



# Full wwPDB X-ray Structure Validation Report

Sep 16, 2014 – 11:07 PM EDT

PDB ID : 4L37  
Title : SP2-SP3 - a complex of two storage proteins from Bombyx mori hemolymph  
Authors : Pietrzyk, A.J.; Bujacz, A.; Mueller-Dieckmann, J.; Jaskolski, M.; Bujacz, G.  
Deposited on : 2013-06-05  
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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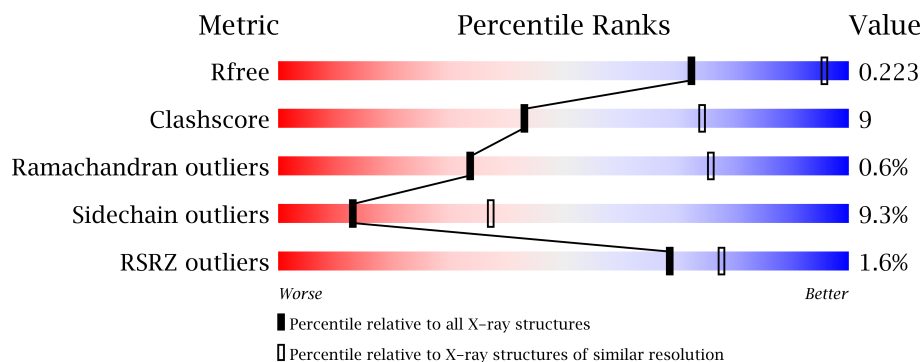
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	680	
2	B	687	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	A	706	-	X
4	SO4	B	706	-	X
6	SCN	A	709	-	X
6	SCN	A	711	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11673 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Silkworm storage protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	1	0
			5723	3780	886	1031	26			

- Molecule 2 is a protein called Arylphorin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	667	Total	C	N	O	S	0	1	0
			5664	3723	892	1024	25			

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	B	5	Total	C	N	O	0	0
			61	34	2	25		

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

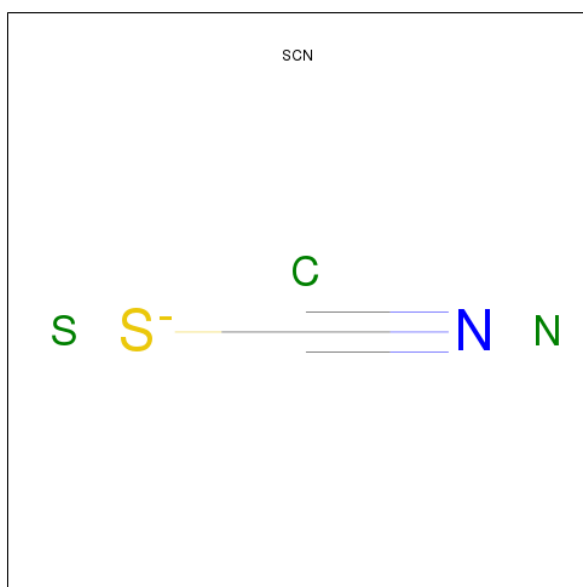


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	S	0	0
			3	1	1	1		
6	A	1	Total	C	N	S	0	0
			3	1	1	1		
6	A	1	Total	C	N	S	0	0
			3	1	1	1		
6	B	1	Total	C	N	S	0	0
			3	1	1	1		
6	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 7 is water.

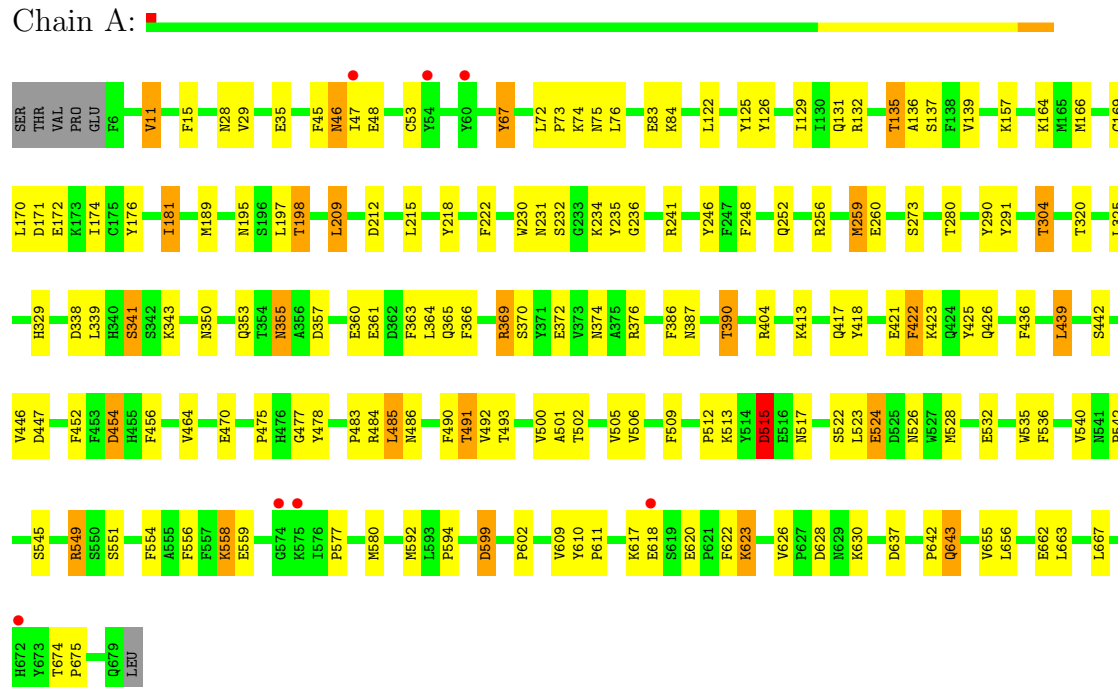
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	84	Total	O	0	0
			84	84		
7	B	52	Total	O	0	0
			52	52		

