



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:57 PM GMT

PDB ID : 4DY0  
Title : Crystal structure of native protease nexin-1 with heparin  
Authors : Huntington, J.A.; Li, W.  
Deposited on : 2012-02-28  
Resolution : 2.35 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

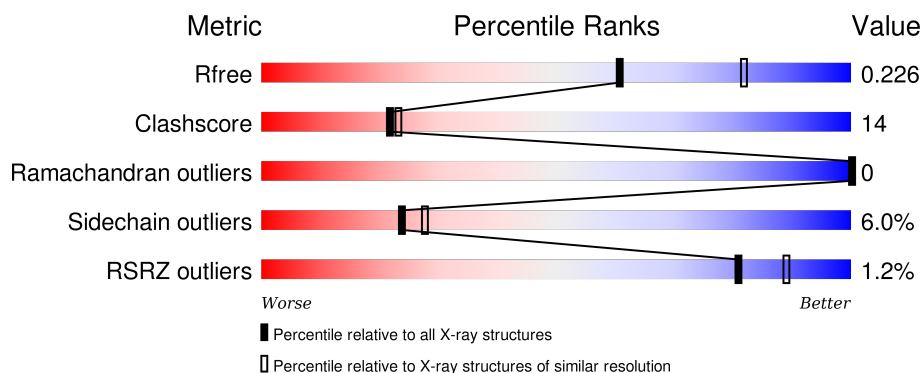
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	A	379	
1	B	379	

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	SO4	A	401	-	-	-	X
3	SGN	A	403	-	-	-	X
4	GOL	B	404	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5947 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 Glia-derived nexin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	1	0
			2759	1780	461	505	13			
1	B	370	Total	C	N	O	S	0	5	0
			2873	1849	485	525	14			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	2	Total	C	N	O	S	0	0
			35	12	1	19	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total	O	0	0
			92	92		
5	B	156	Total	O	0	0
			156	156		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.65Å 140.65Å 93.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.14 – 2.35 68.14 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.14-2.35) 99.9 (68.14-2.35)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.6.0098	Depositor
R, $R_{free}$	0.182 , 0.226 0.180 , 0.226	Depositor DCC
$R_{free}$ test set	1979 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39372 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: GOL, SO4, IDS, SGN

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	0.62	5/2817 (0.2%)	0.54	0/3835
1	B	0.67	4/2932 (0.1%)	0.54	1/3987 (0.0%)
All	All	0.64	9/5749 (0.2%)	0.54	1/7822 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	TYR	CD2-CE2	-7.38	1.28	1.39
1	B	117	CYS	CB-SG	-6.27	1.71	1.82
1	A	197	GLN	CB-CG	-5.79	1.36	1.52
1	B	22	GLN	CB-CG	-5.55	1.37	1.52
1	A	196	TYR	CE1-CZ	-5.46	1.31	1.38
1	A	211	SER	CB-OG	-5.45	1.35	1.42
1	B	22	GLN	CG-CD	-5.18	1.39	1.51
1	A	196	TYR	CD1-CE1	-5.16	1.31	1.39
1	B	117	CYS	C-O	-5.16	1.13	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	GLU	N-CA-C	-5.43	96.33	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	A	2759	0	2723	84	0
1	B	2873	0	2879	74	0
2	A	5	0	0	1	0
2	B	15	0	0	1	0
3	A	35	0	17	3	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
5	A	92	0	0	5	0
5	B	156	0	0	9	0
All	All	5947	0	5635	159	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 14.

