



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:45 am GMT

PDB ID : 4IGB  
Title : Crystal structure of the N-terminal domain of the Streptococcus gordonii adhesin Sgo0707  
Authors : Nylander, A.; Svensater, G.; Senadheera, D.B.; Cvitkovitch, D.G.; Davies, J.R.; Persson, K.  
Deposited on : 2012-12-17  
Resolution : 2.09 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

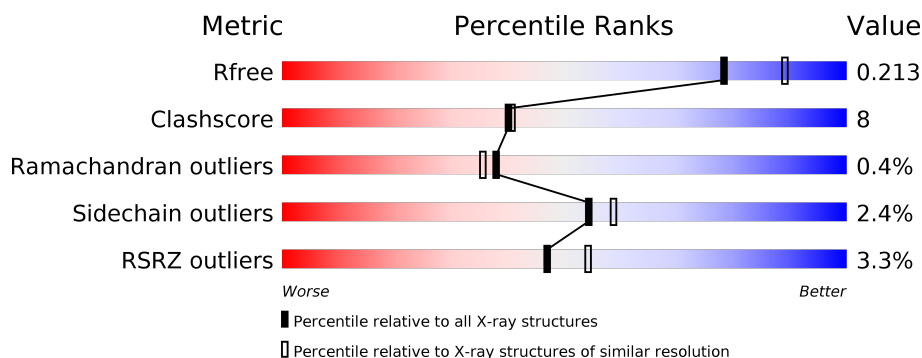
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	430	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>84%</span> <span>15%</span> <span>..</span> </div> </div>
2	B	435	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>3%</span> <span>84%</span> <span>14%</span> <span>.</span> </div> </div>
3	C	436	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>85%</span> <span>13%</span> <span>..</span> </div> </div>
4	D	423	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 7%, orange 1%, yellow 1%, green 91%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>7%</span> <span>80%</span> <span>16%</span> <span>..</span> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	B	501	-	-	-	X
5	SO4	B	502	-	-	-	X
5	SO4	C	502	-	-	-	X
5	SO4	D	502	-	-	-	X
6	GOL	A	503	-	-	-	X
6	GOL	C	503	-	-	-	X
6	GOL	D	503	-	-	X	-
7	ACT	A	504	-	-	-	X
7	ACT	C	504	-	-	X	X
8	NA	D	504	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14782 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 LPXTG cell wall surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	426	3348	2105	547	686	10	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	EXPRESSION TAG	UNP A8AW49
A	-5	TYR	-	EXPRESSION TAG	UNP A8AW49
A	-4	PHE	-	EXPRESSION TAG	UNP A8AW49
A	-3	GLN	-	EXPRESSION TAG	UNP A8AW49
A	-2	GLY	-	EXPRESSION TAG	UNP A8AW49
A	-1	ALA	-	EXPRESSION TAG	UNP A8AW49
A	0	MET	-	EXPRESSION TAG	UNP A8AW49

- Molecule 2 is a protein called LPXTG cell wall surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	435	3417	2146	559	702	10	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	PRO	-	EXPRESSION TAG	UNP A8AW49
B	-10	THR	-	EXPRESSION TAG	UNP A8AW49
B	-9	THR	-	EXPRESSION TAG	UNP A8AW49
B	-8	GLU	-	EXPRESSION TAG	UNP A8AW49
B	-7	ASN	-	EXPRESSION TAG	UNP A8AW49
B	-6	LEU	-	EXPRESSION TAG	UNP A8AW49
B	-5	TYR	-	EXPRESSION TAG	UNP A8AW49
B	-4	PHE	-	EXPRESSION TAG	UNP A8AW49
B	-3	GLN	-	EXPRESSION TAG	UNP A8AW49

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	EXPRESSION TAG	UNP A8AW49
B	-1	ALA	-	EXPRESSION TAG	UNP A8AW49
B	0	MET	-	EXPRESSION TAG	UNP A8AW49

- Molecule 3 is a protein called LPXTG cell wall surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	433	Total	C	N	O	S	0	0	0
			3395	2132	556	697	10			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	ILE	-	EXPRESSION TAG	UNP A8AW49
C	-11	PRO	-	EXPRESSION TAG	UNP A8AW49
C	-10	THR	-	EXPRESSION TAG	UNP A8AW49
C	-9	THR	-	EXPRESSION TAG	UNP A8AW49
C	-8	GLU	-	EXPRESSION TAG	UNP A8AW49
C	-7	ASN	-	EXPRESSION TAG	UNP A8AW49
C	-6	LEU	-	EXPRESSION TAG	UNP A8AW49
C	-5	TYR	-	EXPRESSION TAG	UNP A8AW49
C	-4	PHE	-	EXPRESSION TAG	UNP A8AW49
C	-3	GLN	-	EXPRESSION TAG	UNP A8AW49
C	-2	GLY	-	EXPRESSION TAG	UNP A8AW49
C	-1	ALA	-	EXPRESSION TAG	UNP A8AW49
C	0	MET	-	EXPRESSION TAG	UNP A8AW49

- Molecule 4 is a protein called LPXTG cell wall surface protein.

