Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2017 – 04:39 PM EST

PDB ID	:	5MG8
Title	:	Crystal structure of the S.pombe Smc5/6 hinge domain
Authors	:	Alt, A.; Pearl, L.H.; Oliver, A.W.
Deposited on	:	2016-11-21
Resolution	:	2.75 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:

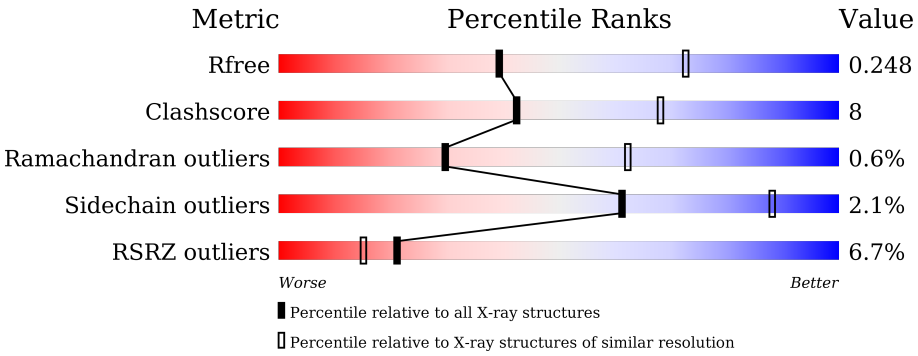
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	347	8% 65% 16% 19%
1	C	347	4% 64% 16% 19%
2	B	294	8% 68% 21% • 10%
2	D	294	2% 70% 20% 10%

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
3	SO4	D	801	-	-	-	X
4	GOL	A	703	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8681 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 Structural maintenance of chromosomes protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	2	0
			2197	1402	364	422	9			
1	C	280	Total	C	N	O	S	0	0	0
			2214	1411	368	426	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	MET	-	initiating methionine	UNP O13710
A	347	GLY	-	expression tag	UNP O13710
A	348	SER	-	expression tag	UNP O13710
A	349	HIS	-	expression tag	UNP O13710
A	350	HIS	-	expression tag	UNP O13710
A	351	HIS	-	expression tag	UNP O13710
A	352	HIS	-	expression tag	UNP O13710
A	353	HIS	-	expression tag	UNP O13710
A	354	HIS	-	expression tag	UNP O13710
A	355	SER	-	expression tag	UNP O13710
A	356	ALA	-	expression tag	UNP O13710
A	357	ALA	-	expression tag	UNP O13710
A	358	LEU	-	expression tag	UNP O13710
A	359	GLU	-	expression tag	UNP O13710
A	360	VAL	-	expression tag	UNP O13710
A	361	LEU	-	expression tag	UNP O13710
A	362	PHE	-	expression tag	UNP O13710
A	363	GLN	-	expression tag	UNP O13710
A	364	GLY	-	expression tag	UNP O13710
A	365	PRO	-	expression tag	UNP O13710
C	346	MET	-	initiating methionine	UNP O13710
C	347	GLY	-	expression tag	UNP O13710
C	348	SER	-	expression tag	UNP O13710
C	349	HIS	-	expression tag	UNP O13710
C	350	HIS	-	expression tag	UNP O13710

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Chain	Residue	Modelled	Actual	Comment	Reference
C	351	HIS	-	expression tag	UNP O13710
C	352	HIS	-	expression tag	UNP O13710
C	353	HIS	-	expression tag	UNP O13710
C	354	HIS	-	expression tag	UNP O13710
C	355	SER	-	expression tag	UNP O13710
C	356	ALA	-	expression tag	UNP O13710
C	357	ALA	-	expression tag	UNP O13710
C	358	LEU	-	expression tag	UNP O13710
C	359	GLU	-	expression tag	UNP O13710
C	360	VAL	-	expression tag	UNP O13710
C	361	LEU	-	expression tag	UNP O13710
C	362	PHE	-	expression tag	UNP O13710
C	363	GLN	-	expression tag	UNP O13710
C	364	GLY	-	expression tag	UNP O13710
C	365	PRO	-	expression tag	UNP O13710

- Molecule 2 is a protein called Structural maintenance of chromosomes protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	264	Total	C	N	O	S	0	2	0
			2027	1278	368	373	8			
2	D	264	Total	C	N	O	S	0	2	0
			2069	1295	376	389	9			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	427	MET	-	initiating methionine	UNP P53692
B	428	ALA	-	expression tag	UNP P53692
B	429	SER	-	expression tag	UNP P53692
B	430	TRP	-	expression tag	UNP P53692
B	431	SER	-	expression tag	UNP P53692
B	432	HIS	-	expression tag	UNP P53692
B	433	PRO	-	expression tag	UNP P53692
B	434	GLN	-	expression tag	UNP P53692
B	435	PHE	-	expression tag	UNP P53692
B	436	GLU	-	expression tag	UNP P53692
B	437	LYS	-	expression tag	UNP P53692
B	438	GLY	-	expression tag	UNP P53692
B	439	ALA	-	expression tag	UNP P53692
B	440	LEU	-	expression tag	UNP P53692
B	441	GLU	-	expression tag	UNP P53692