### 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 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.

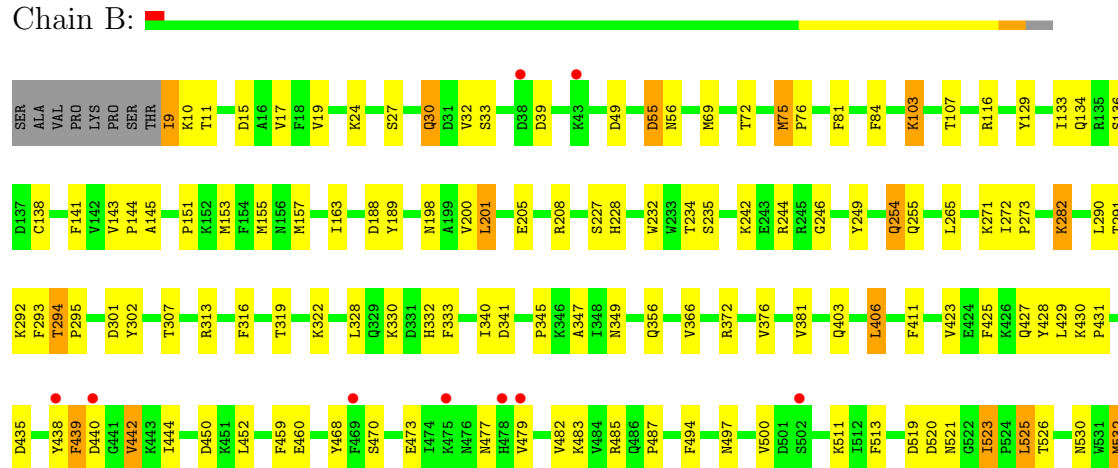
#### • Molecule 1: Silkworm storage protein

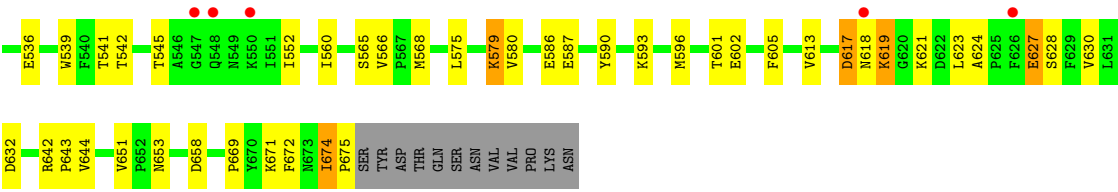
Chain A:



#### • Molecule 2: Arylphorin

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.75Å 192.75Å 180.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.00 – 2.90 48.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.00-2.90) 99.7 (48.19-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.79 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.166 , 0.223 0.166 , 0.223	Depositor DCC
$R_{free}$ test set	1096 reflections (2.54%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 44218 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, NAG, NA, BMA, SO4, MAN