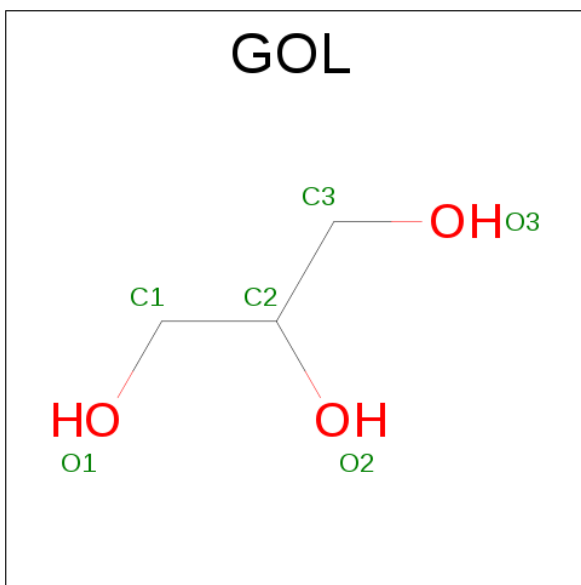
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	416	Total	C	N	O	S	0	0	0
			3264	2049	536	670	9			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



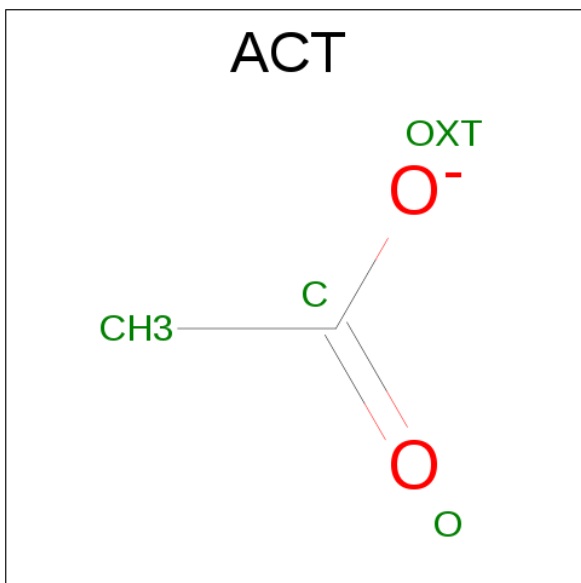
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Na 1 1	0	0
8	A	1	Total Na 1 1	0	0
8	D	1	Total Na 1 1	0	0
8	C	1	Total Na 1 1	0	0

- Molecule 9 is water.

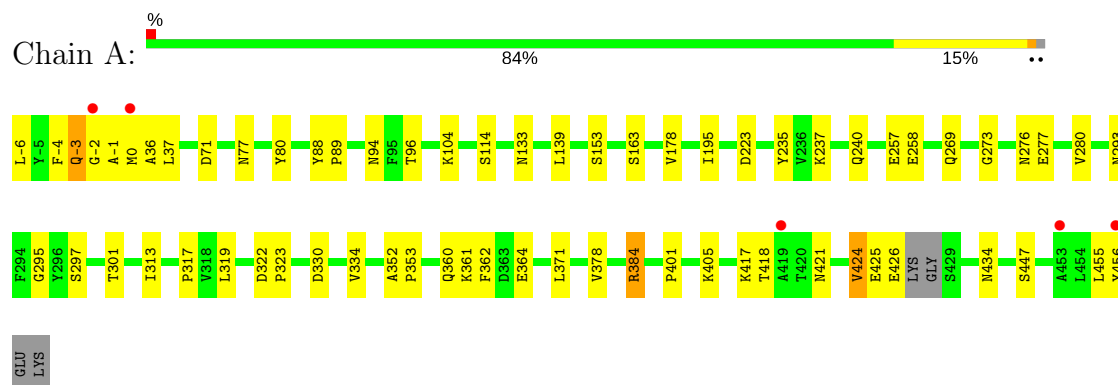
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	408	Total O 408 408	0	0
9	B	352	Total O 352 352	0	0
9	C	267	Total O 267 267	0	0
9	D	255	Total O 255 255	0	0



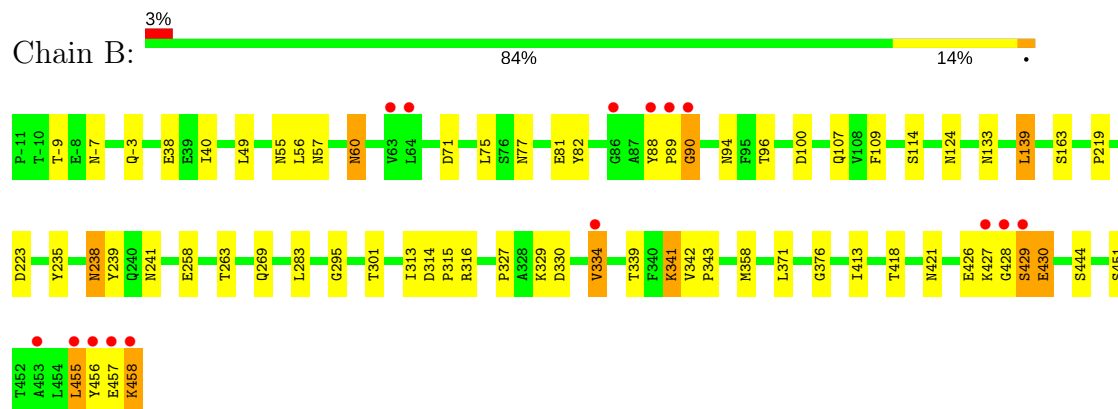
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