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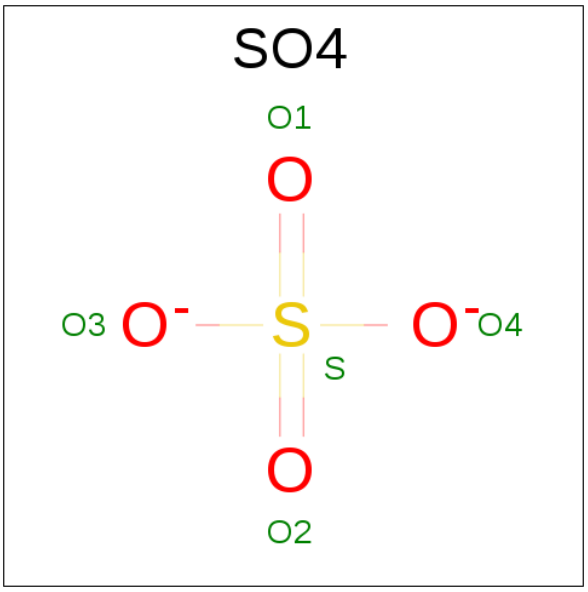
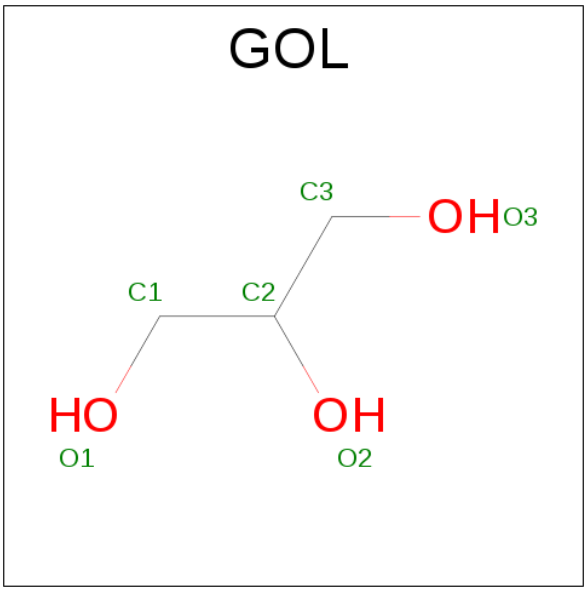
Chain	Residue	Modelled	Actual	Comment	Reference
B	442	VAL	-	expression tag	UNP P53692
B	443	LEU	-	expression tag	UNP P53692
B	444	PHE	-	expression tag	UNP P53692
B	445	GLN	-	expression tag	UNP P53692
B	446	GLY	-	expression tag	UNP P53692
B	447	PRO	-	expression tag	UNP P53692
D	427	MET	-	initiating methionine	UNP P53692
D	428	ALA	-	expression tag	UNP P53692
D	429	SER	-	expression tag	UNP P53692
D	430	TRP	-	expression tag	UNP P53692
D	431	SER	-	expression tag	UNP P53692
D	432	HIS	-	expression tag	UNP P53692
D	433	PRO	-	expression tag	UNP P53692
D	434	GLN	-	expression tag	UNP P53692
D	435	PHE	-	expression tag	UNP P53692
D	436	GLU	-	expression tag	UNP P53692
D	437	LYS	-	expression tag	UNP P53692
D	438	GLY	-	expression tag	UNP P53692
D	439	ALA	-	expression tag	UNP P53692
D	440	LEU	-	expression tag	UNP P53692
D	441	GLU	-	expression tag	UNP P53692
D	442	VAL	-	expression tag	UNP P53692
D	443	LEU	-	expression tag	UNP P53692
D	444	PHE	-	expression tag	UNP P53692
D	445	GLN	-	expression tag	UNP P53692
D	446	GLY	-	expression tag	UNP P53692
D	447	PRO	-	expression tag	UNP P53692

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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



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

- Molecule 5 is water.