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	0.72	0/5924	0.83	5/8026 (0.1%)
2	B	0.68	0/5848	0.79	2/7912 (0.0%)
All	All	0.70	0/11772	0.81	7/15938 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ASP	CB-CA-C	-5.96	98.49	110.40
1	A	355	ASN	CB-CA-C	-5.79	98.81	110.40
2	B	341	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	376	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	A	339	LEU	CB-CG-CD2	5.30	120.00	111.00
1	A	439	LEU	CA-CB-CG	5.17	127.18	115.30
2	B	49	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	477	GLY	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5723	0	5443	111	0
2	B	5664	0	5426	91	0
3	A	61	0	52	0	0
3	B	61	0	52	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	9	0	0	0	0
6	B	6	0	0	1	0
7	A	84	0	0	7	0
7	B	52	0	0	3	0
All	All	11673	0	10973	197	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (197) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:497:ASN:HD22	2:B:552:ILE:HD12	1.22	1.02
1:A:256:ARG:HH12	1:A:260:GLU:HG2	1.31	0.95
1:A:515:ASP:HB3	1:A:517:ASN:H	1.31	0.95
1:A:132:ARG:HB2	1:A:135:THR:HG22	1.49	0.93
2:B:470:SER:HB3	2:B:473:GLU:HG3	1.55	0.85
1:A:132:ARG:HB2	1:A:135:THR:CG2	2.10	0.81
2:B:291:THR:O	2:B:293:PHE:N	2.21	0.74
2:B:56:ASN:HA	2:B:103:LYS:HD3	1.70	0.74
2:B:313[A]:ARG:HD3	2:B:381:VAL:HG12	1.69	0.73
1:A:350:ASN:OD1	1:A:355:ASN:ND2	2.24	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:176:TYR:HD2	1:A:181:ILE:HD11	1.56	0.69
1:A:230:TRP:HZ3	1:A:363:PHE:CZ	2.11	0.68
2:B:27:SER:HA	2:B:30:GLN:HG3	1.75	0.66
1:A:628:ASP:HB3	1:A:630:LYS:H	1.59	0.66
1:A:246:TYR:CE2	1:A:353:GLN:HB2	2.31	0.66
2:B:254:GLN:OE1	2:B:255:GLN:NE2	2.29	0.66
2:B:587:GLU:HG2	2:B:590:TYR:HD2	1.61	0.65
1:A:136:ALA:O	1:A:137:SER:HB3	1.97	0.64
2:B:75:MET:HE3	2:B:81:PHE:HB2	1.78	0.64
1:A:248:PHE:O	1:A:252:GLN:HB2	1.99	0.63
1:A:338:ASP:O	1:A:341:SER:HB3	1.98	0.63
1:A:485:LEU:HD22	1:A:486:ASN:H	1.63	0.63
2:B:163:ILE:HD13	2:B:482:VAL:HG11	1.80	0.63
1:A:256:ARG:NH1	1:A:260:GLU:HG2	2.10	0.62
1:A:509:PHE:CE1	1:A:532:GLU:HG2	2.36	0.61
2:B:460:GLU:HG2	2:B:485:ARG:HB3	1.81	0.61
1:A:536:PHE:CE1	1:A:549:ARG:HG3	2.35	0.61
1:A:132:ARG:CB	1:A:135:THR:HG22	2.27	0.60
2:B:511:LYS:HE3	2:B:539:TRP:HD1	1.65	0.60
1:A:361:GLU:HG2	1:A:363:PHE:O	2.02	0.60
2:B:601:THR:HG23	2:B:605:PHE:HB2	1.84	0.60
1:A:129:ILE:HA	1:A:135:THR:HG21	1.83	0.59
1:A:11:VAL:HG13	1:A:15:PHE:HB3	1.84	0.59
1:A:554:PHE:CE2	1:A:592:MET:HE1	2.38	0.59
1:A:325:LEU:HD21	1:A:422:PHE:HB2	1.85	0.58
2:B:332:HIS:HA	2:B:340:ILE:O	2.04	0.58
1:A:166:MET:CE	2:B:468:TYR:HD1	2.16	0.57
2:B:235:SER:OG	2:B:242:LYS:HG3	2.04	0.57
1:A:361:GLU:CG	1:A:363:PHE:O	2.52	0.57
1:A:620:GLU:OE1	1:A:620:GLU:HA	2.05	0.57
2:B:642:ARG:HB2	2:B:643:PRO:HD2	1.87	0.57
1:A:209:LEU:HG	1:A:260:GLU:HG3	1.87	0.57
1:A:129:ILE:HA	1:A:135:THR:CG2	2.35	0.56
1:A:353:GLN:NE2	1:A:355:ASN:OD1	2.39	0.56
1:A:290:TYR:CD1	2:B:200:VAL:HG21	2.41	0.55
2:B:497:ASN:ND2	2:B:552:ILE:HD12	2.07	0.55
1:A:129:ILE:O	1:A:135:THR:HG23	2.06	0.55
1:A:136:ALA:O	1:A:137:SER:CB	2.54	0.55
1:A:259:MET:HE3	1:A:512:PRO:HD3	1.88	0.55
1:A:423:LYS:HG3	1:A:426:GLN:HE21	1.71	0.55
2:B:587:GLU:HG2	2:B:590:TYR:CD2	2.41	0.55
