Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:16 PM GMT

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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

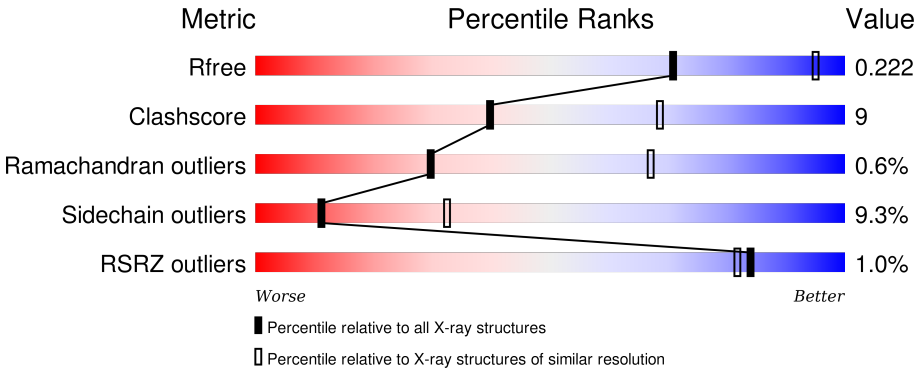
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 >=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 <=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	680	74% 22%
2	B	687	2% 72% 22%

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
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 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 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			

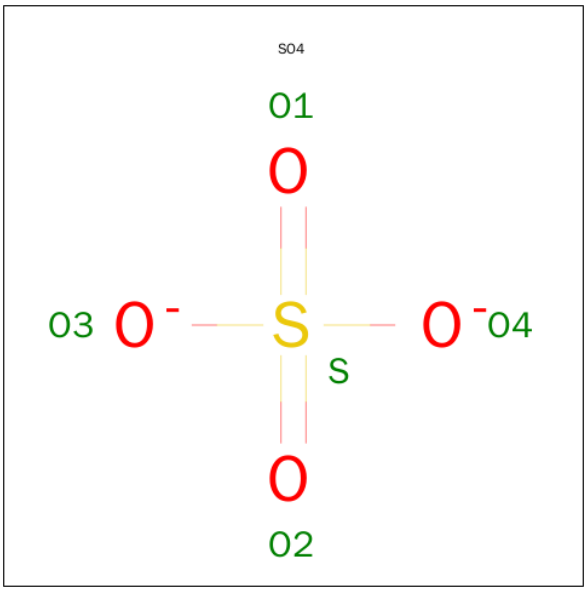
- Molecule 2 is a protein called Arylphorin.

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_4S).

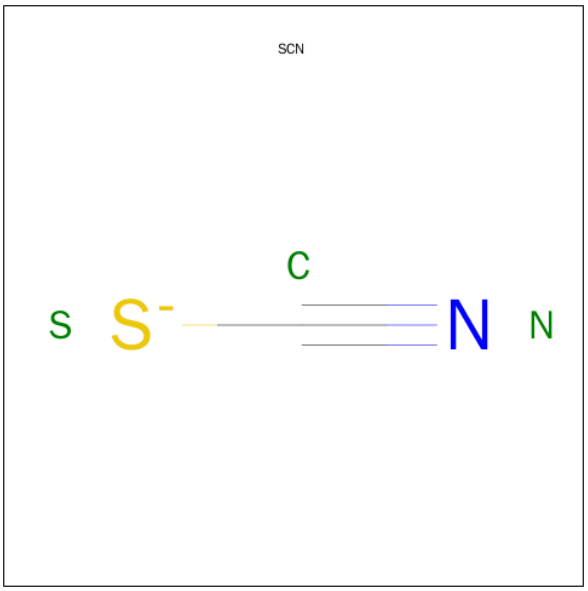


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

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

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

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



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

- Molecule 7 is water.

