Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:13 AM GMT

PDB ID	:	2PWP
Title	:	Crystal structure of spermidine synthase from Plasmodium falciparum in complex with spermidine
Authors	:	Qiu, W.; Dong, A.; Ren, H.; Wu, H.; Zhao, Y.; Schapira, M.; Wasney, G.; Vedadi, M.; Lew, J.; Kozieradzki, I.; Edwards, A.M.; Arrowsmith, C.H.; Weigelt, J.; Sundstrom, M.; Plotnikov, A.N.; Bochkarev, A.; Hui, R.; Structural Genomics Consortium (SGC)
Deposited on	:	2007-05-11
Resolution	:	2.10 Å(reported)

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

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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.10 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	Percentile Ranks	Value
Rfree		0.228
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		1.9%
RSRZ outliers		9.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
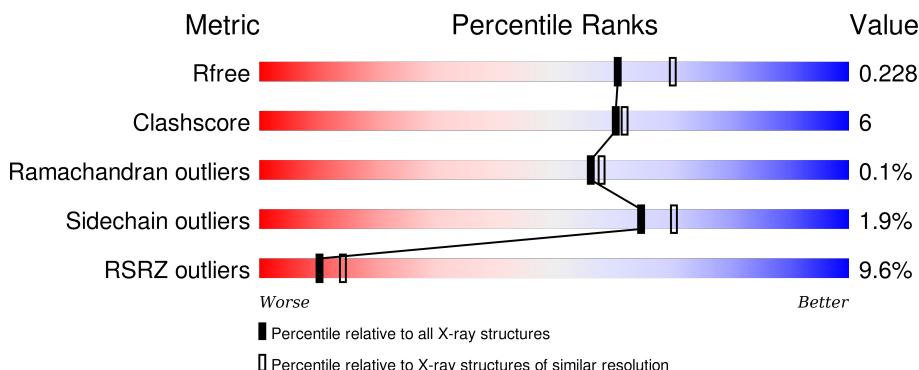
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	282	12% 82% 16% •
1	B	282	7% 83% 13% •
1	C	282	9% 94% 6%
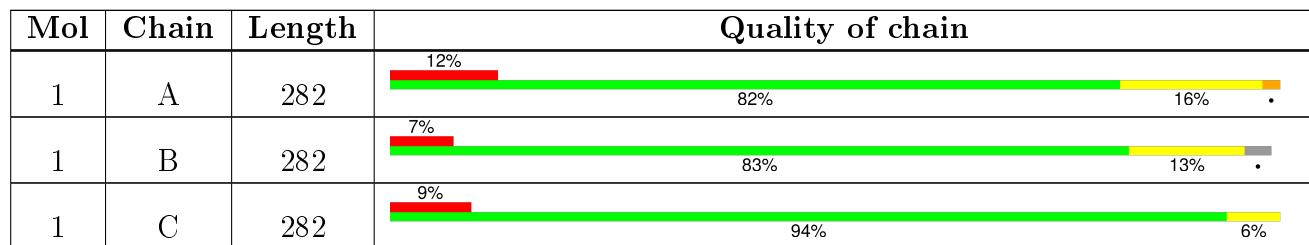
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SPD	A	401	-	-	-	X
2	SPD	B	401	-	-	-	X
2	SPD	C	401	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7110 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 Spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	1	3	0
			2276	1476	356	430	14			
1	B	273	Total	C	N	O	S	6	5	0
			2217	1438	344	420	15			
1	C	281	Total	C	N	O	S	0	1	0
			2260	1468	353	425	14			

- Molecule 2 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).