All (159) 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)
3:A:402:IDS:O1S	3:A:402:IDS:H1	1.44	1.08
1:A:156:ASP:OD2	1:A:159:LEU:HB2	1.60	1.02
1:B:351:TRP:CE3	1:B:353:ILE:HD11	2.06	0.91
1:A:27[B]:ARG:NE	1:A:30:ASP:OD2	2.04	0.90
1:A:8:LEU:HD21	1:A:69:VAL:CG1	2.01	0.90
1:B:309:THR:HG23	1:B:309:THR:O	1.71	0.88
1:B:351:TRP:HE3	1:B:353:ILE:HD11	1.41	0.83
1:B:118:GLU:OE2	1:B:120:ARG:HD3	1.80	0.81
1:A:25:LYS:HE2	5:A:572:HOH:O	1.80	0.81
1:A:274:LEU:HD23	1:A:275:PRO:HD2	1.61	0.81
1:B:309:THR:CG2	1:B:309:THR:O	2.30	0.79
1:A:8:LEU:HD21	1:A:69:VAL:HG11	1.64	0.78
1:B:192:ASP:HB3	1:B:194:LYS:H	1.48	0.78
1:A:156:ASP:OD2	1:A:159:LEU:CB	2.32	0.77
1:A:45:MET:HE2	1:A:164:LEU:HD12	1.68	0.75
1:B:351:TRP:HE3	1:B:353:ILE:CD1	2.01	0.74
1:A:297:MET:HE3	1:A:298:PHE:CZ	2.25	0.71
1:B:149:LEU:HD12	1:B:321:LEU:HD13	1.74	0.70
1:B:27:ARG:NH1	1:B:30:ASP:OD2	2.25	0.69
1:A:94:ALA:HB2	1:A:137:TRP:CH2	2.29	0.67
1:B:379:PRO:O	5:B:599:HOH:O	2.12	0.67
1:B:192:ASP:HB3	1:B:194:LYS:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:HD21	1:B:73:LEU:HD13	1.77	0.66
1:A:8:LEU:CD2	1:A:69:VAL:CG1	2.74	0.65
1:B:309:THR:HG23	1:B:311:GLY:O	1.96	0.65
1:A:147:ASP:OD1	1:A:148:ASN:N	2.27	0.64
1:B:95:VAL:HG22	1:B:164:LEU:HD13	1.80	0.63
1:B:222:PHE:HE1	1:B:265:MET:HG3	1.64	0.62
1:B:284:ASP:OD1	5:B:563:HOH:O	2.16	0.62
1:A:297:MET:CE	1:A:298:PHE:CZ	2.83	0.62
1:A:362:ILE:HB	1:A:372:PHE:HB2	1.82	0.61
1:A:156:ASP:CG	1:A:159:LEU:HB2	2.21	0.60
1:A:45:MET:HE2	1:A:164:LEU:CD1	2.31	0.60
1:A:156:ASP:OD2	1:A:159:LEU:CG	2.49	0.60
1:B:98:LYS:HD3	1:B:161:ARG:HD3	1.84	0.60
1:B:270:VAL:HG12	1:B:350:PRO:HG2	1.84	0.59
1:B:149:LEU:HD12	1:B:321:LEU:CD1	2.32	0.59
1:A:250:ILE:N	1:A:251:PRO:CD	2.65	0.59
1:B:160:THR:OG1	5:B:564:HOH:O	2.07	0.59
1:B:95:VAL:HG22	1:B:164:LEU:CD1	2.32	0.59
1:B:323:LYS:NZ	2:B:403:SO4:O3	2.31	0.58
1:B:333:THR:HG22	1:B:334:LYS:N	2.19	0.58
1:B:269:ARG:NH2	4:B:404:GOL:O3	2.34	0.58
1:B:165:VAL:HG22	1:B:321:LEU:HD11	1.86	0.58
1:A:8:LEU:HD21	1:A:73:LEU:HD13	1.84	0.57
1:B:61:VAL:HG21	1:B:294:ILE:HG13	1.86	0.57
1:A:218:LEU:HD22	1:B:293:GLY:HA2	1.87	0.57
1:A:274:LEU:HD23	1:A:275:PRO:CD	2.35	0.57
1:B:90:THR:HG21	1:B:142:THR:HA	1.86	0.56
1:A:97:VAL:O	1:A:121:ASN:HA	2.06	0.56
1:A:81:VAL:HG12	1:A:81:VAL:O	2.05	0.55
1:A:225:LEU:N	1:A:225:LEU:HD12	2.21	0.55
1:A:100:ALA:CB	1:A:121:ASN:HB3	2.37	0.55
1:B:148:ASN:ND2	5:B:648:HOH:O	2.22	0.55
3:A:402:IDS:O1S	3:A:402:IDS:C1	2.36	0.55