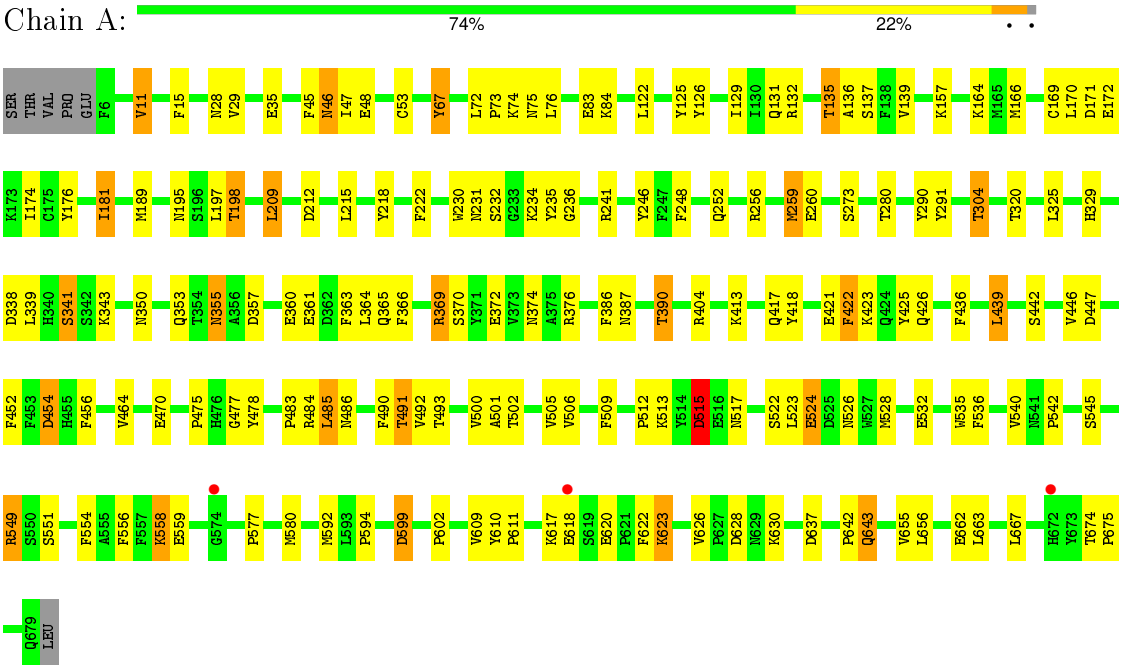
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	84	Total O 84 84	0	0
7	B	52	Total O 52 52	0	0

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.

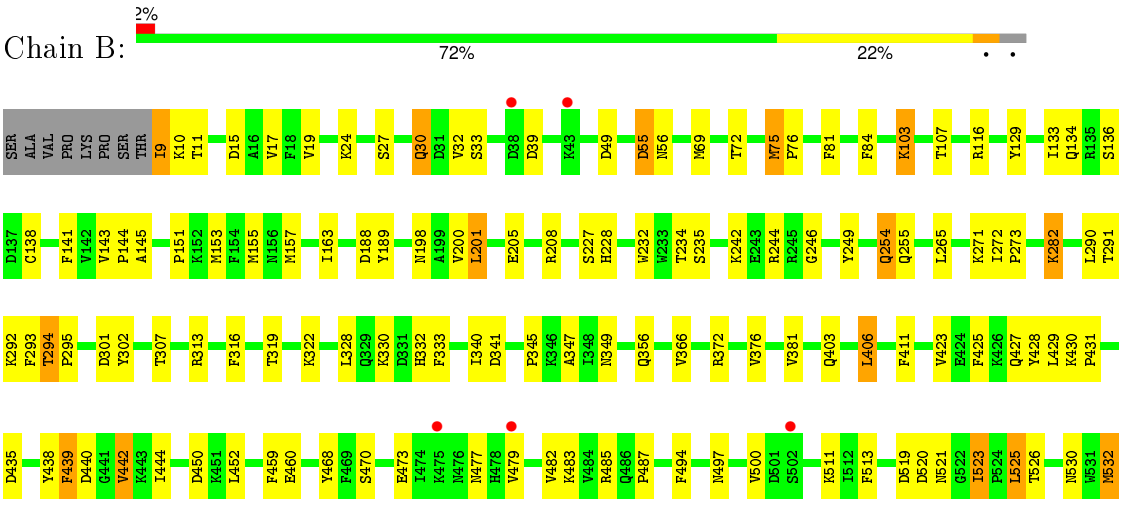
- Molecule 1: Silkworm storage protein

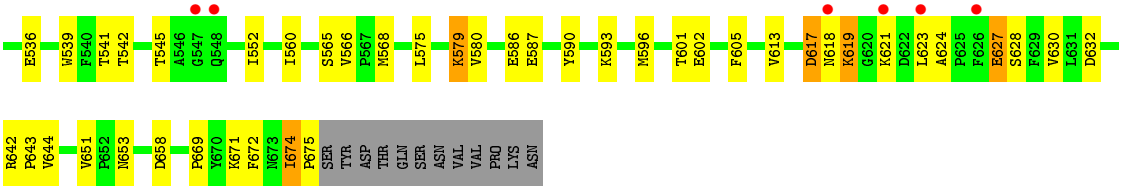
Chain A:



- Molecule 2: Arylphorin

Chain B:




E536
W539
F540
T541
T542
T545
A546
G547
Q548
I552
I560
S565
V566
P567
M568
L575
K579
V580
E586
E587
Y590
K593
M596
T601
E602
F605
V613
D617
W618
K619
G620
K621
D622
L623
A624
P625
F626
E627
S628
F629
V630
L631
D632
R642
P643
V644
V651
F652
N653
D658
P669
Y670
K671
F672
W673
I674
P675
SER
TYR
ASP
THR
GLN
SER
ASN
VAL
VAL
PRO
LYS
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	4.79 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.166 , 0.223 0.166 , 0.222	Depositor DCC
R_{free} test set	1096 reflections (2.54%)	DCC
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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 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	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

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 9.

All (197) 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:497:ASN:HD22	2:B:552:ILE:HD12	1.22	1.02
1:A:515:ASP:HB3	1:A:517:ASN:H	1.31	0.95
1:A:256:ARG:HH12	1:A:260:GLU:HG2	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	Interatomic distance (Å)	Clash overlap (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:338:ASP:O	1:A:341:SER:HB3	1.98	0.63
1:A:248:PHE:O	1:A:252:GLN:HB2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ILE:O	2:B:11:THR:HG23	2.07	0.55
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
2:B:671:LYS:HA	2:B:674:ILE:HD12	1.89	0.54
1:A:535:TRP:HD1	1:A:556:PHE:HE2	1.54	0.54
1:A:73:PRO:HD2	1:A:76:LEU:HD12	1.89	0.54
1:A:369:ARG:NH1	1:A:374:ASN:OD1	2.41	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
2:B:497:ASN:ND2	2:B:552:ILE:HG23	2.23	0.53
2:B:9:ILE:CG2	2:B:10:LYS:N	2.71	0.53
1:A:456:PHE:HB3	1:A:484:ARG:HG3	1.89	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:291:THR:C	2:B:293:PHE:H	2.13	0.51
2:B:11:THR:OG1	2:B:579:LYS:HE3	2.09	0.51
2:B:153:MET:HE1	2:B:403:GLN:NE2	2.25	0.51
2:B:9:ILE:CG2	2:B:10:LYS:H	2.24	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
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:487:PRO:HG3	2:B:672:PHE:HB2	1.93	0.50
2:B:249:TYR:CE1	2:B:356:GLN:HB2	2.46	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
2:B:56:ASN:O	2:B:103:LYS:HB2	2.12	0.49
1:A:524:GLU:HG3	1:A:642:PRO:HG3	1.94	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:139:VAL:HG13	1:A:580:MET:HE2	1.93	0.49
1:A:46:ASN:ND2	1:A:48:GLU:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:VAL:HG23	2:B:427:GLN:HE21	1.78	0.48
2:B:151:PRO:O	2:B:155:MET:HE3	2.14	0.48
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:610:TYR:HB2	1:A:611:PRO:CD	2.43	0.47
1:A:423:LYS:CG	1:A:426:GLN:HE21	2.28	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:505:VAL:HB	1:A:610:TYR:CE2	2.52	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:222:PHE:HD2	1:A:622:PHE:CZ	2.35	0.45
2:B:444:ILE:HD11	2:B:613:VAL:HG23	1.99	0.45
1:A:198:THR:HB	7:A:860:HOH:O	2.16	0.45
1:A:222:PHE:CD2	1:A:622:PHE:CZ	3.04	0.45
2:B:459:PHE:O	2:B:485:ARG:HA	2.17	0.45
1:A:45:PHE:HE2	1:A:47:ILE:HD12	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LYS:HE3	1:A:637:ASP:O	2.18	0.44
2:B:282:LYS:HB2	2:B:302:TYR:CZ	2.53	0.44
2:B:129:TYR:O	2:B:133:ILE:HG13	2.17	0.44
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:272:ILE:HA	2:B:273:PRO:HD3	1.84	0.43
2:B:189:TYR:CD1	2:B:483:LYS:HG3	2.53	0.43
1:A:622:PHE:HE2	7:A:813:HOH:O	2.01	0.43
1:A:234:LYS:HD3	1:A:235:TYR:CZ	2.53	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:554:PHE:CE2	1:A:592:MET:CE	3.01	0.43
1:A:452:PHE:HE1	1:A:454:ASP:OD1	2.02	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
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:171:ASP:HB3	1:A:174:ILE:HD12	2.00	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:291:TYR:OH	2:B:200:VAL:HG22	2.19	0.42
1:A:72:LEU:HA	1:A:73:PRO:HD3	1.82	0.42
2:B:593:LYS:HE3	2:B:593:LYS:HB3	1.79	0.42
2:B:55:ASP:N	2:B:55:ASP:OD1	2.52	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
2:B:525:LEU:HG	2:B:530:ASN:ND2	2.34	0.41
1:A:372:GLU:HB3	7:A:801:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:470:SER:CB	2:B:473:GLU:HG3	2.37	0.41
2:B:430:LYS:HA	2:B:431:PRO:HD3	1.93	0.41
2:B:345:PRO:HB3	2:B:429:LEU:HD13	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:447:ASP:HB2	1:A:490:PHE:HB2	2.02	0.41
1:A:602:PRO:HA	1:A:656:LEU:HD23	2.03	0.41
1:A:215:LEU:O	1:A:218:TYR:HB3	2.21	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
2:B:75:MET:HA	2:B:76:PRO:HD3	1.84	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:617:ASP:O	2:B:618:ASN:C	2.59	0.40
2:B:439:PHE:HB3	2:B:442:VAL:HG22	2.02	0.40
2:B:134:GLN:NE2	2:B:228:HIS:O	2.52	0.40
2:B:265:LEU:HD23	2:B:265:LEU:HA	1.64	0.40
1:A:28:ASN:OD1	1:A:475:PRO:HD2	2.22	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	673/680 (99%)	644 (96%)	25 (4%)	4 (1%)	30 67
2	B	666/687 (97%)	635 (95%)	27 (4%)	4 (1%)	30 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1339/1367 (98%)	1279 (96%)	52 (4%)	8 (1%)	30 67