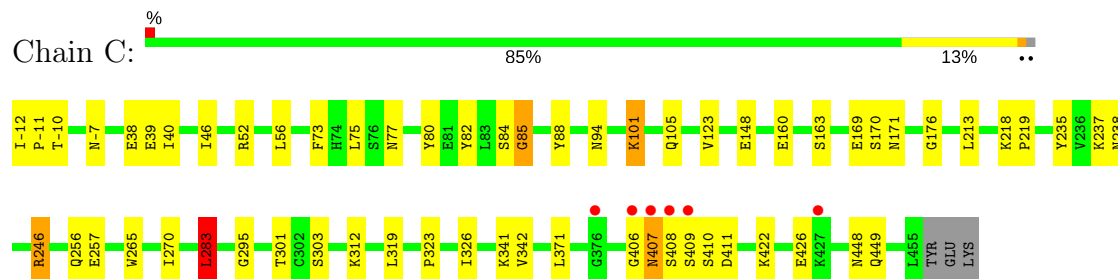
- Molecule 1: LPXTG cell wall surface protein



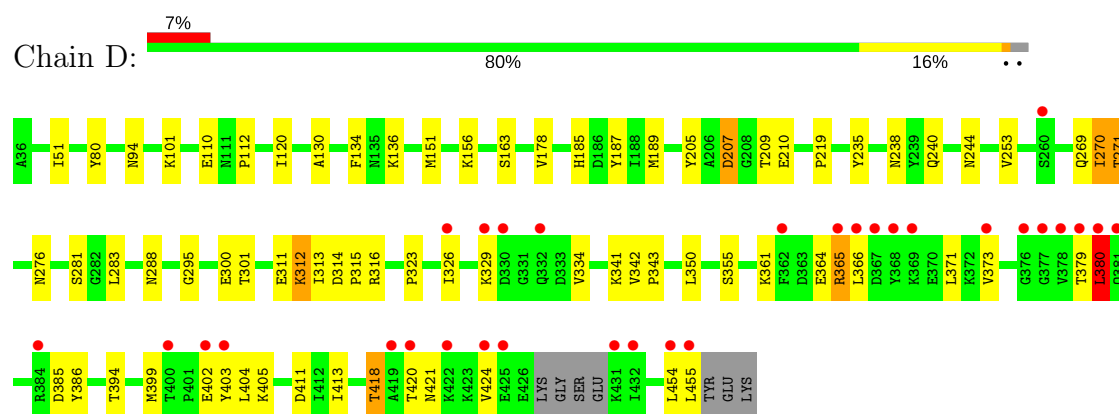
- Molecule 2: LPXTG cell wall surface protein



- Molecule 3: LPXTG cell wall surface protein



- Molecule 4: LPXTG cell wall surface protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.13Å 158.12Å 164.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.07 – 2.09 48.45 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.5 (41.07-2.09) 98.2 (48.45-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.08Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, $R_{free}$	0.179 , 0.225 0.169 , 0.213	Depositor DCC
$R_{free}$ test set	5754 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14782	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, ACT, SO4, NA

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	0.41	0/3407	0.58	0/4622
2	B	0.38	0/3478	0.54	0/4718
3	C	0.36	0/3455	0.54	1/4689 (0.0%)
4	D	0.35	0/3320	0.55	0/4505
All	All	0.38	0/13660	0.55	1/18534 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	283	LEU	CA-CB-CG	5.45	127.83	115.30

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	3348	0	3261	54	0
2	B	3417	0	3330	53	0
3	C	3395	0	3313	47	0
4	D	3264	0	3184	69	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	10	0	0	0	0
5	D	10	0	0	1	0
6	A	6	0	8	3	0
6	B	6	0	8	1	0
6	C	6	0	8	0	0
6	D	6	0	8	5	0
7	A	4	0	3	1	0
7	C	4	0	3	3	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	408	0	0	4	0
9	B	352	0	0	3	0
9	C	267	0	0	2	0
9	D	255	0	0	5	0
All	All	14782	0	13126	220	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 8.