1:B:351:TRP:CE3	1:B:353:ILE:CD1	2.82	0.55
1:B:138:VAL:HG11	1:B:149:LEU:HD23	1.87	0.55
1:A:95:VAL:CG1	1:A:162:LEU:HD11	2.37	0.55
1:A:8:LEU:CD2	1:A:69:VAL:HG13	2.37	0.55
1:A:21:ASN:O	1:A:25:LYS:HE3	2.07	0.55
1:B:190:ALA:HB3	1:B:192:ASP:HB2	1.89	0.54
1:B:250:ILE:N	1:B:251:PRO:CD	2.70	0.54
1:A:224:GLU:C	1:A:225:LEU:HD12	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ASN:O	1:B:138:VAL:HG12	2.08	0.53
1:B:96:PHE:HB3	1:B:122:VAL:CG1	2.38	0.53
1:A:287:GLU:HB2	1:A:288:PRO:HD3	1.91	0.52
1:B:378:LYS:CB	5:B:585:HOH:O	2.57	0.52
1:B:27:ARG:HB3	1:B:30:ASP:OD2	2.09	0.52
1:A:105:VAL:HB	1:A:106:PRO:HD3	1.92	0.51
1:B:162:LEU:HB2	1:B:316:HIS:O	2.10	0.51
1:A:8:LEU:CD2	1:A:69:VAL:HG11	2.39	0.51
1:B:250:ILE:HB	1:B:251:PRO:HD3	1.91	0.51
1:A:268:LYS:O	1:A:270:VAL:HG23	2.10	0.51
1:B:69:VAL:HG13	1:B:73:LEU:HD22	1.93	0.51
1:B:250:ILE:N	1:B:251:PRO:HD2	2.26	0.51
1:B:48:LEU:CD1	1:B:66:VAL:HG11	2.41	0.51
1:B:378:LYS:HB2	5:B:585:HOH:O	2.11	0.50
1:A:156:ASP:OD2	1:A:159:LEU:HG	2.12	0.50
1:B:105:VAL:N	1:B:106:PRO:CD	2.75	0.50
1:B:124:PHE:O	1:B:157:GLY:HA2	2.12	0.50
1:B:216:ASN:O	1:B:217:ASP:HB2	2.12	0.50
1:A:218:LEU:CD2	1:B:293:GLY:HA2	2.42	0.49
1:A:108:VAL:HA	1:A:119:VAL:HG11	1.93	0.49
1:A:151:SER:HB3	1:A:153:ASP:OD1	2.12	0.49
1:B:147:ASP:OD1	1:B:148:ASN:N	2.38	0.49
1:B:201:LEU:HD22	1:B:330:GLU:HG3	1.95	0.49
1:A:150:LEU:HD12	1:A:150:LEU:N	2.27	0.48
1:A:45:MET:CE	1:A:164:LEU:CD1	2.90	0.48
1:B:95:VAL:HB	1:B:119:VAL:HB	1.94	0.48
1:B:48:LEU:HD13	1:B:66:VAL:HG11	1.96	0.48
1:A:204:LEU:HG	1:A:271:GLN:HG2	1.95	0.48
1:A:222:PHE:HA	1:A:236:ILE:O	2.13	0.48
1:A:119:VAL:HG12	5:A:540:HOH:O	2.14	0.48
1:B:85:ASN:O	1:B:86:LYS:HB2	2.14	0.47
1:A:159:LEU:HA	1:A:159:LEU:HD23	1.45	0.47
1:A:62:MET:O	1:A:63:ARG:HB2	2.14	0.47
1:A:100:ALA:HB3	1:A:121:ASN:HB3	1.95	0.47
1:A:34:ILE:HG22	1:A:35:SER:N	2.29	0.47
1:B:333:THR:CG2	1:B:334:LYS:N	2.77	0.47
1:B:287:GLU:HB2	1:B:288:PRO:HD3	1.96	0.47
1:A:159:LEU:N	1:A:159:LEU:HD23	2.21	0.47
1:B:222:PHE:HA	1:B:236:ILE:O	2.15	0.46
1:B:378:LYS:HA	5:B:585:HOH:O	2.13	0.46
1:A:314:ASN:CB	5:A:541:HOH:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:VAL:CG1	1:A:69:VAL:O	2.64	0.46
1:A:283:THR:HG23	1:A:285:LEU:HD13	1.97	0.46
1:A:108:VAL:HG13	1:A:119:VAL:HG13	1.98	0.46
1:A:200:MET:HG2	1:A:275:PRO:HA	1.97	0.46
1:B:222:PHE:CE1	1:B:265:MET:HG3	2.47	0.46
1:A:250:ILE:O	1:A:253:ILE:HG13	2.16	0.46
1:A:216:ASN:O	1:A:217:ASP:HB2	2.15	0.46
