



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 12:11 pm GMT

PDB ID : 3S3N  
Title : Crystal structure of the Prototype Foamy Virus (PFV) S217H mutant intasome in complex with magnesium and Dolutegravir (S/GSK1349572)  
Authors : Hare, S.; Cherepanov, P.  
Deposited on : 2011-05-18  
Resolution : 2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

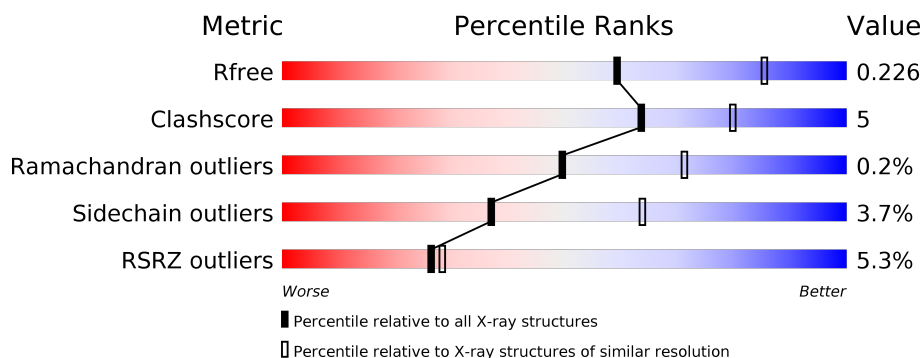
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	395	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 7%</div> </div> </div>
1	B	395	<div> <div>5%</div> <div> <div></div> <div>39%</div> <div>6%</div> <div>• 54%</div> </div> </div>
2	C	19	<div> <div>47%</div> <div>37%</div> <div>16%</div> </div>
3	D	17	<div> <div>53%</div> <div>41%</div> <div>6%</div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5411 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 PFV integrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	1	0
			2936	1882	518	532	4			
1	B	181	Total	C	N	O	S	0	0	0
			1421	924	230	266	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P14350
A	-1	PRO	-	EXPRESSION TAG	UNP P14350
A	0	GLY	-	EXPRESSION TAG	UNP P14350
A	217	HIS	GLY	ENGINEERED MUTATION	UNP P14350
A	218	GLY	SER	VARIANT	UNP P14350
B	-2	GLY	-	EXPRESSION TAG	UNP P14350
B	-1	PRO	-	EXPRESSION TAG	UNP P14350
B	0	GLY	-	EXPRESSION TAG	UNP P14350
B	217	HIS	GLY	VARIANT	UNP P14350
B	218	GLY	SER	VARIANT	UNP P14350

- Molecule 2 is a DNA chain called 5'-D(\*AP\*TP\*TP\*GP\*TP\*CP\*AP\*TP\*GP\*GP\*AP\*A P\*TP\*TP\*TP\*CP\*GP\*CP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	19	Total	C	N	O	P	0	1	0
			405	197	73	117	18			

- Molecule 3 is a DNA chain called 5'-D(\*TP\*GP\*CP\*GP\*AP\*AP\*AP\*TP\*TP\*CP\*CP\*A P\*TP\*GP\*AP\*CP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	17	Total	C	N	O	P	0	1	0
			366	176	70	103	17			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

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



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

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



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

- Molecule 7 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).

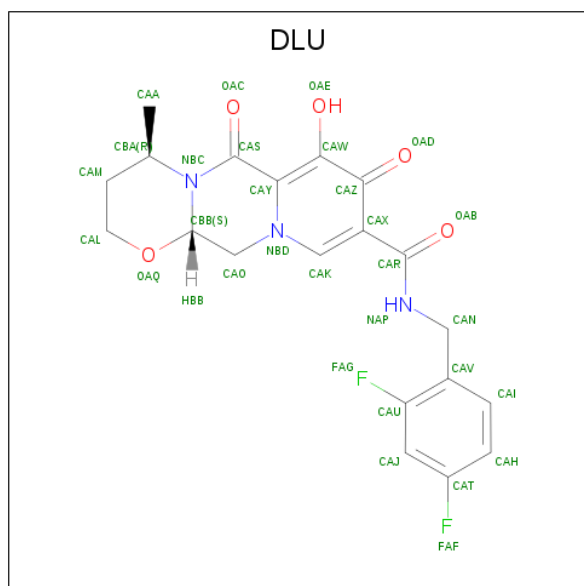


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total N 1 1	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Mg 2 2	0	0

- Molecule 9 is (4R,12aS)-N-(2,4-difluorobenzyl)-7-hydroxy-4-methyl-6,8-dioxo-3,4,6,8,12,12a-hexahydro-2H-pyrido[1',2':4,5]pyrazino[2,1-b][1,3]oxazine-9-carboxamide (three-letter code: DLU) (formula: C<sub>20</sub>H<sub>19</sub>F<sub>2</sub>N<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C F N O 30 20 2 3 5	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	143	Total O 143 143	0	0
10	B	30	Total O 30 30	0	0
10	C	21	Total O 21 21	0	0