All (220) 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:B:457:GLU:O	2:B:458:LYS:HB2	1.57	1.01
1:A:313:ILE:H	6:A:503:GOL:H12	1.26	0.98
3:C:319:LEU:H	3:C:448:ASN:HD21	1.18	0.92
1:A:237:LYS:HZ3	1:A:293:ASN:HD21	0.93	0.91
2:B:38:GLU:OE2	2:B:40:ILE:HD11	1.74	0.87
3:C:-12:ILE:O	3:C:-10:THR:HG23	1.74	0.86
3:C:169:GLU:OE2	9:C:834:HOH:O	1.95	0.85
1:A:-6:LEU:HD23	1:A:-4:PHE:H	1.45	0.81
4:D:314:ASP:OD1	4:D:315:PRO:HA	1.81	0.81
1:A:-1:ALA:O	1:A:0:MET:HG3	1.80	0.81
4:D:334:VAL:O	4:D:418:THR:HG22	1.81	0.79
1:A:421:ASN:O	1:A:424:VAL:HG22	1.82	0.79
4:D:271:THR:HG21	4:D:281:SER:OG	1.84	0.78
2:B:457:GLU:O	2:B:458:LYS:CB	2.32	0.78
1:A:237:LYS:NZ	1:A:293:ASN:HD21	1.78	0.77
2:B:100:ASP:H	2:B:107:GLN:HE22	1.31	0.77
1:A:37:LEU:HD23	3:C:-7:ASN:ND2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:316:ARG:HH22	6:D:503:GOL:H11	1.51	0.76
1:A:237:LYS:HZ3	1:A:293:ASN:ND2	1.78	0.74
1:A:313:ILE:H	6:A:503:GOL:C1	1.99	0.74
3:C:246:ARG:HH21	3:C:256:GLN:HE22	1.36	0.73
2:B:427:LYS:HA	2:B:428:GLY:C	2.08	0.73
4:D:366:LEU:HD13	4:D:418:THR:HG21	1.71	0.73
3:C:246:ARG:C	3:C:246:ARG:HD2	2.09	0.72
1:A:313:ILE:N	6:A:503:GOL:H12	2.04	0.72
3:C:73:PHE:HE1	3:C:75:LEU:HD11	1.58	0.69
2:B:334:VAL:HG22	2:B:418:THR:OG1	1.92	0.69
4:D:420:THR:HB	4:D:424:VAL:HG11	1.75	0.68
3:C:38:GLU:OE2	3:C:40:ILE:HD11	1.94	0.67
4:D:373:VAL:HG22	4:D:380:LEU:HD22	1.76	0.66
4:D:270:ILE:HD13	4:D:271:THR:N	2.11	0.66
4:D:316:ARG:HH22	6:D:503:GOL:C1	2.08	0.66
2:B:427:LYS:HG2	2:B:429:SER:HB2	1.80	0.64
2:B:429:SER:OG	2:B:430:GLU:HA	1.98	0.63
3:C:56:LEU:H	3:C:171:ASN:HB3	1.64	0.62
1:A:-1:ALA:O	1:A:0:MET:CG	2.47	0.62
4:D:421:ASN:O	4:D:424:VAL:HG22	2.00	0.62
3:C:-7:ASN:HB3	3:C:39:GLU:HB2	1.81	0.62
4:D:379:THR:HG22	4:D:379:THR:O	1.99	0.62
2:B:427:LYS:HA	2:B:428:GLY:O	1.99	0.61
2:B:339:THR:HG23	2:B:413:ILE:CD1	2.31	0.61
2:B:427:LYS:HE2	2:B:429:SER:OG	2.01	0.61
3:C:303:SER:OG	7:C:504:ACT:H3	2.00	0.61
4:D:210:GLU:H	4:D:210:GLU:CD	2.04	0.60
2:B:426:GLU:O	2:B:428:GLY:HA3	2.01	0.60
3:C:256:GLN:HE21	3:C:265:TRP:HE1	1.49	0.60
3:C:94:ASN:HD22	3:C:163:SER:HB3	1.65	0.60
2:B:371:LEU:C	2:B:371:LEU:HD12	2.22	0.59
3:C:301:THR:O	3:C:301:THR:HG23	2.02	0.59
2:B:77:ASN:HA	2:B:88:TYR:O	2.02	0.59
3:C:341:LYS:HG2	3:C:411:ASP:OD1	2.03	0.59
4:D:420:THR:HB	4:D:424:VAL:CG1	2.33	0.59
4:D:373:VAL:CG2	4:D:380:LEU:HD22	2.33	0.58
4:D:402:GLU:O	4:D:405:LYS:HG2	2.03	0.58
2:B:427:LYS:HG2	2:B:429:SER:CB	2.34	0.58
2:B:57:ASN:H	2:B:60:ASN:HD21	1.52	0.58
4:D:364:GLU:O	4:D:365:ARG:HB2	2.03	0.58
4:D:402:GLU:HA	4:D:405:LYS:HE3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:380:LEU:HD23	4:D:386:TYR:HD2	1.69	0.58
4:D:51:ILE:HA	9:D:831:HOH:O	2.04	0.57
1:A:319:LEU:HD21	1:A:434:ASN:HD22	1.70	0.57
4:D:219:PRO:HD2	4:D:283:LEU:O	2.05	0.57
4:D:207:ASP:HB3	4:D:209:THR:H	1.70	0.56
3:C:246:ARG:HD2	3:C:246:ARG:O	2.05	0.56
1:A:94:ASN:HD22	1:A:163:SER:HB3	1.71	0.56
4:D:244:ASN:HB2	4:D:288:ASN:ND2	2.20	0.56
1:A:114:SER:HB2	1:A:133:ASN:ND2	2.21	0.56
3:C:406:GLY:C	3:C:408:SER:H	2.09	0.56
2:B:239:TYR:HD2	2:B:263:THR:HG1	1.54	0.56
2:B:429:SER:CB	2:B:430:GLU:HA	2.34	0.56
3:C:407:ASN:H	3:C:407:ASN:HD22	1.52	0.56
3:C:270:ILE:H	3:C:270:ILE:HD12	1.70	0.56
