR	C12-O1-C1	-2.49	110.71	117.45
4	A	201	SCR	O10-C15-C16	-2.23	104.39	109.49
4	A	201	SCR	O4-C4-C3	2.05	113.19	108.49
4	A	201	SCR	C2-O2-S2	2.42	123.38	118.77
4	A	201	SCR	O2-C2-C1	3.01	112.00	107.62
4	A	201	SCR	O1-C12-C11	3.48	121.17	109.72
4	A	201	SCR	C1-O5-C5	3.52	120.64	113.74
3	B	201	NAG	C8-C7-N2	3.53	122.87	116.10
4	A	201	SCR	O10-C15-C14	3.65	109.67	103.48
4	A	201	SCR	C14-O71-S13	4.09	126.56	118.77
4	A	201	SCR	C13-O91-S12	4.85	126.73	118.44

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	202	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	SCR	S12-O91-C13-C14

There are no ring outliers.

3 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	201	SCR	27	4
3	B	201	NAG	2	0
3	B	202	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	124/149 (83%)	-0.31	2 (1%) 74 47	80, 113, 144, 164	0
2	A	100/122 (81%)	-0.31	0 100 100	79, 107, 142, 151	0
All	All	224/271 (82%)	-0.31	2 (0%) 85 64	79, 110, 143, 164	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	ASP	3.9
1	B	165	GLU	2.6

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SCR	A	201	55/55	0.85	0.13	-1.74	91,125,150,162	55

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	202	14/15	0.78	0.28	-	98,107,119,120	0
3	NAG	B	201	14/15	0.86	0.27	-	73,87,92,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.