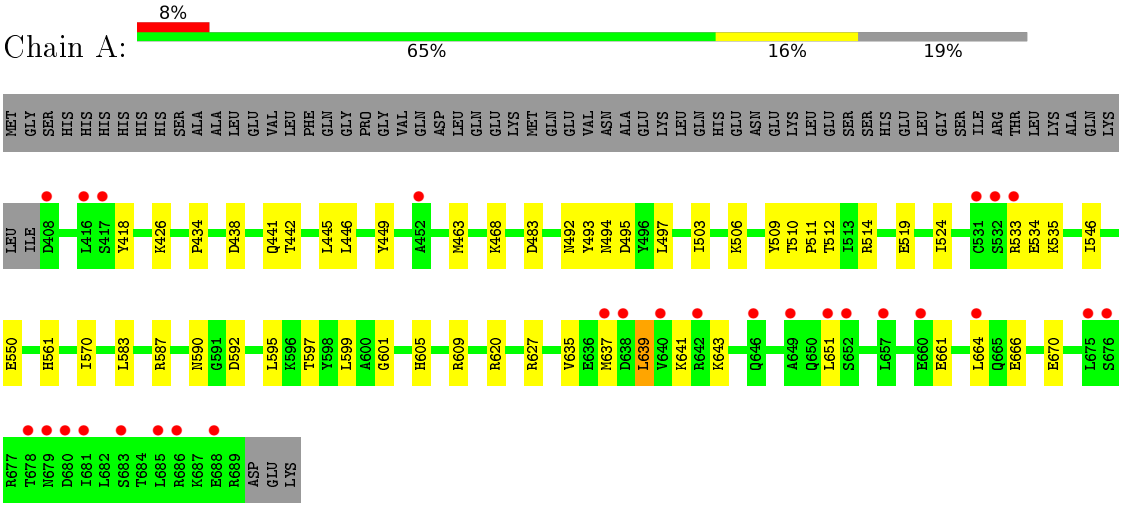
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	22	Total O 22 22	0	0
5	B	29	Total O 29 29	0	0
5	C	19	Total O 19 19	0	0
5	D	35	Total O 35 35	0	0

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.

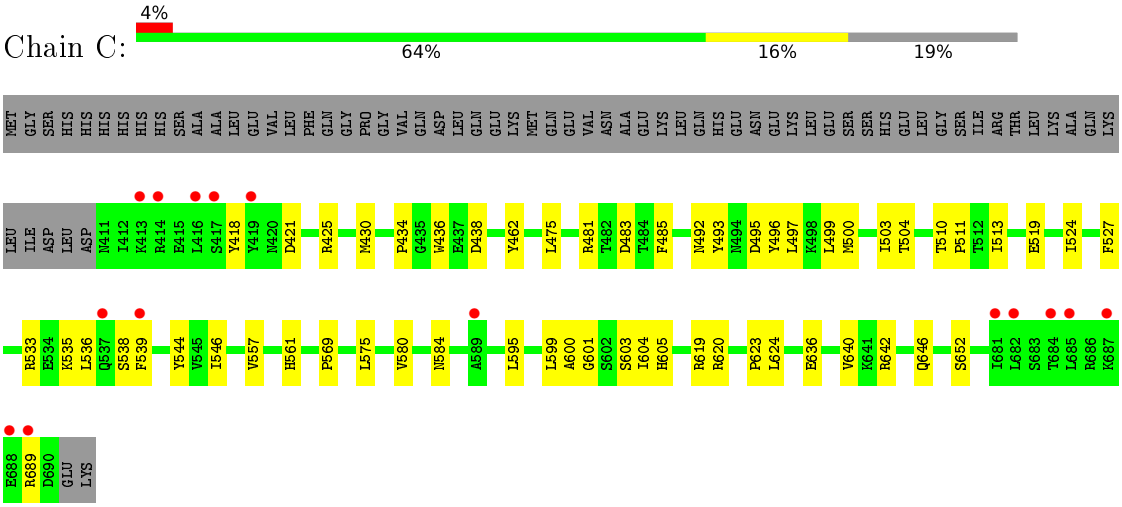
- Molecule 1: Structural maintenance of chromosomes protein 5

Chain A:



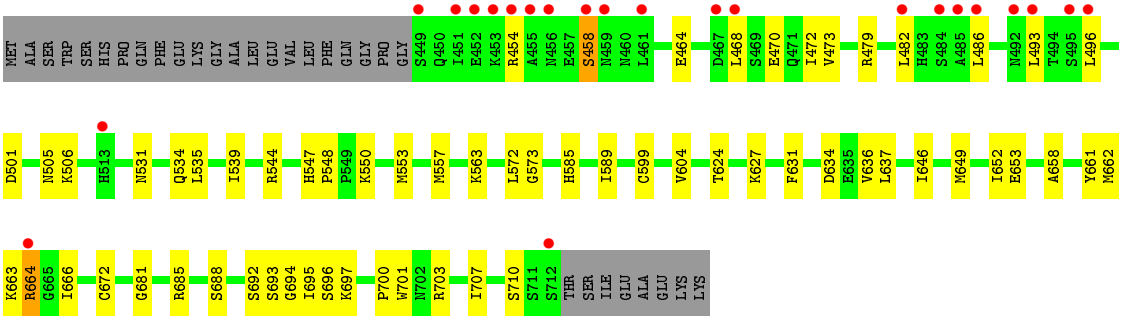
- Molecule 1: Structural maintenance of chromosomes protein 5