2:B:124:ASN:HA	2:B:316:ARG:HD2	1.88	0.55
2:B:456:TYR:O	2:B:457:GLU:HG3	2.05	0.55
3:C:73:PHE:CE1	3:C:75:LEU:HD11	2.41	0.55
3:C:-11:PRO:HD3	4:D:276:ASN:OD1	2.07	0.55
3:C:256:GLN:NE2	3:C:265:TRP:HE1	2.05	0.55
3:C:371:LEU:HD12	3:C:371:LEU:C	2.28	0.54
1:A:77:ASN:HA	1:A:88:TYR:O	2.08	0.54
4:D:334:VAL:HB	4:D:418:THR:CG2	2.37	0.54
4:D:314:ASP:OD1	4:D:315:PRO:CA	2.54	0.54
1:A:360:GLN:HE21	1:A:361:LYS:H	1.55	0.53
2:B:109:PHE:HE1	2:B:139:LEU:HD22	1.73	0.53
3:C:319:LEU:H	3:C:448:ASN:ND2	1.98	0.53
4:D:253:VAL:HG21	4:D:269:GLN:HG2	1.91	0.53
4:D:94:ASN:HD22	4:D:163:SER:HB3	1.73	0.53
4:D:399:MET:HB2	4:D:404:LEU:HD11	1.91	0.53
2:B:109:PHE:CE1	2:B:139:LEU:HD22	2.42	0.53
1:A:269:GLN:HG3	9:A:704:HOH:O	2.08	0.53
3:C:323:PRO:HG2	3:C:326:ILE:HG22	1.91	0.53
4:D:244:ASN:HB2	4:D:288:ASN:HD22	1.75	0.52
4:D:364:GLU:O	4:D:365:ARG:CB	2.57	0.52
1:A:0:MET:SD	1:A:36:ALA:N	2.82	0.52
2:B:313:ILE:HB	6:B:503:GOL:H2	1.92	0.52
3:C:342:VAL:HG11	3:C:409:SER:HA	1.92	0.52
1:A:114:SER:OG	7:A:504:ACT:H3	2.08	0.52
4:D:120:ILE:HD13	4:D:130:ALA:HB2	1.92	0.52
1:A:258:GLU:HG3	9:C:754:HOH:O	2.10	0.52
1:A:360:GLN:HG2	1:A:362:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-6:LEU:HB3	1:A:-3:GLN:HG3	1.91	0.51
4:D:373:VAL:O	4:D:380:LEU:HB3	2.11	0.51
2:B:329:LYS:NZ	2:B:458:LYS:HG2	2.26	0.51
3:C:246:ARG:NH2	3:C:256:GLN:HE22	2.08	0.51
1:A:371:LEU:C	1:A:371:LEU:HD12	2.31	0.51
4:D:112:PRO:HD2	4:D:134:PHE:O	2.11	0.51
1:A:257:GLU:HG3	3:C:257:GLU:OE2	2.11	0.51
3:C:77:ASN:HA	3:C:88:TYR:O	2.10	0.51
2:B:223:ASP:HB2	2:B:269:GLN:O	2.11	0.50
4:D:316:ARG:NH1	6:D:503:GOL:O1	2.40	0.50
1:A:384:ARG:HD2	9:A:674:HOH:O	2.11	0.50
4:D:205:TYR:HB3	4:D:207:ASP:HB2	1.94	0.50
4:D:312:LYS:HG3	9:D:821:HOH:O	2.10	0.50
1:A:301:THR:HG23	1:A:301:THR:O	2.11	0.50
2:B:235:TYR:CZ	2:B:295:GLY:HA3	2.46	0.49
4:D:341:LYS:HD2	4:D:411:ASP:OD1	2.12	0.49
2:B:55:ASN:C	2:B:56:LEU:HD12	2.33	0.49
1:A:-6:LEU:HD23	1:A:-4:PHE:N	2.22	0.49
2:B:330:ASP:OD1	2:B:421:ASN:HA	2.13	0.49
5:D:501:SO4:O2	9:D:748:HOH:O	2.19	0.49
2:B:81:GLU:HG2	2:B:82:TYR:CD2	2.49	0.48
4:D:311:GLU:O	6:D:503:GOL:H12	2.13	0.48
3:C:246:ARG:HH21	3:C:256:GLN:NE2	2.07	0.48
4:D:316:ARG:NH2	6:D:503:GOL:H11	2.25	0.48
4:D:380:LEU:HD23	4:D:386:TYR:CD2	2.48	0.48
4:D:380:LEU:HD11	4:D:403:TYR:CE1	2.48	0.48
2:B:314:ASP:O	2:B:341:LYS:HE2	2.13	0.48
4:D:326:ILE:HG13	4:D:454:LEU:HD23	1.96	0.48
4:D:329:LYS:C	4:D:424:VAL:HG21	2.34	0.48
3:C:80:TYR:OH	7:C:504:ACT:H1	2.14	0.47
1:A:240:GLN:HE22	3:C:-7:ASN:HD22	1.62	0.47
4:D:185:HIS:HA	4:D:187:TYR:CE1	2.49	0.47
4:D:380:LEU:CD2	4:D:386:TYR:HD2	2.25	0.47
3:C:94:ASN:ND2	3:C:160:GLU:OE2	2.37	0.47
2:B:57:ASN:H	2:B:60:ASN:ND2	2.12	0.47
4:D:355:SER:HA	4:D:404:LEU:HD21	1.96	0.47
1:A:223:ASP:HB2	1:A:269:GLN:O	2.13	0.47
1:A:71:ASP:HB3	1:A:96:THR:OG1	2.13	0.47
3:C:235:TYR:CZ	3:C:295:GLY:HA3	2.49	0.47
4:D:80:TYR:CZ	4:D:178:VAL:HG11	2.50	0.47
4:D:156:LYS:HB3	4:D:189:MET:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-2:GLY:O	1:A:-1:ALA:C	2.53	0.46
3:C:123:VAL:HG11	3:C:213:LEU:HD21	1.97	0.46
2:B:458:LYS:HD2	2:B:458:LYS:HA	1.65	0.46
1:A:114:SER:CB	1:A:133:ASN:HD22	2.29	0.46
2:B:327:PRO:HB2	2:B:329:LYS:HD2	1.97	0.46
1:A:114:SER:HB2	1:A:133:ASN:HD22	1.79	0.46