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 (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	612/617 (99%)	556 (91%)	56 (9%)	11 33
2	B	608/626 (97%)	551 (91%)	57 (9%)	11 32
All	All	1220/1243 (98%)	1107 (91%)	113 (9%)	11 32

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 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)

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	14,14,15	0.72	0	15,19,21	1.01	1 (6%)
3	NAG	A	702	3	14,14,15	0.88	1 (7%)	15,19,21	2.15	5 (33%)
3	BMA	A	703	3	11,11,12	0.96	0	14,15,17	1.63	3 (21%)
3	MAN	A	704	3	11,11,12	0.89	0	14,15,17	2.20	4 (28%)
3	MAN	A	705	3	11,11,12	0.78	0	14,15,17	2.13	3 (21%)
3	NAG	B	701	3,2	14,14,15	0.71	0	15,19,21	1.17	1 (6%)
3	NAG	B	702	3	14,14,15	0.81	0	15,19,21	1.53	4 (26%)
3	BMA	B	703	3	11,11,12	0.79	0	14,15,17	2.88	5 (35%)
3	MAN	B	704	3	11,11,12	0.66	0	14,15,17	1.23	1 (7%)
3	MAN	B	705	3	11,11,12	0.86	1 (9%)	14,15,17	1.54	3 (21%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAG	O5-C1	-2.33	1.39	1.43
3	B	705	MAN	C2-C3	2.07	1.55	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	703	BMA	C1-C2-C3	-5.12	103.49	109.54
3	A	705	MAN	O2-C2-C3	-4.28	101.50	110.12
3	A	705	MAN	O5-C1-C2	-3.55	105.10	110.86
3	A	702	NAG	O7-C7-C8	-3.06	116.45	122.06
3	B	701	NAG	C2-N2-C7	-2.92	119.28	123.04
3	B	702	NAG	O4-C4-C3	-2.89	103.83	110.34
3	A	701	NAG	C2-N2-C7	-2.62	119.67	123.04
3	B	702	NAG	O7-C7-C8	-2.60	117.29	122.06
3	B	702	NAG	O3-C3-C4	-2.56	104.58	110.34
3	A	702	NAG	O5-C5-C6	-2.53	101.88	107.35
3	B	702	NAG	C2-N2-C7	-2.35	120.02	123.04
3	B	705	MAN	C3-C4-C5	2.03	113.73	110.20
3	B	703	BMA	O2-C2-C1	2.08	113.37	109.21
3	A	703	BMA	O5-C5-C6	2.08	111.85	107.35
3	A	703	BMA	C3-C4-C5	2.11	113.87	110.20
3	A	704	MAN	O3-C3-C2	2.14	113.86	110.00
3	A	702	NAG	O7-C7-N2	2.34	126.64	121.86
3	A	702	NAG	O4-C4-C3	2.47	115.91	110.34
3	A	704	MAN	C1-C2-C3	2.56	112.57	109.54
3	B	704	MAN	C1-C2-C3	2.69	112.72	109.54
3	B	705	MAN	C2-C3-C4	2.70	115.62	111.04
3	B	703	BMA	C3-C4-C5	2.75	115.00	110.20
3	A	704	MAN	O5-C1-C2	3.12	115.91	110.86
3	B	705	MAN	C1-C2-C3	3.94	114.20	109.54
3	A	703	BMA	O3-C3-C2	4.17	117.54	110.00
3	A	705	MAN	C1-C2-C3	4.70	115.11	109.54
3	A	702	NAG	C1-O5-C5	4.88	118.44	112.25
3	B	703	BMA	O5-C1-C2	5.22	119.32	110.86
3	A	704	MAN	C1-O5-C5	6.02	119.88	112.25
3	B	703	BMA	C1-O5-C5	6.49	120.48	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	NAG	1	0