Chain C:

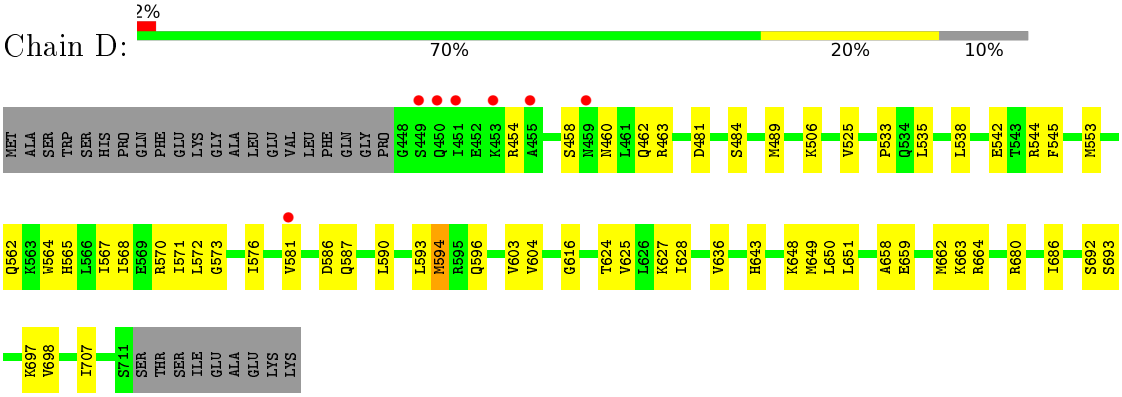


- Molecule 2: Structural maintenance of chromosomes protein 6

Chain B:



- Molecule 2: Structural maintenance of chromosomes protein 6



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	172.56Å 196.46Å 122.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.58 – 2.75 45.58 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.58-2.75) 100.0 (45.58-2.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.209 , 0.249 0.207 , 0.248	Depositor DCC
R_{free} test set	2728 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	63.2	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8681	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.72% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, SO4