3:C:408:SER:C	3:C:410:SER:H	2.19	0.46
3:C:270:ILE:N	3:C:270:ILE:HD12	2.30	0.46
4:D:334:VAL:HB	4:D:418:THR:HG22	1.98	0.45
1:A:-6:LEU:HB3	1:A:-3:GLN:CG	2.45	0.45
2:B:-3:GLN:HG2	2:B:241:ASN:HD21	1.81	0.45
3:C:52:ARG:HB2	3:C:312:LYS:HD2	1.99	0.45
4:D:379:THR:O	4:D:380:LEU:O	2.35	0.45
4:D:323:PRO:HG2	4:D:326:ILE:HG22	1.99	0.45
2:B:81:GLU:HG2	2:B:82:TYR:CE2	2.51	0.45
2:B:219:PRO:HD2	2:B:283:LEU:O	2.17	0.45
4:D:235:TYR:CZ	4:D:295:GLY:HA3	2.51	0.44
4:D:413:ILE:HD12	9:D:720:HOH:O	2.17	0.44
2:B:334:VAL:HG22	2:B:418:THR:HG1	1.82	0.44
2:B:94:ASN:HD22	2:B:163:SER:HB3	1.83	0.44
1:A:104:LYS:HE3	9:A:897:HOH:O	2.17	0.44
1:A:235:TYR:CZ	1:A:295:GLY:HA3	2.53	0.44
2:B:258:GLU:HG2	2:B:263:THR:OG1	2.18	0.44
1:A:273:GLY:O	1:A:277:GLU:HG3	2.18	0.43
3:C:101:LYS:HG2	3:C:101:LYS:H	1.53	0.43
1:A:195:ILE:O	1:A:297:SER:HA	2.18	0.43
1:A:322:ASP:HA	1:A:323:PRO:HA	1.87	0.43
4:D:373:VAL:HA	4:D:413:ILE:O	2.17	0.43
4:D:94:ASN:ND2	4:D:163:SER:HB3	2.33	0.43
4:D:238:ASN:OD1	4:D:240:GLN:NE2	2.52	0.43
1:A:-6:LEU:HD22	1:A:-3:GLN:HG2	2.00	0.43
1:A:139:LEU:HD12	1:A:195:ILE:HG22	1.99	0.42
4:D:301:THR:HG23	4:D:301:THR:O	2.19	0.42
1:A:425:GLU:O	1:A:426:GLU:C	2.57	0.42
1:A:317:PRO:HB2	1:A:447:SER:HB3	2.00	0.42
2:B:358:MET:N	2:B:358:MET:SD	2.92	0.42
4:D:364:GLU:HG2	9:D:760:HOH:O	2.19	0.42
3:C:219:PRO:HD2	3:C:283:LEU:O	2.20	0.42
1:A:80:TYR:CZ	1:A:178:VAL:HG11	2.55	0.42
2:B:427:LYS:CE	2:B:429:SER:OG	2.66	0.42
2:B:455:LEU:HD12	2:B:455:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLN:HE21	1:A:361:LYS:N	2.17	0.42
1:A:360:GLN:CG	1:A:362:PHE:CZ	3.02	0.42
1:A:401:PRO:O	1:A:405:LYS:HG3	2.20	0.42
2:B:376:GLY:HA2	9:B:734:HOH:O	2.20	0.42
3:C:82:TYR:O	3:C:85:GLY:N	2.53	0.42
2:B:89:PRO:HA	2:B:90:GLY:HA2	1.69	0.42
3:C:170:SER:O	3:C:171:ASN:C	2.57	0.42
4:D:101:LYS:HE2	4:D:151:MET:O	2.20	0.42
4:D:371:LEU:HD12	4:D:371:LEU:C	2.40	0.42
1:A:334:VAL:HG22	1:A:418:THR:OG1	2.19	0.42
4:D:271:THR:HG21	4:D:281:SER:HG	1.83	0.42
2:B:71:ASP:HB3	2:B:96:THR:OG1	2.20	0.41
4:D:361:LYS:HD3	4:D:394:THR:OG1	2.19	0.41
1:A:417:LYS:HD2	9:A:842:HOH:O	2.19	0.41
1:A:88:TYR:HA	1:A:89:PRO:HD3	1.80	0.41
2:B:316:ARG:CZ	9:B:833:HOH:O	2.68	0.41
1:A:455:LEU:O	1:A:456:TYR:HB2	2.21	0.41
3:C:176:GLY:HA3	3:C:303:SER:HB3	2.03	0.41
1:A:276:ASN:O	1:A:280:VAL:HB	2.21	0.41
1:A:352:ALA:HA	1:A:353:PRO:HD3	1.90	0.41
4:D:365:ARG:O	4:D:420:THR:HA	2.21	0.41
3:C:406:GLY:C	3:C:408:SER:N	2.72	0.41
4:D:300:GLU:HG3	4:D:301:THR:HG22	2.01	0.41
2:B:301:THR:O	2:B:301:THR:HG23	2.20	0.41
2:B:-9:THR:HG22	9:B:867:HOH:O	2.21	0.41
2:B:315:PRO:HD2	2:B:341:LYS:HG3	2.03	0.41
1:A:330:ASP:OD1	1:A:421:ASN:HA	2.22	0.41
2:B:114:SER:HB2	2:B:133:ASN:OD1	2.20	0.41
4:D:313:ILE:HB	4:D:316:ARG:NH1	2.35	0.41
3:C:46:ILE:HG22	3:C:218:LYS:HD2	2.03	0.40
4:D:342:VAL:HA	4:D:343:PRO:HD3	1.93	0.40
4:D:380:LEU:HD21	4:D:385:ASP:HB3	2.03	0.40
2:B:238:ASN:HA	2:B:238:ASN:HD22	1.69	0.40
3:C:237:LYS:HE2	3:C:237:LYS:HB3	1.90	0.40
4:D:110:GLU:OE2	4:D:136:LYS:HE2	2.22	0.40
3:C:80:TYR:OH	7:C:504:ACT:CH3	2.69	0.40
4:D:207:ASP:HB3	4:D:209:THR:HG23	2.02	0.40
2:B:235:TYR:CE2	2:B:295:GLY:HA3	2.57	0.40
2:B:342:VAL:HA	2:B:343:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