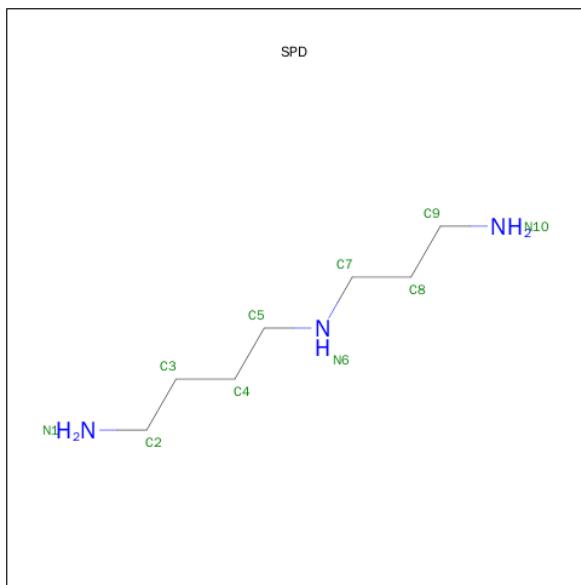
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	7	3		
2	B	1	Total	C	N	0	0
			10	7	3		
2	C	1	Total	C	N	0	0
			10	7	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
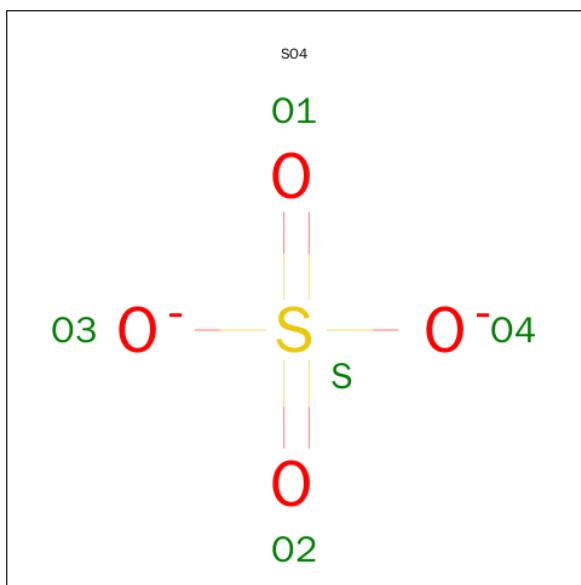
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	S 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
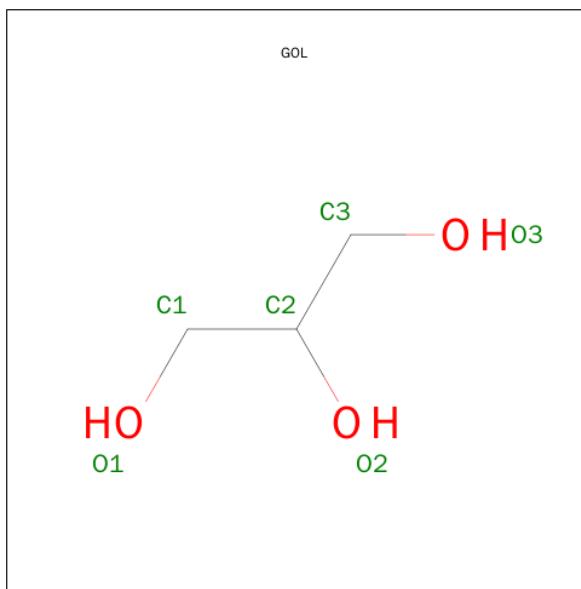
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total 63	O 63	0	0
5	B	92	Total 92	O 92	0	0
5	C	149	Total 149	O 149	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Spermidine synthase
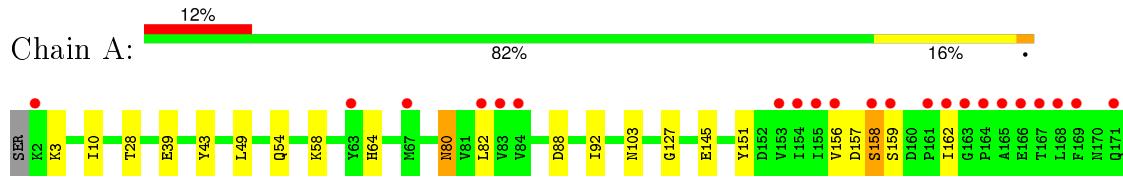
• Molecule 1: Spermidine synthase
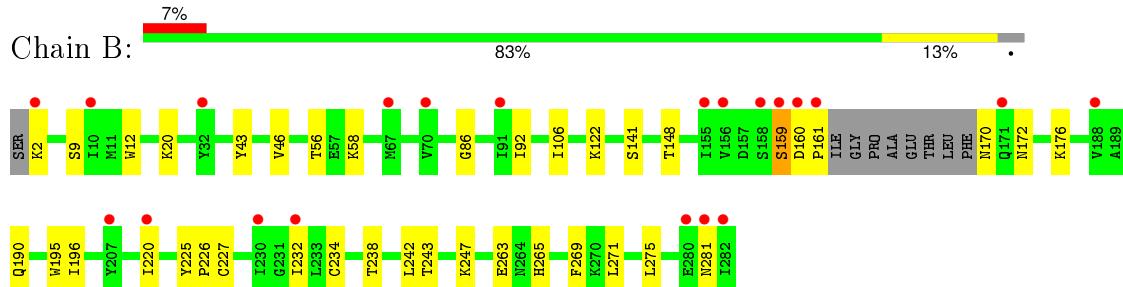
• Molecule 1: Spermidine synthase
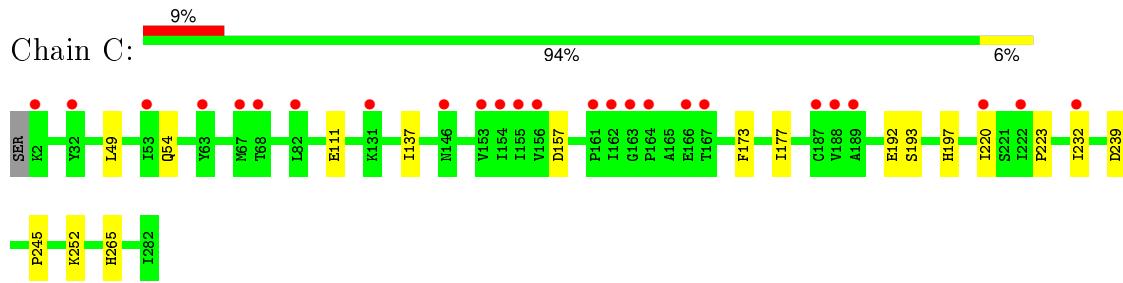
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	198.97Å　　134.50Å　　48.71Å 90.00°　　　95.88°　　　90.00°	Depositor
Resolution (Å)	30.00　–　2.10 29.62　–　2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.10) 99.3 (29.62-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.195　,　0.232 0.192　,　0.228	Depositor DCC
R_{free} test set	3734 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 74726 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7110	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SPD, 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	0.33	0/2330	0.52	0/3147
1	B	0.39	0/2276	0.55	1/3072 (0.0%)
1	C	0.41	0/2313	0.53	0/3122
All	All	0.37	0/6919	0.53	1/9341 (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
1	B	0	1
All	All	0	3

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	B	161	PRO	N-CA-C	-5.72	97.24	112.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ASP	Peptide
1	A	279	ILE	Peptide
1	B	160	ASP	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	2276	0	2275	37	0
1	B	2217	0	2220	27	0
1	C	2260	0	2278	15	0
2	A	10	0	19	5	0
2	B	10	0	19	2	0
2	C	10	0	19	1	0
3	B	5	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
5	A	63	0	0	0	0
5	B	92	0	0	1	0
5	C	149	0	0	1	0
All	All	7110	0	6854	77	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 6.