2:B:9:ILE:O	2:B:11:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:TRP:CZ3	1:A:363:PHE:CE1	2.95	0.54
1:A:230:TRP:CZ3	1:A:363:PHE:CZ	2.95	0.54
1:A:535:TRP:HD1	1:A:556:PHE:HE2	1.54	0.54
2:B:671:LYS:HA	2:B:674:ILE:HD12	1.89	0.54
1:A:369:ARG:NH1	1:A:374:ASN:OD1	2.41	0.54
1:A:73:PRO:HD2	1:A:76:LEU:HD12	1.89	0.54
2:B:618:ASN:O	2:B:619:LYS:CB	2.55	0.54
2:B:84:PHE:HD1	2:B:376:VAL:HG22	1.72	0.54
1:A:387:ASN:OD1	1:A:390:THR:HG23	2.07	0.54
1:A:456:PHE:HB3	1:A:484:ARG:HG3	1.89	0.53
2:B:9:ILE:CG2	2:B:10:LYS:N	2.71	0.53
2:B:497:ASN:ND2	2:B:552:ILE:HG23	2.23	0.53
2:B:406:LEU:HD22	2:B:411:PHE:CE2	2.44	0.53
1:A:166:MET:HE2	2:B:468:TYR:HD1	1.73	0.53
2:B:618:ASN:O	2:B:619:LYS:HB2	2.07	0.52
1:A:74:LYS:O	1:A:75:ASN:HB2	2.08	0.52
2:B:198:ASN:HA	2:B:201:LEU:O	2.10	0.52
1:A:491:THR:HG22	7:A:866:HOH:O	2.09	0.52
2:B:232:TRP:O	2:B:366:VAL:HA	2.10	0.51
2:B:11:THR:OG1	2:B:579:LYS:HE3	2.09	0.51
2:B:291:THR:C	2:B:293:PHE:H	2.13	0.51
2:B:153:MET:HE1	2:B:403:GLN:NE2	2.25	0.51
2:B:519:ASP:CG	2:B:523:ILE:HG12	2.32	0.51
2:B:624:ALA:O	2:B:628:SER:HB2	2.09	0.51
2:B:9:ILE:CG2	2:B:10:LYS:H	2.24	0.51
1:A:610:TYR:HB2	1:A:611:PRO:HD2	1.93	0.51
1:A:241:ARG:NH2	1:A:630:LYS:O	2.45	0.50
2:B:249:TYR:CE1	2:B:356:GLN:HB2	2.46	0.50
2:B:487:PRO:HG3	2:B:672:PHE:HB2	1.93	0.50
1:A:83:GLU:CD	1:A:366:PHE:HB2	2.32	0.50
1:A:577:PRO:HB2	1:A:580:MET:HG3	1.94	0.49
1:A:628:ASP:HB2	7:A:834:HOH:O	2.11	0.49
1:A:524:GLU:HG3	1:A:642:PRO:HG3	1.94	0.49
2:B:56:ASN:O	2:B:103:LYS:HB2	2.12	0.49
1:A:662:GLU:OE1	1:A:667:LEU:HD13	2.12	0.49
2:B:658:ASP:HB3	7:B:848:HOH:O	2.12	0.49
1:A:164:LYS:NZ	1:A:470:GLU:OE1	2.44	0.49
1:A:446:VAL:HG13	1:A:492:VAL:HG22	1.94	0.49
1:A:46:ASN:ND2	1:A:48:GLU:OE1	2.46	0.49
1:A:139:VAL:HG13	1:A:580:MET:HE2	1.93	0.49
2:B:151:PRO:O	2:B:155:MET:HE3	2.14	0.48
2:B:423:VAL:HG23	2:B:427:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:ASN:HB3	1:A:197:LEU:H	1.79	0.48
1:A:304:THR:HB	7:A:836:HOH:O	2.13	0.47
2:B:330:LYS:HD3	2:B:333:PHE:HB3	1.95	0.47
1:A:259:MET:HE1	1:A:512:PRO:N	2.29	0.47
2:B:316:PHE:CE1	2:B:372:ARG:HD3	2.49	0.47
2:B:328:LEU:O	2:B:428:TYR:OH	2.32	0.47
1:A:164:LYS:HG2	1:A:478:TYR:OH	2.14	0.47
1:A:67:TYR:CD2	1:A:67:TYR:C	2.87	0.47
1:A:454:ASP:O	1:A:483:PRO:HA	2.15	0.47
2:B:144:PRO:HB3	2:B:568:MET:HG3	1.95	0.47
1:A:423:LYS:CG	1:A:426:GLN:HE21	2.28	0.47
1:A:610:TYR:HB2	1:A:611:PRO:CD	2.43	0.47
2:B:9:ILE:HG23	2:B:10:LYS:N	2.30	0.46
1:A:125:TYR:CZ	1:A:129:ILE:HD11	2.50	0.46
1:A:522:SER:HB2	1:A:524:GLU:OE1	2.15	0.46
2:B:205:GLU:O	2:B:208:ARG:HB2	2.15	0.46
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.71	0.46
2:B:513:PHE:CE2	2:B:536:GLU:HB2	2.51	0.46
1:A:554:PHE:CD2	1:A:592:MET:CE	2.98	0.46
1:A:361:GLU:CD	1:A:365:GLN:HG2	2.36	0.46
2:B:294:THR:HG22	2:B:295:PRO:HD2	1.96	0.46
2:B:619:LYS:C	2:B:621:LYS:H	2.19	0.45
1:A:554:PHE:CD2	1:A:592:MET:HE3	2.51	0.45
2:B:627:GLU:HA	2:B:630:VAL:HG22	1.98	0.45
2:B:188:ASP:N	2:B:188:ASP:OD1	2.50	0.45
1:A:404:ARG:NH1	7:A:806:HOH:O	2.48	0.45
1:A:413:LYS:O	1:A:417:GLN:HG2	2.15	0.45
1:A:505:VAL:HB	1:A:610:TYR:CE2	2.52	0.45
1:A:222:PHE:HD2	1:A:622:PHE:CZ	2.35	0.45
1:A:198:THR:HB	7:A:860:HOH:O	2.16	0.45
2:B:444:ILE:HD11	2:B:613:VAL:HG23	1.99	0.45
1:A:222:PHE:CD2	1:A:622:PHE:CZ	3.04	0.45
1:A:45:PHE:HE2	1:A:47:ILE:HD12	1.81	0.45