## 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	A	422/430 (98%)	403 (96%)	18 (4%)	1 (0%)	51	52
2	B	433/435 (100%)	413 (95%)	19 (4%)	1 (0%)	51	52
3	C	431/436 (99%)	407 (94%)	21 (5%)	3 (1%)	25	20
4	D	412/423 (97%)	389 (94%)	21 (5%)	2 (0%)	32	28
All	All	1698/1724 (98%)	1612 (95%)	79 (5%)	7 (0%)	38	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	365	ARG
4	D	380	LEU
3	C	407	ASN
3	C	426	GLU
1	A	364	GLU
3	C	85	GLY
2	B	90	GLY

### 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	377/380 (99%)	372 (99%)	5 (1%)	73	80
2	B	385/385 (100%)	371 (96%)	14 (4%)	40	41
3	C	383/386 (99%)	374 (98%)	9 (2%)	56	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	369/375 (98%)	361 (98%)	8 (2%)	57	62
All	All	1514/1526 (99%)	1478 (98%)	36 (2%)	54	59

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

Mol	Chain	Res	Type
1	A	-3	GLN
1	A	153	SER
1	A	378	VAL
1	A	384	ARG
1	A	424	VAL
2	B	-7	ASN
2	B	49	LEU
2	B	60	ASN
2	B	75	LEU
2	B	139	LEU
2	B	238	ASN
2	B	334	VAL
2	B	341	LYS
2	B	429	SER
2	B	430	GLU
2	B	444	SER
2	B	451	SER
2	B	455	LEU
2	B	458	LYS
3	C	84	SER
3	C	101	LYS
3	C	105	GLN
3	C	148	GLU
3	C	238	ASN
3	C	246	ARG
3	C	283	LEU
3	C	422	LYS
3	C	449	GLN
4	D	207	ASP
4	D	270	ILE
4	D	271	THR
4	D	312	LYS
4	D	350	LEU
4	D	380	LEU
4	D	418	THR
4	D	455	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	111	ASN
1	A	133	ASN
1	A	293	ASN
1	A	360	GLN
1	A	434	ASN
2	B	60	ASN
2	B	94	ASN
2	B	107	GLN
2	B	152	ASN
2	B	185	HIS
2	B	238	ASN
2	B	241	ASN
2	B	407	ASN
3	C	-7	ASN
3	C	59	ASN
3	C	94	ASN
3	C	105	GLN
3	C	238	ASN
3	C	241	ASN
3	C	250	ASN
3	C	256	GLN
3	C	293	ASN
3	C	381	GLN
3	C	407	ASN
3	C	448	ASN
3	C	449	GLN
4	D	94	ASN
4	D	288	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z  > 2$
5	SO4	A	501	-	4,4,4	0.11	0	6,6,6	0.18	0
5	SO4	A	502	8	4,4,4	0.14	0	6,6,6	0.17	0
6	GOL	A	503	-	5,5,5	0.36	0	5,5,5	0.54	0
7	ACT	A	504	-	1,3,3	1.51	0	0,3,3	0.00	-
5	SO4	B	501	-	4,4,4	0.11	0	6,6,6	0.19	0
5	SO4	B	502	8	4,4,4	0.15	0	6,6,6	0.13	0
6	GOL	B	503	-	5,5,5	0.29	0	5,5,5	0.59	0
5	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.13	0
5	SO4	C	502	8	4,4,4	0.14	0	6,6,6	0.05	0
6	GOL	C	503	-	5,5,5	0.29	0	5,5,5	0.57	0
7	ACT	C	504	-	1,3,3	2.03	1 (100%)	0,3,3	0.00	-
5	SO4	D	501	-	4,4,4	0.08	0	6,6,6	0.21	0
5	SO4	D	502	-	4,4,4	0.31	0	6,6,6	0.22	0
6	GOL	D	503	-	5,5,5	0.29	0	5,5,5	0.56	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
5	SO4	A	501	-	-	0/0/0/0	0/0/0/0
5	SO4	A	502	8	-	0/0/0/0	0/0/0/0
6	GOL	A	503	-	-	0/4/4/4	0/0/0/0
7	ACT	A	504	-	-	0/0/0/0	0/0/0/0
5	SO4	B	501	-	-	0/0/0/0	0/0/0/0
5	SO4	B	502	8	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	503	-	-	0/4/4/4	0/0/0/0
5	SO4	C	501	-	-	0/0/0/0	0/0/0/0
5	SO4	C	502	8	-	0/0/0/0	0/0/0/0