All (77) 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:192:GLU:HB3	1:C:197:HIS:CD2	1.82	1.14
1:C:192:GLU:HB3	1:C:197:HIS:HD2	1.29	0.97
1:B:2:LYS:HD2	1:B:20:LYS:HE2	1.46	0.94
1:A:192:GLU:HB3	1:A:197[A]:HIS:CD2	2.11	0.86
1:A:80:ASN:HD21	1:A:103:ASN:HD22	1.33	0.77
1:C:193:SER:H	1:C:197:HIS:HD2	1.33	0.77
1:A:192:GLU:HB3	1:A:197[A]:HIS:NE2	2.05	0.71
1:A:192:GLU:CB	1:A:197[A]:HIS:CD2	2.80	0.64
1:A:43:TYR:CD2	1:A:58:LYS:HD3	2.36	0.61
1:A:158:SER:O	1:A:159:SER:HB3	2.02	0.60
1:A:245:PRO:HG2	1:A:262:TYR:CE1	2.37	0.60
1:C:239:ASP:HB2	5:C:588:HOH:O	2.02	0.60
1:B:170:ASN:HD21	1:B:172:ASN:HB3	1.65	0.59
1:A:88:ASP:OD2	2:A:401:SPD:H92	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:PHE:CZ	1:C:177:ILE:HD11	2.37	0.58
1:C:193:SER:H	1:C:197:HIS:CD2	2.19	0.58
1:B:243:THR:HG22	1:B:269:PHE:CG	2.37	0.58
1:C:111:GLU:HB3	1:C:137:ILE:HD12	1.86	0.57
1:A:178:TYR:CE1	1:A:237:LYS:HE2	2.39	0.57
1:C:173:PHE:O	1:C:177:ILE:HD13	2.05	0.55
1:B:86:GLY:CA	1:B:106:ILE:HD11	2.36	0.55
1:B:170:ASN:HD22	1:B:172:ASN:H	1.56	0.54
1:A:280:GLU:O	1:A:281:ASN:HB2	2.06	0.54
1:A:80:ASN:ND2	1:A:103:ASN:HD22	2.01	0.54
1:B:226:PRO:O	1:B:227:CYS:HB2	2.08	0.54
1:B:243:THR:HG22	1:B:269:PHE:CD1	2.43	0.53
1:B:43:TYR:CD2	1:B:58:LYS:HD3	2.45	0.52
1:A:190:GLN:HE22	2:A:401:SPD:H52	1.75	0.52
1:C:245:PRO:HG3	1:C:265:HIS:CG	2.44	0.51
1:C:245:PRO:HG3	1:C:265:HIS:ND1	2.25	0.51
1:B:220:ILE:HD11	1:B:232:ILE:HD11	1.93	0.50
1:B:170:ASN:ND2	1:B:172:ASN:HB3	2.26	0.50
1:A:280:GLU:C	1:A:282:ILE:H	2.15	0.50
1:B:225:TYR:CE1	2:B:401:SPD:H82	2.47	0.50
1:B:92:ILE:HD11	1:B:106:ILE:HD13	1.94	0.49
1:B:86:GLY:C	1:B:106:ILE:HD11	2.33	0.49
1:C:192:GLU:HB3	1:C:197:HIS:CG	2.40	0.48
1:B:86:GLY:HA3	1:B:106:ILE:HD11	1.97	0.47
1:A:54:GLN:O	2:A:401:SPD:H82	2.15	0.47
1:A:3:LYS:HB2	1:A:3:LYS:HE3	1.52	0.47
1:B:86:GLY:HA3	1:B:106:ILE:CD1	2.45	0.47
1:B:170:ASN:ND2	1:B:172:ASN:H	2.13	0.46
1:A:28:THR:OG1	1:B:122:LYS:HD2	2.16	0.46
1:B:195:TRP:CE2	1:C:223:PRO:HD3	2.50	0.46
1:A:279:ILE:HA	1:A:282:ILE:HD11	1.97	0.45
1:B:46:VAL:HG22	1:B:56:THR:HG22	1.97	0.45
1:C:157:ASP:OD1	2:C:401:SPD:H72	2.16	0.45
1:A:214:LYS:HB3	1:A:236:SER:HB2	1.99	0.45
1:A:204:MET:HB3	1:A:233:LEU:HD22	2.00	0.44
1:C:220:ILE:HD11	1:C:232:ILE:HD11	1.99	0.44
1:B:263:GLU:HG3	5:B:619:HOH:O	2.17	0.44
1:B:9:SER:HB3	1:B:12:TRP:CE2	2.53	0.43
1:A:64:HIS:NE2	2:A:401:SPD:N10	2.67	0.43
1:A:226:PRO:O	1:A:227:CYS:HB2	2.18	0.43
1:A:156:VAL:HG12	1:A:158:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ILE:HG12	1:B:227:CYS:SG	2.58	0.43