2:B:459:PHE:O	2:B:485:ARG:HA	2.17	0.45
1:A:674:THR:HA	1:A:675:PRO:HD3	1.76	0.44
2:B:138:CYS:O	2:B:141:PHE:HB2	2.16	0.44
2:B:532:MET:N	2:B:532:MET:SD	2.87	0.44
1:A:626:VAL:O	1:A:628:ASP:N	2.46	0.44
1:A:610:TYR:OH	1:A:628:ASP:OD2	2.24	0.44
1:A:423:LYS:HE3	1:A:637:ASP:O	2.18	0.44
2:B:129:TYR:O	2:B:133:ILE:HG13	2.17	0.44
2:B:282:LYS:HB2	2:B:302:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:319:THR:HG22	7:B:839:HOH:O	2.17	0.44
2:B:494:PHE:HZ	2:B:596:MET:HE1	1.83	0.43
1:A:554:PHE:HD2	1:A:592:MET:HE3	1.83	0.43
2:B:189:TYR:CD1	2:B:483:LYS:HG3	2.53	0.43
2:B:272:ILE:HA	2:B:273:PRO:HD3	1.84	0.43
1:A:234:LYS:HD3	1:A:235:TYR:CZ	2.53	0.43
1:A:622:PHE:HE2	7:A:813:HOH:O	2.01	0.43
1:A:260:GLU:OE2	1:A:594:PRO:HA	2.19	0.43
1:A:599:ASP:N	1:A:599:ASP:OD1	2.51	0.43
2:B:347:ALA:HA	7:B:830:HOH:O	2.18	0.43
1:A:355:ASN:HB3	1:A:357:ASP:H	1.84	0.43
1:A:452:PHE:HE1	1:A:454:ASP:OD1	2.02	0.43
1:A:554:PHE:CE2	1:A:592:MET:CE	3.01	0.43
2:B:675:PRO:HG3	3:B:702:NAG:H61	2.00	0.43
1:A:501:ALA:HA	1:A:540:VAL:O	2.19	0.43
2:B:669:PRO:HD2	6:B:709:SCN:S	2.59	0.43
1:A:171:ASP:HB3	1:A:174:ILE:HD12	2.00	0.43
2:B:291:THR:C	2:B:293:PHE:N	2.72	0.43
2:B:9:ILE:HG22	2:B:10:LYS:H	1.83	0.43
1:A:290:TYR:CD1	2:B:200:VAL:CG2	3.02	0.42
1:A:386:PHE:HB3	1:A:390:THR:OG1	2.19	0.42
1:A:72:LEU:HA	1:A:73:PRO:HD3	1.82	0.42
1:A:291:TYR:OH	2:B:200:VAL:HG22	2.19	0.42
2:B:55:ASP:N	2:B:55:ASP:OD1	2.52	0.42
2:B:593:LYS:HE3	2:B:593:LYS:HB3	1.79	0.42
2:B:145:ALA:HB2	2:B:565:SER:CB	2.49	0.42
1:A:506:VAL:HG22	1:A:609:VAL:HG22	2.00	0.42
2:B:32:VAL:HA	2:B:116:ARG:HH12	1.85	0.42
2:B:246:GLY:HA3	2:B:349:ASN:HA	2.00	0.42
1:A:325:LEU:O	1:A:425:TYR:OH	2.31	0.42
1:A:524:GLU:HG3	1:A:642:PRO:CG	2.49	0.42
1:A:642:PRO:HD2	1:A:643:GLN:OE1	2.20	0.42
1:A:353:GLN:HG2	1:A:353:GLN:O	2.20	0.42
1:A:418:TYR:O	1:A:421:GLU:HB3	2.19	0.42
1:A:558:LYS:HD2	1:A:559:GLU:O	2.19	0.42
2:B:133:ILE:HD12	2:B:227:SER:HB3	2.02	0.41
1:A:372:GLU:HB3	7:A:801:HOH:O	2.21	0.41
2:B:525:LEU:HG	2:B:530:ASN:ND2	2.34	0.41
1:A:506:VAL:O	1:A:535:TRP:HA	2.21	0.41
2:B:438:TYR:CE1	2:B:440:ASP:HA	2.56	0.41
2:B:345:PRO:HB3	2:B:429:LEU:HD13	2.03	0.41
2:B:430:LYS:HA	2:B:431:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:470:SER:CB	2:B:473:GLU:HG3	2.37	0.41
1:A:447:ASP:HB2	1:A:490:PHE:HB2	2.02	0.41
1:A:215:LEU:O	1:A:218:TYR:HB3	2.21	0.41
1:A:602:PRO:HA	1:A:656:LEU:HD23	2.03	0.41
2:B:468:TYR:CD2	2:B:468:TYR:N	2.87	0.41
2:B:672:PHE:CD1	2:B:672:PHE:N	2.89	0.41
1:A:181:ILE:HA	1:A:181:ILE:HD13	1.72	0.41
2:B:19:VAL:HG13	2:B:575:LEU:HB3	2.02	0.41
1:A:212:ASP:OD2	1:A:484:ARG:NH1	2.54	0.40
1:A:164:LYS:HG3	1:A:464:VAL:HG13	2.03	0.40
1:A:501:ALA:HB2	1:A:542:PRO:HD3	2.02	0.40
1:A:512:PRO:HG2	1:A:526:ASN:OD1	2.21	0.40
2:B:613:VAL:O	2:B:653:ASN:HB2	2.21	0.40
2:B:75:MET:HA	2:B:76:PRO:HD3	1.84	0.40
2:B:439:PHE:HB3	2:B:442:VAL:HG22	2.02	0.40
2:B:617:ASP:O	2:B:618:ASN:C	2.59	0.40
2:B:134:GLN:NE2	2:B:228:HIS:O	2.52	0.40
1:A:28:ASN:OD1	1:A:475:PRO:HD2	2.22	0.40
2:B:265:LEU:HD23	2:B:265:LEU:HA	1.64	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	673/680 (99%)	644 (96%)	25 (4%)	4 (1%)	33	76
2	B	666/687 (97%)	635 (95%)	27 (4%)	4 (1%)	33	76
All	All	1339/1367 (98%)	1279 (96%)	52 (4%)	8 (1%)	33	76