1:A:277:PHE:CE2	1:A:279:ALA:HB2	2.50	0.46
1:B:378:LYS:CA	5:B:585:HOH:O	2.63	0.46
1:B:128:ALA:HA	1:B:152:PRO:HG3	1.98	0.46
1:A:178:PHE:CD2	1:A:201:LEU:HB3	2.50	0.46
1:B:198:VAL:HG13	5:B:541:HOH:O	2.15	0.45
1:B:8:LEU:CD2	1:B:73:LEU:HD13	2.45	0.45
1:B:69:VAL:CG1	1:B:73:LEU:HD22	2.47	0.45
1:A:69:VAL:HG12	1:A:69:VAL:O	2.17	0.45
1:A:225:LEU:CD1	1:A:225:LEU:N	2.79	0.45
1:B:96:PHE:HB3	1:B:122:VAL:HG11	1.99	0.44
1:A:97:VAL:HG11	1:A:103:ILE:HD11	1.99	0.44
1:A:95:VAL:HG13	1:A:162:LEU:HD11	1.99	0.44
1:A:173:LEU:HB2	1:A:228:HIS:ND1	2.33	0.44
1:A:250:ILE:N	1:A:251:PRO:HD3	2.32	0.44
1:A:151:SER:CB	1:A:153:ASP:OD1	2.66	0.44
1:A:42:VAL:HG11	1:A:320:ILE:HG21	2.00	0.44
1:A:179:GLN:HA	1:A:180:PRO:HD3	1.81	0.43
1:A:305:PHE:HB3	1:A:308:ILE:HD12	2.00	0.43
1:A:115:PHE:C	1:A:116:GLN:NE2	2.72	0.43
1:B:310:THR:O	1:B:310:THR:HG22	2.18	0.43
1:B:211:SER:HB3	1:B:221:ASN:OD1	2.18	0.43
1:A:214:ALA:HB1	1:A:215:PRO:HD2	2.01	0.43
1:A:34:ILE:CG2	1:A:35:SER:N	2.81	0.42
1:B:81:VAL:CG1	1:B:81:VAL:O	2.67	0.42
1:A:103:ILE:HG12	1:A:103:ILE:H	1.67	0.42
1:A:146:ILE:HA	2:A:401:SO4:O3	2.18	0.42
1:A:365:ASN:N	1:A:366:PRO:CD	2.82	0.42
1:A:282:GLN:HG2	1:A:283:THR:N	2.33	0.42
1:A:81:VAL:CG1	1:A:81:VAL:O	2.68	0.42
1:B:131:CYS:SG	1:B:155:ILE:HD12	2.60	0.42
1:B:34[A]:ILE:HD13	1:B:34[A]:ILE:HA	1.87	0.42
1:B:137:TRP:CE2	1:B:141:GLU:HG3	2.55	0.42
3:A:402:IDS:C6	3:A:403:SGN:H5	2.49	0.41
1:A:283:THR:HG23	1:A:285:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ILE:O	1:A:262:MET:HG2	2.20	0.41
1:A:67:ASN:HB2	5:A:507:HOH:O	2.20	0.41
1:A:362:ILE:CB	1:A:372:PHE:HB2	2.50	0.41
1:B:81:VAL:HG12	1:B:81:VAL:O	2.20	0.41
1:A:166:ASN:O	1:A:322:GLN:HA	2.20	0.41
1:A:4:ASN:OD1	1:A:4:ASN:C	2.58	0.41
1:B:213:SER:HB3	1:B:219:TRP:CE2	2.56	0.41
1:A:53:ARG:HB3	1:A:296:ASP:OD2	2.19	0.41
1:B:35:SER:HB2	1:B:168[A]:VAL:HG11	2.02	0.41
1:B:34[A]:ILE:CG2	1:B:35:SER:N	2.84	0.41
1:A:100:ALA:H	1:A:121:ASN:HB2	1.86	0.40
1:A:89:VAL:HG22	1:A:170:PHE:CD1	2.56	0.40
1:A:250:ILE:HG13	5:A:530:HOH:O	2.21	0.40
1:B:205:SER:OG	1:B:206:VAL:N	2.54	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	357/379 (94%)	348 (98%)	9 (2%)	0	100	100
1	B	371/379 (98%)	361 (97%)	10 (3%)	0	100	100
All	All	728/758 (96%)	709 (97%)	19 (3%)	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	292/332 (88%)	276 (94%)	16 (6%)	27	32
1	B	311/332 (94%)	291 (94%)	20 (6%)	22	24
All	All	603/664 (91%)	567 (94%)	36 (6%)	24	28