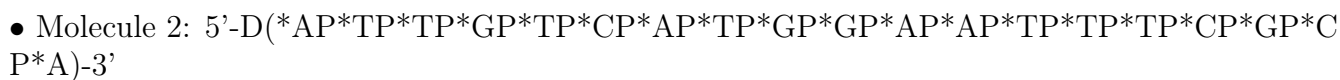
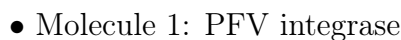
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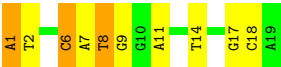
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	16	Total	O	0	0
			16	16		



- Molecule 1: PFV integrase







● Molecule 3: 5'-D(\*TP\*GP\*CP\*GP\*AP\*AP\*AP\*TP\*TP\*CP\*CP\*AP\*TP\*GP\*AP\*CP\*A)-3',



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.05Å 160.05Å 123.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.16 – 2.49 39.16 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.0 (39.16-2.49) 94.0 (39.16-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.209 , 0.232 0.204 , 0.226	Depositor DCC
$R_{free}$ test set	2723 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5411	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, MG, NH4, SO4, DLU

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	0.61	0/3019	0.70	3/4120 (0.1%)
1	B	0.63	0/1459	0.62	0/1994
2	C	1.02	0/454	1.71	11/700 (1.6%)
3	D	1.05	0/410	1.99	10/628 (1.6%)
All	All	0.70	0/5342	0.99	24/7442 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	15	DA	O4'-C1'-N9	15.31	118.72	108.00
3	D	1	DT	P-O3'-C3'	9.18	130.71	119.70
2	C	7	DA	O4'-C1'-N9	-7.88	102.49	108.00
2	C	8	DT	O4'-C4'-C3'	-7.77	101.34	106.00
3	D	8	DT	O4'-C1'-N1	-6.66	103.34	108.00
3	D	7	DA	O4'-C1'-N9	-6.39	103.53	108.00
3	D	15	DA	P-O3'-C3'	6.28	127.23	119.70
3	D	14	DG	N1-C6-O6	-6.25	116.15	119.90
1	A	69	ARG	NE-CZ-NH2	-6.09	117.25	120.30
2	C	11	DA	O4'-C1'-N9	-6.09	103.74	108.00
1	A	69	ARG	NE-CZ-NH1	6.02	123.31	120.30
3	D	15	DA	P-O5'-C5'	5.93	130.39	120.90
2	C	14	DT	P-O3'-C3'	5.72	126.56	119.70
2	C	18	DC	C1'-O4'-C4'	-5.64	104.46	110.10
2	C	14	DT	N3-C4-O4	5.56	123.23	119.90
2	C	17	DG	O4'-C1'-N9	-5.48	104.16	108.00
2	C	1[A]	DA	O4'-C4'-C3'	-5.34	102.36	104.50
2	C	1[B]	DA	O4'-C4'-C3'	-5.34	102.36	104.50
2	C	8	DT	OP2-P-O3'	5.34	116.94	105.20
2	C	6	DC	O4'-C1'-N1	5.22	111.65	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	14	DG	O4'-C1'-N9	-5.18	104.37	108.00
1	A	173	LEU	CA-CB-CG	5.14	127.13	115.30
3	D	8	DT	N1-C1'-C2'	5.11	122.31	112.60
3	D	13	DT	C5-C4-O4	-5.08	121.34	124.90

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	2936	0	2966	29	0
1	B	1421	0	1401	11	0
2	C	405	0	230	6	0
3	D	366	0	205	2	0
4	A	1	0	0	0	0
5	A	10	0	0	1	0
5	B	5	0	0	1	0
6	A	24	0	32	1	0
7	A	1	0	0	0	0
8	A	2	0	0	0	0
9	A	30	0	18	2	0
10	A	143	0	0	1	0
10	B	30	0	0	0	0
10	C	21	0	0	0	0
10	D	16	0	0	0	0
All	All	5411	0	4852	46	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 5.