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	ASP
2	B	292	LYS
2	B	477	ASN
2	B	450	ASP
2	B	619	LYS
1	A	623	LYS
1	A	343	LYS
1	A	236	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	612/617 (99%)	556 (91%)	56 (9%)	13	38
2	B	608/626 (97%)	551 (91%)	57 (9%)	13	36
All	All	1220/1243 (98%)	1107 (91%)	113 (9%)	13	37

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	29	VAL
1	A	35	GLU
1	A	46	ASN
1	A	53	CYS
1	A	67	TYR
1	A	84	LYS
1	A	126	TYR
1	A	131	GLN
1	A	135	THR
1	A	157	LYS
1	A	169	CYS
1	A	170	LEU
1	A	172	GLU
1	A	181	ILE
1	A	189	MET
1	A	198	THR
1	A	209	LEU

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Mol	Chain	Res	Type
1	A	231	ASN
1	A	232	SER
1	A	259	MET
1	A	273	SER
1	A	280	THR
1	A	304	THR
1	A	320	THR
1	A	329	HIS
1	A	341	SER
1	A	364	LEU
1	A	369	ARG
1	A	370	SER
1	A	390	THR
1	A	422	PHE
1	A	436	PHE
1	A	439	LEU
1	A	442	SER
1	A	454	ASP
1	A	485	LEU
1	A	491	THR
1	A	493	THR
1	A	500	VAL
1	A	502	THR
1	A	513	LYS
1	A	523	LEU
1	A	524	GLU
1	A	528	MET
1	A	545	SER
1	A	549	ARG
1	A	551	SER
1	A	558	LYS
1	A	599	ASP
1	A	617	LYS
1	A	618	GLU
1	A	623	LYS
1	A	643	GLN
1	A	655	VAL
1	A	663	LEU
2	B	9	ILE
2	B	15	ASP
2	B	17	VAL
2	B	24	LYS