6	GOL	C	503	-	-	0/4/4/4	0/0/0/0
7	ACT	C	504	-	-	0/0/0/0	0/0/0/0
5	SO4	D	501	-	-	0/0/0/0	0/0/0/0
5	SO4	D	502	-	-	0/0/0/0	0/0/0/0
6	GOL	D	503	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	504	ACT	CH3-C	2.03	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	503	GOL	3	0
7	A	504	ACT	1	0
6	B	503	GOL	1	0
7	C	504	ACT	3	0
5	D	501	SO4	1	0
6	D	503	GOL	5	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, 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	426/430 (99%)	0.30	5 (1%) 79 82	12, 25, 45, 89	0
2	B	435/435 (100%)	0.32	15 (3%) 46 53	14, 26, 48, 112	0
3	C	433/436 (99%)	0.13	6 (1%) 75 79	14, 28, 49, 89	0
4	D	416/423 (98%)	0.40	31 (7%) 15 19	16, 29, 53, 88	0
All	All	1710/1724 (99%)	0.28	57 (3%) 47 54	12, 27, 49, 112	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	428	GLY	7.1
4	D	455	LEU	5.3
2	B	427	LYS	5.0
1	A	0	MET	4.0
4	D	432	ILE	3.8
4	D	376	GLY	3.8
2	B	458	LYS	3.6
4	D	369	LYS	3.5
1	A	456	TYR	3.5
4	D	381	GLN	3.5
3	C	408	SER	3.4
4	D	366	LEU	3.1
4	D	454	LEU	3.1
4	D	362	PHE	3.1
4	D	378	VAL	3.1
2	B	456	TYR	3.0
3	C	409	SER	2.9
2	B	429	SER	2.9
4	D	403	TYR	2.9
4	D	384	ARG	2.8
1	A	453	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	373	VAL	2.7
4	D	380	LEU	2.7
4	D	326	ILE	2.7
2	B	89	PRO	2.7
2	B	453	ALA	2.7
3	C	406	GLY	2.6
4	D	260	SER	2.6
4	D	422	LYS	2.6
4	D	402	GLU	2.6
2	B	455	LEU	2.5
1	A	-2	GLY	2.5
3	C	427	LYS	2.5
2	B	86	GLY	2.4
4	D	431	LYS	2.4
4	D	368	TYR	2.4
4	D	365	ARG	2.4
4	D	367	ASP	2.4
3	C	376	GLY	2.4
4	D	419	ALA	2.4
4	D	424	VAL	2.4
4	D	329	LYS	2.4
3	C	407	ASN	2.4
1	A	419	ALA	2.3
2	B	334	VAL	2.3
4	D	400	THR	2.2
2	B	64	LEU	2.2
4	D	420	THR	2.2
4	D	425	GLU	2.2
4	D	379	THR	2.2
2	B	88	TYR	2.1
4	D	377	GLY	2.1
2	B	457	GLU	2.1
4	D	332	GLN	2.1
4	D	330	ASP	2.1
2	B	90	GLY	2.1
2	B	63	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
5	SO4	D	502	5/5	0.85	0.36	15.82	43,60,74,78	5
5	SO4	C	502	5/5	0.76	0.27	9.97	54,60,74,75	5
6	GOL	A	503	6/6	0.83	0.27	9.26	20,28,30,32	6
7	ACT	A	504	4/4	0.90	0.39	8.57	28,30,37,55	4
8	NA	D	504	1/1	0.73	0.26	8.42	49,49,49,49	0
5	SO4	B	502	5/5	0.92	0.22	7.16	29,42,53,57	5
5	SO4	B	501	5/5	0.92	0.21	5.47	38,48,55,79	5
6	GOL	C	503	6/6	0.77	0.21	5.06	45,51,63,75	0
7	ACT	C	504	4/4	0.75	0.20	4.11	25,37,52,55	0
6	GOL	B	503	6/6	0.94	0.16	1.54	20,27,32,33	6
6	GOL	D	503	6/6	0.80	0.20	1.40	33,47,52,58	6
5	SO4	A	502	5/5	0.94	0.19	0.19	23,28,36,44	5
8	NA	B	504	1/1	0.90	0.11	-0.51	31,31,31,31	1
8	NA	A	505	1/1	0.96	0.11	-2.09	29,29,29,29	0
5	SO4	D	501	5/5	0.92	0.25	-	35,36,47,61	5
5	SO4	A	501	5/5	0.98	0.13	-	27,27,36,42	5
5	SO4	C	501	5/5	0.94	0.19	-	35,38,45,47	5
8	NA	C	505	1/1	0.28	0.33	-	40,40,40,40	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.