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	0.26	0/2247	0.44	1/3049 (0.0%)
1	C	0.25	0/2261	0.40	0/3063
2	B	0.26	0/2070	0.47	0/2803
2	D	0.25	0/2113	0.43	0/2856
All	All	0.25	0/8691	0.43	1/11771 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	639	LEU	CA-CB-CG	5.38	127.68	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2197	0	2070	41	0
1	C	2214	0	2109	38	0
2	B	2027	0	1974	43	0
2	D	2069	0	2021	38	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	20	0	0	2	0
3	D	10	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
4	D	12	0	16	1	0
5	A	22	0	0	1	0
5	B	29	0	0	0	0
5	C	19	0	0	0	0
5	D	35	0	0	1	0
All	All	8681	0	8206	140	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 (140) 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)
1:C:599:LEU:HD13	1:C:604:ILE:HD12	1.37	1.06
1:C:599:LEU:HD13	1:C:604:ILE:CD1	2.04	0.87
2:B:634:ASP:H	4:B:802:GOL:H31	1.45	0.81
2:B:547:HIS:HD2	2:B:548:PRO:HD2	1.46	0.80
1:C:535:LYS:O	1:C:538:SER:HB2	1.83	0.79
2:D:625:VAL:HG21	2:D:649:MET:HE2	1.69	0.75
2:B:664[A]:ARG:HG2	2:B:664[A]:ARG:HH21	1.51	0.74
1:A:524:ILE:HD11	1:A:546:ILE:HD11	1.73	0.70
2:D:538:LEU:HB3	2:D:593:LEU:HD21	1.74	0.70
1:C:599:LEU:CD1	1:C:604:ILE:CD1	2.72	0.67
1:A:661:GLU:OE1	2:B:479:ARG:NH2	2.27	0.66
1:A:570:ILE:HD12	1:A:599:LEU:HB2	1.76	0.66
2:D:460:ASN:O	2:D:463:ARG:HB2	1.96	0.66
2:D:659:GLU:HG2	2:D:686:ILE:HD13	1.78	0.66
1:A:587:ARG:NH1	3:A:701:SO4:O2	2.29	0.65
2:B:563:LYS:NZ	2:B:653:GLU:OE2	2.29	0.64
1:A:503:ILE:HG13	1:A:511:PRO:HG3	1.81	0.63
1:C:569:PRO:HG2	1:C:595:LEU:HD13	1.81	0.62
1:C:603:SER:HB3	1:C:623:PRO:HA	1.82	0.62
1:A:583:LEU:HD11	1:A:595:LEU:HD12	1.83	0.61
2:D:590:LEU:O	2:D:594:MET:HB2	2.01	0.61
1:A:637:MET:O	1:A:641:LYS:HB2	2.01	0.61
1:C:580:VAL:O	1:C:584:ASN:ND2	2.34	0.60
2:D:568:ILE:HA	2:D:571:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ASN:HD21	1:A:592:ASP:HB2	1.67	0.59
1:A:441:GLN:HG3	1:A:509:TYR:CE2	2.37	0.59
1:C:510:THR:HB	2:D:697:LYS:HD2	1.86	0.58
1:A:664:LEU:HB2	2:B:472:ILE:HD11	1.85	0.58
1:A:534:GLU:OE1	1:A:534:GLU:N	2.29	0.58
1:C:599:LEU:CD1	1:C:604:ILE:HD13	2.34	0.57
1:C:511:PRO:HG2	1:C:513:ILE:HD11	1.87	0.57
1:C:475:LEU:HD23	1:C:624:LEU:HD21	1.87	0.56
2:D:568:ILE:HD11	2:D:628:ILE:HD11	1.89	0.55
2:B:557:MET:HB2	2:B:707:ILE:HD12	1.89	0.54
1:A:449:TYR:OH	1:A:506:LYS:NZ	2.41	0.54
1:C:599:LEU:HD11	1:C:604:ILE:HD13	1.89	0.54
1:A:627:ARG:HD3	2:B:505:ASN:HB3	1.89	0.54
1:A:510:THR:HB	2:B:697:LYS:HB2	1.89	0.53
1:C:524:ILE:HD11	1:C:546:ILE:HD11	1.90	0.53
2:B:535:LEU:O	2:B:539:ILE:HG13	2.09	0.53
1:C:620:ARG:HG3	2:D:604:VAL:HG22	1.89	0.53
2:D:538:LEU:CB	2:D:593:LEU:HD21	2.38	0.52
1:A:514[A]:ARG:HD3	2:B:694:GLY:HA3	1.90	0.52
1:A:627:ARG:HG3	1:A:627:ARG:HH21	1.74	0.51