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Mol	Chain	Res	Type
2	B	30	GLN
2	B	33	SER
2	B	39	ASP
2	B	55	ASP
2	B	69	MET
2	B	72	THR
2	B	75	MET
2	B	103	LYS
2	B	107	THR
2	B	136	SER
2	B	143	VAL
2	B	157	MET
2	B	201	LEU
2	B	234	THR
2	B	244	ARG
2	B	254	GLN
2	B	271	LYS
2	B	282	LYS
2	B	290	LEU
2	B	294	THR
2	B	301	ASP
2	B	307	THR
2	B	322	LYS
2	B	406	LEU
2	B	425	PHE
2	B	435	ASP
2	B	439	PHE
2	B	442	VAL
2	B	452	LEU
2	B	479	VAL
2	B	500	VAL
2	B	520	ASP
2	B	521	ASN
2	B	523	ILE
2	B	525	LEU
2	B	526	THR
2	B	532	MET
2	B	541	THR
2	B	542	THR
2	B	545	THR
2	B	560	ILE
2	B	566	VAL

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Mol	Chain	Res	Type
2	B	579	LYS
2	B	580	VAL
2	B	586	GLU
2	B	602	GLU
2	B	617	ASP
2	B	623	LEU
2	B	627	GLU
2	B	632	ASP
2	B	644	VAL
2	B	651	VAL
2	B	674	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	417	GLN
1	A	426	GLN
1	A	431	GLN
2	B	427	GLN
2	B	497	ASN
2	B	530	ASN
2	B	548	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

10 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	NAG	A	701	1,3	12,14,15	1.12	1 (8%)	15,19,21	1.54	2 (13%)
3	NAG	A	702	3	12,14,15	1.06	1 (8%)	15,19,21	2.05	4 (26%)
3	BMA	A	703	3	10,11,12	0.88	0	11,15,17	2.51	4 (36%)
3	MAN	A	704	3	10,11,12	0.51	0	11,15,17	1.55	3 (27%)
3	MAN	A	705	3	10,11,12	0.74	0	11,15,17	1.62	1 (9%)
3	NAG	B	701	3,2	12,14,15	0.95	1 (8%)	15,19,21	1.38	2 (13%)
3	NAG	B	702	3	12,14,15	1.05	1 (8%)	15,19,21	1.62	4 (26%)
3	BMA	B	703	3	10,11,12	0.61	0	11,15,17	1.53	2 (18%)
3	MAN	B	704	3	10,11,12	0.91	1 (10%)	11,15,17	1.23	1 (9%)
3	MAN	B	705	3	10,11,12	0.88	0	11,15,17	1.71	1 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	702	3	-	0/6/23/26	0/1/1/1
3	BMA	A	703	3	-	0/2/19/22	0/1/1/1
3	MAN	A	704	3	-	0/2/19/22	0/1/1/1
3	MAN	A	705	3	-	0/2/19/22	0/1/1/1
3	NAG	B	701	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	702	3	-	0/6/23/26	0/1/1/1
3	BMA	B	703	3	-	0/2/19/22	0/1/1/1
3	MAN	B	704	3	-	0/2/19/22	0/1/1/1
3	MAN	B	705	3	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	NAG	O5-C5	-3.54	1.39	1.45
3	A	702	NAG	O5-C5	-3.23	1.40	1.45
3	B	702	NAG	O5-C5	-3.04	1.40	1.45
3	B	701	NAG	O5-C5	-2.67	1.41	1.45
3	B	704	MAN	O5-C5	-2.21	1.42	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAG	O5-C5-C6	-4.86	101.88	106.98
3	A	703	BMA	O5-C5-C6	4.64	111.85	106.98
3	B	705	MAN	C4-C3-C2	4.50	115.62	110.61
3	A	703	BMA	O3-C3-C2	4.29	117.54	109.74
3	A	701	NAG	O5-C5-C4	-4.14	105.40	110.65
3	A	705	MAN	O2-C2-C3	-4.06	101.50	110.10
3	A	703	BMA	O5-C5-C4	-3.78	105.85	110.65
3	B	701	NAG	C2-N2-C7	-3.40	119.28	123.39
3	A	701	NAG	C2-N2-C7	-3.07	119.67	123.39
3	B	702	NAG	O4-C4-C3	-2.92	103.83	110.36
3	A	702	NAG	O7-C7-C8	-2.92	116.45	122.04
3	B	702	NAG	C2-N2-C7	-2.79	120.02	123.39
3	B	703	BMA	O5-C5-C6	2.76	109.88	106.98
3	B	703	BMA	C3-C4-C5	2.69	115.00	110.17
3	B	702	NAG	O3-C3-C4	-2.59	104.58	110.36
3	A	702	NAG	O4-C4-C3	2.49	115.91	110.36
3	B	702	NAG	O7-C7-C8	-2.48	117.29	122.04
3	B	701	NAG	O5-C5-C6	2.43	109.53	106.98
3	A	704	MAN	O5-C5-C4	2.39	113.68	110.65
3	A	702	NAG	O7-C7-N2	2.33	126.64	121.90
3	A	704	MAN	O5-C5-C6	2.27	109.37	106.98
3	A	704	MAN	O3-C3-C2	2.26	113.86	109.74
3	B	704	MAN	C4-C3-C2	2.11	112.97	110.61
3	A	703	BMA	C3-C4-C5	2.06	113.87	110.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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
4	SO4	A	706	-	4,4,4	0.53	0	6,6,6	0.73	0
6	SCN	A	709	-	2,2,2	1.34	0	1,1,1	0.29	0
6	SCN	A	710	-	2,2,2	1.87	1 (50%)	1,1,1	0.59	0
6	SCN	A	711	-	2,2,2	1.71	1 (50%)	1,1,1	0.54	0
4	SO4	B	706	-	4,4,4	0.51	0	6,6,6	0.37	0
6	SCN	B	708	-	2,2,2	1.75	1 (50%)	1,1,1	0.45	0
6	SCN	B	709	-	2,2,2	1.33	0	1,1,1	0.42	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	SO4	A	706	-	-	0/0/0/0	0/0/0/0
6	SCN	A	709	-	-	0/0/0/0	0/0/0/0
6	SCN	A	710	-	-	0/0/0/0	0/0/0/0
6	SCN	A	711	-	-	0/0/0/0	0/0/0/0
4	SO4	B	706	-	-	0/0/0/0	0/0/0/0
6	SCN	B	708	-	-	0/0/0/0	0/0/0/0
6	SCN	B	709	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	710	SCN	C-S	-2.64	1.46	1.63
6	B	708	SCN	C-S	-2.47	1.48	1.63
6	A	711	SCN	C-S	-2.42	1.48	1.63