1:A:216:GLU:OE2	1:A:243:THR:HG23	2.19	0.43
1:A:82:LEU:HB2	1:A:151:TYR:CE1	2.54	0.42
1:B:271:LEU:HD13	1:B:275:LEU:HD23	2.01	0.42
1:B:172:ASN:OD1	1:B:176:LYS:HE3	2.20	0.42
1:A:249:LEU:HB3	1:A:254:PHE:CG	2.55	0.42
1:A:49:LEU:HG	1:A:54:GLN:HG3	2.02	0.42
1:B:234:CYS:HB3	1:B:242:LEU:CD1	2.50	0.41
1:A:92:ILE:HG22	1:A:127:GLY:HA3	2.02	0.41
1:A:279:ILE:HA	1:A:282:ILE:CD1	2.50	0.41
1:A:265:HIS:C	1:A:265:HIS:CD2	2.93	0.41
1:A:196:ILE:HG12	1:A:227:CYS:SG	2.61	0.41
1:A:212:PHE:CG	1:A:235:CYS:HB3	2.56	0.41
1:A:10:ILE:HD11	1:A:162:ILE:HD13	2.01	0.41
1:B:265:HIS:CD2	1:B:265:HIS:C	2.94	0.41
1:A:280:GLU:C	1:A:282:ILE:N	2.72	0.41
1:A:145[A]:GLU:OE1	1:A:176:LYS:HE2	2.21	0.41
1:A:158:SER:O	1:A:159:SER:CB	2.68	0.41
1:C:49:LEU:HG	1:C:54:GLN:HG3	2.02	0.40
1:A:190:GLN:NE2	2:A:401:SPD:H52	2.36	0.40
1:B:225:TYR:OH	2:B:401:SPD:H31	2.21	0.40
1:A:280:GLU:HB2	1:A:281:ASN:H	1.78	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	282/282 (100%)	276 (98%)	6 (2%)	0	100	100
1	B	274/282 (97%)	265 (97%)	8 (3%)	1 (0%)	39	37
1	C	280/282 (99%)	271 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	836/846 (99%)	812 (97%)	23 (3%)	1 (0%)	56 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	SER

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	255/254 (100%)	248 (97%)	7 (3%)	52 56
1	B	250/254 (98%)	243 (97%)	7 (3%)	51 55
1	C	254/254 (100%)	253 (100%)	1 (0%)	93 96
All	All	759/762 (100%)	744 (98%)	15 (2%)	65 68

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	80	ASN
1	A	158	SER
1	A	197[A]	HIS
1	A	197[B]	HIS
1	A	251	SER
1	A	280	GLU
1	B	141	SER
1	B	148	THR
1	B	159	SER
1	B	190	GLN
1	B	238	THR
1	B	247	LYS
1	B	281	ASN
1	C	252	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	80	ASN
1	A	134	ASN
1	A	179	ASN
1	A	190	GLN
1	B	103	ASN
1	B	170	ASN
1	B	246	ASN
1	C	134	ASN
1	C	171	GLN
1	C	172	ASN
1	C	197	HIS
1	C	246	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SPD	A	401	-	9,9,9	0.53	0	8,8,8	2.95	3 (37%)
4	GOL	A	501	-	5,5,5	0.32	0	5,5,5	0.30	0
2	SPD	B	401	-	9,9,9	0.50	0	8,8,8	0.56	0
4	GOL	B	501	-	5,5,5	0.36	0	5,5,5	0.27	0
3	SO4	B	601	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SPD	C	401	-	9,9,9	0.41	0	8,8,8	0.95	0
4	GOL	C	501	-	5,5,5	0.30	0	5,5,5	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SPD	A	401	-	-	0/7/7/7	0/0/0/0
4	GOL	A	501	-	-	0/4/4/4	0/0/0/0
2	SPD	B	401	-	-	0/7/7/7	0/0/0/0
4	GOL	B	501	-	-	0/4/4/4	0/0/0/0
3	SO4	B	601	-	-	0/0/0/0	0/0/0/0
2	SPD	C	401	-	-	0/7/7/7	0/0/0/0