1:A:434:PRO:HD2	2:B:506:LYS:HD3	1.93	0.51
2:D:593:LEU:O	2:D:596:GLN:N	2.43	0.51
1:C:493:TYR:O	1:C:497:LEU:HD12	2.10	0.51
1:A:512:THR:HG23	2:B:696:SER:HB3	1.93	0.51
2:D:581:VAL:HG13	2:D:586:ASP:HB2	1.91	0.51
1:A:661:GLU:HG3	2:B:472:ILE:HD12	1.94	0.50
1:C:430:MET:HG2	1:C:436:TRP:CE3	2.47	0.50
1:C:462:TYR:HB2	1:C:485:PHE:HB3	1.94	0.50
2:D:542:GLU:OE1	2:D:544:ARG:HG2	2.10	0.50
2:B:688:SER:HA	2:B:693:SER:HA	1.92	0.50
1:A:426:LYS:HD3	1:A:463:MET:HA	1.94	0.50
2:D:587:GLN:HG3	2:D:603:VAL:HG11	1.93	0.50
2:D:458:SER:O	2:D:462:GLN:HG3	2.12	0.49
1:C:539:PHE:O	1:C:575:LEU:HD23	2.12	0.49
2:D:697:LYS:NZ	4:D:803:GOL:O2	2.44	0.49
1:A:535:LYS:NZ	5:A:803:HOH:O	2.46	0.49
1:C:600:ALA:HB3	1:C:605:HIS:CE1	2.47	0.49
2:D:525:VAL:HG13	2:D:533:PRO:HG3	1.93	0.49
2:D:664:ARG:NH1	5:D:902:HOH:O	2.45	0.49
1:C:536:LEU:HD11	1:C:544:TYR:CZ	2.48	0.49
2:B:534:GLN:OE1	2:B:534:GLN:N	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:681:GLY:C	2:B:700:PRO:HG3	2.34	0.48
2:B:663:LYS:NZ	2:B:693:SER:HB3	2.29	0.48
1:C:421:ASP:O	1:C:425:ARG:HG3	2.13	0.47
1:C:500:MET:O	1:C:504:THR:HG23	2.14	0.47
1:C:499:LEU:O	1:C:503:ILE:HG12	2.15	0.47
2:D:564:TRP:O	2:D:568:ILE:HG13	2.14	0.47
2:B:631:PHE:CD2	2:B:637:LEU:HD12	2.50	0.47
1:C:493:TYR:CZ	1:C:497:LEU:HD11	2.50	0.47
1:A:635:VAL:HG23	2:B:501:ASP:HB3	1.97	0.47
2:B:482:LEU:HD23	2:B:486:LEU:HB2	1.96	0.47
2:D:576:ILE:HD12	2:D:707:ILE:HD11	1.97	0.46
2:B:553:MET:HB3	2:B:636:VAL:HG13	1.97	0.46
2:B:652:ILE:HB	2:B:658:ALA:HB2	1.98	0.46
2:D:481:ASP:O	2:D:484:SER:HB2	2.15	0.46
2:D:535:LEU:CD1	2:D:593:LEU:HD22	2.46	0.46
1:C:519:GLU:HG2	1:C:561:HIS:NE2	2.30	0.46
1:A:442:THR:O	1:A:446:LEU:HB2	2.16	0.46
2:D:572:LEU:HB2	2:D:576:ILE:HD13	1.98	0.46
1:A:493:TYR:CE2	1:A:497:LEU:HD11	2.51	0.46
1:A:627:ARG:HG3	1:A:627:ARG:NH2	2.31	0.45
2:B:550:LYS:HE2	2:B:550:LYS:HB2	1.82	0.45
2:B:454:ARG:O	2:B:458:SER:HB3	2.16	0.45
1:A:503:ILE:HG21	1:A:511:PRO:HD3	1.99	0.45
1:A:441:GLN:O	1:A:445:LEU:HG	2.17	0.45
1:A:492:ASN:ND2	1:A:495:ASP:H	2.14	0.45
2:B:547:HIS:CD2	2:B:548:PRO:HD2	2.38	0.45
1:C:642:ARG:O	1:C:646:GLN:HG3	2.17	0.44
1:A:666:GLU:O	1:A:670:GLU:HG3	2.17	0.44
1:C:533:ARG:O	1:C:536:LEU:HB2	2.17	0.44
1:C:492:ASN:ND2	1:C:495:ASP:H	2.16	0.44
2:D:625:VAL:HG13	2:D:651:LEU:HD21	2.00	0.44
2:B:544:ARG:HB2	2:B:589:ILE:HD13	2.00	0.44
2:B:701:TRP:CE2	2:B:703:ARG:HB2	2.52	0.43
1:C:619:ARG:NH2	3:C:701:SO4:O3	2.47	0.43
2:B:624:THR:OG1	2:B:627:LYS:HG3	2.18	0.43
2:B:646:ILE:HA	2:B:649:MET:SD	2.58	0.43
1:A:468:LYS:HE2	1:A:550:GLU:HG3	2.00	0.43
1:C:620:ARG:HB2	2:D:643:HIS:CE1	2.54	0.43
1:A:620:ARG:HG3	2:B:604:VAL:HG22	2.00	0.43
1:A:639:LEU:HD11	2:B:496:LEU:HD22	2.01	0.43