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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	674/680 (99%)	-0.34	7 (1%) 79 86	26, 43, 78, 141	0
2	B	667/687 (97%)	-0.37	14 (2%) 60 69	26, 49, 94, 170	0
All	All	1341/1367 (98%)	-0.35	21 (1%) 68 78	26, 46, 88, 170	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	475	LYS	4.5
2	B	618	ASN	3.8
2	B	548	GLN	3.7
1	A	672	HIS	3.3
2	B	479	VAL	3.0
1	A	54	TYR	2.8
1	A	574	GLY	2.6
2	B	440	ASP	2.6
1	A	60	TYR	2.6
2	B	478	HIS	2.5
1	A	618	GLU	2.5
2	B	43	LYS	2.4
2	B	547	GLY	2.4
2	B	38	ASP	2.3
2	B	550	LYS	2.3
2	B	626	PHE	2.3
2	B	469	PHE	2.3
2	B	502	SER	2.2
1	A	47	ILE	2.2
2	B	438	TYR	2.2
1	A	575	LYS	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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	B	704	11/12	0.23	1.15	113,119,128,138	0
3	MAN	A	704	11/12	0.20	0.17	91,114,121,122	0
3	NAG	A	702	14/15	0.18	-0.12	46,59,65,70	0
3	NAG	A	701	14/15	0.11	-0.96	32,45,56,58	0
3	NAG	B	702	14/15	0.14	-1.05	51,53,59,76	0
3	NAG	B	701	14/15	0.09	-1.43	35,40,49,52	0
3	BMA	A	703	11/12	0.19	-	79,83,98,106	0
3	BMA	B	703	11/12	0.14	-	71,86,103,110	0
3	MAN	A	705	11/12	0.32	-	91,106,111,112	0
3	MAN	B	705	11/12	0.22	-	97,121,129,132	0

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	SCN	A	711	3/3	0.39	7.51	61,61,73,76	0
4	SO4	A	706	5/5	0.25	4.27	37,45,47,50	5
4	SO4	B	706	5/5	0.26	3.85	69,78,81,81	5
6	SCN	A	709	3/3	0.21	2.62	59,59,74,75	0
6	SCN	A	710	3/3	0.16	0.60	72,72,72,77	0
6	SCN	B	709	3/3	0.14	0.47	68,68,75,80	0
6	SCN	B	708	3/3	0.13	-0.58	64,64,71,75	0
5	NA	B	707	1/1	0.11	-2.02	38,38,38,38	0
5	NA	A	707	1/1	0.11	-2.06	46,46,46,46	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NA	A	708	1/1	0.08	-4.56	36,36,36,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.