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	53	ARG
1	A	73	LEU
1	A	116	GLN
1	A	119	VAL
1	A	121	ASN
1	A	141	GLU
1	A	197	GLN
1	A	204	LEU
1	A	211	SER
1	A	218	LEU
1	A	271	GLN
1	A	274	LEU
1	A	285	LEU
1	A	331	ASP
1	A	375	GLN
1	B	7	SER
1	B	24	VAL
1	B	27	ARG
1	B	46	LEU
1	B	48	LEU
1	B	67	ASN
1	B	69	VAL
1	B	73	LEU
1	B	118	GLU
1	B	119	VAL
1	B	122	VAL
1	B	156	ASP
1	B	162	LEU
1	B	198	VAL
1	B	268	LYS
1	B	269	ARG
1	B	271	GLN

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Mol	Chain	Res	Type
1	B	310	THR
1	B	314	ASN
1	B	315	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	116	GLN
1	A	271	GLN
1	B	18	GLN
1	B	271	GLN
1	B	377	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 ⓘ

2 carbohydrates 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$
3	IDS	A	402	3	12,16,17	1.23	2 (16%)	14,24,26	0.80	0
3	SGN	A	403	3	16,19,20	4.17	4 (25%)	15,29,31	0.90	1 (6%)

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	IDS	A	402	3	-	1/5/25/29	1/1/1/1
3	SGN	A	403	3	-	0/11/27/31	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	SGN	O4S-S2	2.24	1.53	1.45
3	A	403	SGN	O5S-S2	2.31	1.53	1.45
3	A	402	IDS	O1S-S	2.33	1.53	1.45
3	A	402	IDS	O2S-S	2.61	1.54	1.45
3	A	403	SGN	O1S-S1	11.43	1.53	1.42
3	A	403	SGN	O2S-S1	11.46	1.53	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	SGN	C1-O5-C5	-2.22	109.38	113.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	IDS	S-O2-C2-C1

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	IDS	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	IDS	3	0
3	A	403	SGN	1	0

## 5.6 Ligand geometry

6 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	SO4	A	401	-	4,4,4	0.36	0	6,6,6	0.12	0
4	GOL	A	404	-	5,5,5	0.25	0	5,5,5	0.20	0
2	SO4	B	401	-	4,4,4	0.30	0	6,6,6	0.10	0
2	SO4	B	402	-	4,4,4	0.39	0	6,6,6	0.09	0
2	SO4	B	403	-	4,4,4	0.38	0	6,6,6	0.06	0
4	GOL	B	404	-	5,5,5	0.29	0	5,5,5	0.32	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
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
4	GOL	A	404	-	-	0/4/4/4	0/0/0/0
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0
2	SO4	B	403	-	-	0/0/0/0	0/0/0/0
4	GOL	B	404	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	1	0
2	B	403	SO4	1	0
4	B	404	GOL	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	A	362/379 (95%)	-0.00	8 (2%) 65 77	17, 37, 66, 96	0
1	B	370/379 (97%)	-0.14	1 (0%) 94 97	19, 31, 60, 94	0
All	All	732/758 (96%)	-0.07	9 (1%) 81 89	17, 34, 64, 96	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ASN	2.7
1	A	67	ASN	2.6
1	A	6	LEU	2.4
1	B	72	ILE	2.2
1	A	66	VAL	2.2
1	A	60	MET	2.2
1	A	10	GLU	2.2
1	A	3	PHE	2.1
1	A	68	GLY	2.0

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

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

### 6.3 Carbohydrates [i](#)

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( $\text{\AA}^2$ )	Q<0.9
3	SGN	A	403	19/20	0.66	0.37	5.07	79,136,164,176	0
3	IDS	A	402	16/17	0.57	0.38	-	105,172,206,219	0

## 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	401	5/5	0.94	0.22	9.83	74,80,99,101	0
4	GOL	B	404	6/6	0.80	0.24	5.05	56,76,89,107	0
2	SO4	B	401	5/5	0.99	0.14	1.91	37,39,44,51	0
4	GOL	A	404	6/6	0.87	0.17	1.81	63,72,73,77	0
2	SO4	B	402	5/5	0.97	0.11	-0.51	61,62,72,73	0
2	SO4	B	403	5/5	0.89	0.14	-	67,81,90,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.