1:A:643:LYS:HB3	2:B:493:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:LEU:HG	2:B:486:LEU:HD11	2.01	0.43
2:B:464:GLU:O	2:B:468:LEU:HD22	2.18	0.43
1:C:434:PRO:HD2	2:D:506:LYS:HD3	2.00	0.43
2:D:624:THR:OG1	2:D:627:LYS:HG3	2.18	0.43
1:A:519:GLU:OE2	2:B:692:SER:HB3	2.19	0.43
1:A:492:ASN:HD22	1:A:494:ASN:H	1.66	0.42
1:C:636:GLU:O	1:C:640:VAL:HG13	2.19	0.42
2:D:562:GLN:O	2:D:564:TRP:N	2.53	0.42
2:B:563:LYS:H	2:B:563:LYS:HG3	1.65	0.42
1:C:493:TYR:O	1:C:496:TYR:HB3	2.20	0.42
3:C:703:SO4:O2	2:D:454:ARG:NH2	2.47	0.42
2:B:470:GLU:HA	2:B:473:VAL:HG12	2.02	0.42
2:B:661:TYR:CE2	2:B:666:ILE:HG13	2.54	0.42
2:D:624:THR:HG22	2:D:650:LEU:HD23	2.01	0.42
1:C:600:ALA:HB3	1:C:605:HIS:HE1	1.83	0.42
1:A:519:GLU:HG2	1:A:561:HIS:NE2	2.35	0.41
1:A:441:GLN:HG3	1:A:509:TYR:HE2	1.85	0.41
1:C:503:ILE:HG13	1:C:511:PRO:HG3	2.01	0.41
1:C:519:GLU:OE2	2:D:692:SER:HB3	2.19	0.41
1:A:597:THR:HA	1:A:605:HIS:O	2.19	0.41
2:B:544:ARG:O	2:B:585:HIS:HE1	2.04	0.41
2:B:531:ASN:HB2	2:B:599:CYS:HB2	2.02	0.41
2:D:616:GLY:O	2:D:648:LYS:HE3	2.20	0.41
2:B:685:ARG:O	2:B:695:ILE:HA	2.20	0.41
2:B:664[A]:ARG:HG2	2:B:664[A]:ARG:NH2	2.26	0.41
1:C:496:TYR:CZ	2:D:693:SER:HB3	2.56	0.41
2:D:570:ARG:HG3	2:D:570:ARG:O	2.21	0.41
2:D:538:LEU:HB3	2:D:593:LEU:HD11	2.03	0.41
1:A:590:ASN:HD22	1:A:609:ARG:NH2	2.18	0.41
2:D:567:ILE:HG23	2:D:698:VAL:HG11	2.03	0.41
2:D:553:MET:HB3	2:D:636:VAL:HG13	2.03	0.40
1:A:442:THR:OG1	1:A:511:PRO:HB3	2.22	0.40
1:C:527:PHE:HE1	1:C:557:VAL:HG13	1.87	0.40
2:D:658:ALA:O	2:D:662:MET:HG2	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	281/347 (81%)	274 (98%)	6 (2%)	1 (0%)	39	72
1	C	278/347 (80%)	272 (98%)	4 (1%)	2 (1%)	26	59
2	B	264/294 (90%)	254 (96%)	8 (3%)	2 (1%)	24	55
2	D	264/294 (90%)	247 (94%)	15 (6%)	2 (1%)	24	55
All	All	1087/1282 (85%)	1047 (96%)	33 (3%)	7 (1%)	30	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	573	GLY
1	C	601	GLY
2	D	565	HIS
2	B	572	LEU
1	C	481	ARG
2	D	573	GLY
1	A	601	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	226/313 (72%)	222 (98%)	4 (2%)	66	90
1	C	232/313 (74%)	227 (98%)	5 (2%)	60	87
2	B	211/263 (80%)	205 (97%)	6 (3%)	51	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	222/263 (84%)	217 (98%)	5 (2%)	58 87
All	All	891/1152 (77%)	871 (98%)	20 (2%)	61 87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	TYR
1	A	438	ASP
1	A	483	ASP
1	A	533	ARG
2	B	458	SER
2	B	662	MET
2	B	664[A]	ARG
2	B	664[B]	ARG
2	B	672	CYS
2	B	710	SER
1	C	418	TYR
1	C	438	ASP
1	C	483	ASP
1	C	652	SER
1	C	689	ARG
2	D	489	MET
2	D	545	PHE
2	D	594	MET
2	D	663	LYS
2	D	680	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	492	ASN
1	A	590	ASN
1	A	679	ASN
2	B	546	GLN
2	B	547	HIS
2	B	584	HIS
2	B	585	HIS
2	B	587	GLN
2	B	638	HIS
1	C	492	ASN
1	C	605	HIS