4	GOL	C	501	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	SPD	C4-C5-N6	-5.34	98.62	111.96
2	A	401	SPD	C8-C7-N6	-4.75	100.10	111.96
2	A	401	SPD	C7-N6-C5	3.58	126.03	113.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SPD	5	0
2	B	401	SPD	2	0
2	C	401	SPD	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	281/282 (99%)	0.45	34 (12%)	6	7	30, 45, 80, 101	13 (4%)
1	B	273/282 (96%)	0.22	21 (7%)	16	22	21, 36, 66, 110	10 (3%)
1	C	281/282 (99%)	0.19	25 (8%)	12	16	21, 33, 62, 86	4 (1%)
All	All	835/846 (98%)	0.28	80 (9%)	10	14	21, 38, 72, 110	27 (3%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	ILE	6.6
1	B	161	PRO	6.3
1	C	162	ILE	5.8
1	B	282	ILE	5.5
1	A	155	ILE	4.6
1	B	281	ASN	4.5
1	A	167	THR	4.5
1	B	10	ILE	4.4
1	A	281	ASN	4.3
1	A	156	VAL	4.1
1	A	282	ILE	4.0
1	C	167	THR	3.9
1	A	169	PHE	3.9
1	C	166	GLU	3.8
1	A	166	GLU	3.7
1	A	164	PRO	3.7
1	B	171	GLN	3.7
1	A	188	VAL	3.7
1	B	232	ILE	3.6
1	A	154	ILE	3.5
1	A	163	GLY	3.5
1	A	240	THR	3.4
1	A	2	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	161	PRO	3.3
1	A	82	LEU	3.2
1	C	163	GLY	3.2
1	C	188	VAL	3.2
1	B	32	TYR	3.2
1	B	188	VAL	3.1
1	A	84	VAL	3.1
1	C	68	THR	3.0
1	C	154	ILE	2.9
1	A	83	VAL	2.9
1	B	156	VAL	2.9
1	C	155	ILE	2.9
1	A	161	PRO	2.8
1	A	168	LEU	2.8
1	A	262	TYR	2.8
1	A	67	MET	2.8
1	B	159	SER	2.8
1	B	280[A]	GLU	2.8
1	B	67	MET	2.7
1	B	155	ILE	2.7
1	C	164	PRO	2.7
1	A	230	ILE	2.7
1	B	91	ILE	2.7
1	A	239	ASP	2.6
1	C	156	VAL	2.6
1	A	63	TYR	2.6
1	A	153	VAL	2.6
1	C	63	TYR	2.6
1	A	171	GLN	2.5
1	C	67	MET	2.5
1	A	232	ILE	2.5
1	B	230	ILE	2.5
1	B	160	ASP	2.5
1	C	131	LYS	2.5
1	C	220	ILE	2.5
1	A	187	CYS	2.5
1	A	159	SER	2.4
1	A	158	SER	2.4
1	B	2	LYS	2.4
1	C	189	ALA	2.3
1	C	82	LEU	2.3
1	C	187	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	32	TYR	2.3
1	B	70	VAL	2.3
1	C	232	ILE	2.3
1	B	207	TYR	2.2
1	C	146	ASN	2.2
1	C	153	VAL	2.2
1	A	165	ALA	2.1
1	B	158	SER	2.1
1	C	53	ILE	2.1
1	A	280	GLU	2.1
1	A	199	GLY	2.1
1	A	231	GLY	2.1
1	C	222	ILE	2.0
1	B	220	ILE	2.0
1	C	2	LYS	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, 95th 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
2	SPD	B	401	10/10	0.91	0.40	4.05	27,46,55,59	0
2	SPD	C	401	10/10	0.95	0.35	3.79	25,39,54,54	0
2	SPD	A	401	10/10	0.93	0.31	2.68	32,43,63,68	0
3	SO4	B	601	5/5	0.95	0.13	0.12	54,56,75,92	0
4	GOL	C	501	6/6	0.95	0.11	-	42,50,61,63	0
4	GOL	B	501	6/6	0.96	0.15	-	29,43,47,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	A	501	6/6	0.94	0.18	-	51,57,62,74	0

6.5 Other polymers (i)

There are no such residues in this entry.