5.6 Ligand geometry (i)

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	1.32	0	1,1,1	0.31	0
6	SCN	A	710	-	2,2,2	1.85	1 (50%)	1,1,1	0.59	0
6	SCN	A	711	-	2,2,2	1.69	1 (50%)	1,1,1	0.54	0
4	SO4	B	706	-	4,4,4	0.51	0	6,6,6	0.38	0
6	SCN	B	708	-	2,2,2	1.73	1 (50%)	1,1,1	0.46	0
6	SCN	B	709	-	2,2,2	1.31	0	1,1,1	0.44	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	-2.61	1.46	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	708	SCN	C-S	-2.43	1.48	1.63
6	A	711	SCN	C-S	-2.39	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	709	SCN	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

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	674/680 (99%)	-0.40	3 (0%)	93	92	26, 43, 78, 141	0
2	B	667/687 (97%)	-0.41	11 (1%)	74	72	26, 49, 94, 170	0
All	All	1341/1367 (98%)	-0.40	14 (1%)	84	82	26, 46, 88, 170	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	618	ASN	4.1
2	B	475	LYS	3.8
2	B	548	GLN	3.5
1	A	672	HIS	3.0
2	B	623	LEU	2.7
2	B	479	VAL	2.6
2	B	38	ASP	2.6
2	B	621	LYS	2.6
1	A	618	GLU	2.4
2	B	626	PHE	2.3
2	B	502	SER	2.2
2	B	547	GLY	2.1
2	B	43	LYS	2.1
1	A	574	GLY	2.1

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^{th} 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^2)	Q<0.9
3	NAG	A	701	14/15	0.97	0.11	-1.17	32,45,56,58	0
3	NAG	B	702	14/15	0.96	0.14	-1.24	51,53,59,76	0
3	NAG	B	701	14/15	0.97	0.09	-1.57	35,40,49,52	0
3	BMA	A	703	11/12	0.88	0.18	-	79,83,98,106	0
3	BMA	B	703	11/12	0.93	0.14	-	71,86,103,110	0
3	MAN	A	705	11/12	0.80	0.33	-	91,106,111,112	0
3	MAN	A	704	11/12	0.85	0.22	-	91,114,121,122	0
3	MAN	B	704	11/12	0.88	0.20	-	113,119,128,138	0
3	NAG	A	702	14/15	0.96	0.14	-	46,59,65,70	0
3	MAN	B	705	11/12	0.84	0.23	-	97,121,129,132	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^{th} 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^2)	Q<0.9
6	SCN	A	711	3/3	0.77	0.35	6.29	61,61,73,76	0
4	SO4	A	706	5/5	0.94	0.22	4.02	37,45,47,50	5
4	SO4	B	706	5/5	0.96	0.23	3.72	69,78,81,81	5
6	SCN	A	709	3/3	0.87	0.21	2.19	59,59,74,75	0
6	SCN	B	708	3/3	0.92	0.16	1.11	64,64,71,75	0
6	SCN	B	709	3/3	0.92	0.14	-0.05	68,68,75,80	0
5	NA	A	707	1/1	0.98	0.13	-1.18	46,46,46,46	0
5	NA	B	707	1/1	0.95	0.11	-1.91	38,38,38,38	0
5	NA	A	708	1/1	0.98	0.10	-2.21	36,36,36,36	0
6	SCN	A	710	3/3	0.85	0.17	-	72,72,72,77	0

6.5 Other polymers (i)

There are no such residues in this entry.