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Mol	Chain	Res	Type
1	C	648	ASN
1	C	658	GLN
1	C	665	GLN
2	D	638	HIS
2	D	668	ASN
2	D	679	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	701	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	A	702	-	4,4,4	0.25	0	6,6,6	0.07	0
4	GOL	A	703	-	5,5,5	0.35	0	5,5,5	0.24	0
3	SO4	B	801	-	4,4,4	0.25	0	6,6,6	0.07	0
4	GOL	B	802	-	5,5,5	0.35	0	5,5,5	0.23	0
3	SO4	C	701	-	4,4,4	0.26	0	6,6,6	0.07	0
3	SO4	C	702	-	4,4,4	0.26	0	6,6,6	0.07	0
3	SO4	C	703	-	4,4,4	0.26	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	C	704	-	4,4,4	0.26	0	6,6,6	0.05	0
3	SO4	D	801	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	D	802	-	4,4,4	0.26	0	6,6,6	0.06	0
4	GOL	D	803	-	5,5,5	0.35	0	5,5,5	0.22	0
4	GOL	D	804	-	5,5,5	0.36	0	5,5,5	0.21	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
3	SO4	A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	A	702	-	-	0/0/0/0	0/0/0/0
4	GOL	A	703	-	-	0/4/4/4	0/0/0/0
3	SO4	B	801	-	-	0/0/0/0	0/0/0/0
4	GOL	B	802	-	-	0/4/4/4	0/0/0/0
3	SO4	C	701	-	-	0/0/0/0	0/0/0/0
3	SO4	C	702	-	-	0/0/0/0	0/0/0/0
3	SO4	C	703	-	-	0/0/0/0	0/0/0/0
3	SO4	C	704	-	-	0/0/0/0	0/0/0/0
3	SO4	D	801	-	-	0/0/0/0	0/0/0/0
3	SO4	D	802	-	-	0/0/0/0	0/0/0/0
4	GOL	D	803	-	-	0/4/4/4	0/0/0/0
4	GOL	D	804	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	SO4	1	0
4	B	802	GOL	1	0
3	C	701	SO4	1	0
3	C	703	SO4	1	0
4	D	803	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	282/347 (81%)	0.54	28 (9%) 9 6	44, 72, 128, 181	0
1	C	280/347 (80%)	0.40	15 (5%) 29 22	50, 77, 130, 170	0
2	B	264/294 (89%)	0.55	23 (8%) 13 8	47, 74, 147, 182	0
2	D	264/294 (89%)	0.33	7 (2%) 58 51	46, 75, 143, 209	0
All	All	1090/1282 (85%)	0.46	73 (6%) 21 15	44, 75, 139, 209	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	SER	5.7
2	B	461	LEU	5.6
1	A	679	ASN	5.6
2	B	468	LEU	5.3
2	B	456	ASN	5.0
2	B	486	LEU	4.9
2	B	454	ARG	4.6
1	C	413	LYS	4.6
1	A	664	LEU	4.5
2	B	451	ILE	4.4
1	A	637	MET	4.4
1	A	675	LEU	4.2
2	B	449	SER	4.2
1	A	678	THR	3.9
2	B	452	GLU	3.9
2	B	458	SER	3.7
2	B	492	ASN	3.7
2	B	485	ALA	3.6
2	B	455	ALA	3.6
2	B	482	LEU	3.6
1	C	589	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	640	VAL	3.5
2	D	451	ILE	3.5
1	C	685	LEU	3.4
1	C	414	ARG	3.3
2	B	496	LEU	3.3
1	A	416	LEU	3.3
1	C	419	TYR	3.2
1	A	685	LEU	3.2
1	A	533	ARG	3.2
2	B	453	LYS	3.1
2	B	493	LEU	3.1
1	A	680	ASP	3.0
1	C	417	SER	2.9
1	C	416	LEU	2.9
2	D	455	ALA	2.9
1	A	657	LEU	2.8
1	C	689	ARG	2.8
1	A	646	GLN	2.8
1	C	537	GLN	2.8
1	A	531	CYS	2.8
1	C	682	LEU	2.7
2	B	484	SER	2.6
1	C	687	LYS	2.6
1	C	684	THR	2.6
2	D	453	LYS	2.6
2	D	459	ASN	2.5
1	A	649	ALA	2.5
1	A	417	SER	2.5
1	A	686	ARG	2.5
2	B	513	HIS	2.5
2	B	459	ASN	2.5
1	A	681	ILE	2.4
1	A	688	GLU	2.4
1	A	660	GLU	2.3
1	A	676	SER	2.3
1	A	408	ASP	2.3
2	D	449	SER	2.3
1	A	642	ARG	2.3
2	B	495	SER	2.3
2	B	664[A]	ARG	2.2
2	D	450	GLN	2.2
1	C	688	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	651	LEU	2.1
1	A	532	SER	2.1
1	A	452	ALA	2.1
1	A	638	ASP	2.1
2	B	712	SER	2.1
1	C	681	ILE	2.1
1	A	652	SER	2.1
2	D	581	VAL	2.1
2	B	467	ASP	2.1
1	C	539	PHE	2.0

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

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

6.3 Carbohydrates (i)

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^{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	SO4	D	801	5/5	0.69	0.41	5.19	204,204,205,205	0
4	GOL	A	703	6/6	0.89	0.27	3.07	81,87,91,95	0
4	GOL	D	803	6/6	0.81	0.23	1.85	84,95,98,100	0
4	GOL	B	802	6/6	0.83	0.15	-1.23	90,96,98,99	0
3	SO4	C	702	5/5	0.93	0.12	-	126,128,130,133	0
3	SO4	D	802	5/5	0.74	0.18	-	176,178,179,179	0
3	SO4	C	704	5/5	0.90	0.28	-	148,150,153,153	0
3	SO4	C	703	5/5	0.95	0.17	-	158,159,160,162	0
3	SO4	A	701	5/5	0.83	0.23	-	141,141,144,146	0
3	SO4	C	701	5/5	0.83	0.31	-	172,172,175,176	0
4	GOL	D	804	6/6	0.70	0.20	-	80,94,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	A	702	5/5	0.93	0.15	-	113,120,120,125	0
3	SO4	B	801	5/5	0.92	0.23	-	167,167,168,170	0

6.5 Other polymers (i)

There are no such residues in this entry.