All (46) 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:A:174:THR:HB	1:A:178:ILE:HD13	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:SER:O	1:B:261:LEU:O	2.06	0.73
1:A:358:LEU:N	1:A:359:GLY:HA2	2.08	0.69
1:A:221:GLU:O	1:A:224:ASN:HB2	1.93	0.68
3:D:15:DA:H4'	3:D:16:DC:OP1	1.93	0.66
1:B:233:LYS:O	1:B:236:VAL:HG22	1.97	0.63
1:A:162:SER:HB2	6:A:801:GOL:H2	1.82	0.61
1:A:108:ALA:O	1:A:314:SER:HA	2.03	0.58
1:B:155:LEU:HD12	1:B:250:GLN:HG3	1.84	0.58
1:B:127:ILE:HG22	1:B:145:VAL:HG22	1.87	0.56
2:C:1[A]:DA:C2'	2:C:2:DT:OP1	2.55	0.55
1:A:73:LEU:HD13	1:A:86:ARG:HG3	1.88	0.55
1:A:295:LEU:HD21	1:A:299:ARG:CZ	2.37	0.54
1:A:215[A]:GLN:HG3	9:A:398:DLU:FAF	1.98	0.54
1:B:127:ILE:HA	1:B:144:VAL:O	2.08	0.53
1:A:174:THR:HB	1:A:178:ILE:CD1	2.35	0.52
1:A:114:ARG:NH1	5:A:399:SO4:O3	2.36	0.51
1:A:76:ILE:HG22	1:A:85:MET:CE	2.42	0.50
1:A:295:LEU:HD21	1:A:299:ARG:NH2	2.28	0.49
1:B:283:THR:C	1:B:285:ASP:H	2.17	0.49
1:A:67:THR:HB	1:A:71:ALA:HB3	1.94	0.48
2:C:1[A]:DA:N3	2:C:1[A]:DA:O4'	2.45	0.48
1:A:145:VAL:HG11	1:A:173:LEU:HD21	1.97	0.47
1:B:290:GLU:HA	1:B:293:SER:HB2	1.97	0.47
1:A:221:GLU:OE1	1:A:221:GLU:HA	2.16	0.46
1:A:219:LYS:HE3	2:C:6:DC:OP1	2.17	0.45
1:B:120:LYS:O	1:B:123:ASP:HB2	2.16	0.45
1:A:157:PRO:HD3	1:A:246:LEU:HD12	1.99	0.45
1:B:222:ARG:NE	5:B:393:SO4:O3	2.33	0.45
1:A:358:LEU:H	1:A:359:GLY:HA2	1.81	0.44
2:C:8:DT:H2''	2:C:9:DG:H5'	2.00	0.44
1:A:366:ILE:HD13	1:A:366:ILE:HG21	1.65	0.43
2:C:1[B]:DA:H2''	2:C:2:DT:C6	2.52	0.43
9:A:398:DLU:CAR	3:D:17[A]:DA:H2'	2.49	0.43
2:C:8:DT:H2'	2:C:9:DG:C8	2.53	0.43
1:A:163:THR:HG23	1:A:195:PHE:HB2	2.01	0.43
1:A:122:PHE:O	1:A:179:PRO:HA	2.19	0.42
1:A:358:LEU:N	1:A:359:GLY:CA	2.80	0.42
1:A:276:THR:HG22	1:B:178:ILE:HD12	2.01	0.42
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.90	0.42
1:A:97:GLN:OE1	1:A:339:LYS:HG2	2.19	0.42
1:A:315:TRP:CE2	1:A:371:PRO:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:THR:HG23	1:B:195:PHE:HB2	2.02	0.41
1:A:341:SER:HB2	1:A:355:LEU:O	2.20	0.41
1:A:112:ILE:HG23	10:A:435:HOH:O	2.21	0.41
1:A:69:ARG:HD2	1:A:70:GLU:OE2	2.21	0.41

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	367/395 (93%)	355 (97%)	11 (3%)	1 (0%)	43	64
1	B	177/395 (45%)	168 (95%)	9 (5%)	0	100	100
All	All	544/790 (69%)	523 (96%)	20 (4%)	1 (0%)	49	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	GLU

### 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	329/354 (93%)	321 (98%)	8 (2%)	52	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	156/354 (44%)	146 (94%)	10 (6%)	19	36
All	All	485/708 (68%)	467 (96%)	18 (4%)	37	64

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	73	LEU
1	A	137	GLN
1	A	149	MET
1	A	312	SER
1	A	356	ASP
1	A	357	HIS
1	A	361	ASN
1	B	149	MET
1	B	164	SER
1	B	261	LEU
1	B	274	SER
1	B	281	GLN
1	B	285	ASP
1	B	286	LEU
1	B	288	ARG
1	B	293	SER
1	B	297	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

Of 12 ligands modelled in this entry, 1 is modelled with single atom and 3 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	A	394	-	4,4,4	0.14	0	6,6,6	0.28	0
9	DLU	A	398	8	26,33,33	1.18	2 (7%)	34,49,49	2.11	10 (29%)
5	SO4	A	399	-	4,4,4	0.34	0	6,6,6	0.34	0
6	GOL	A	801	-	5,5,5	0.49	0	5,5,5	0.78	0
6	GOL	A	802	-	5,5,5	0.48	0	5,5,5	0.57	0
6	GOL	A	803	-	5,5,5	0.36	0	5,5,5	0.50	0
6	GOL	A	805	-	5,5,5	0.43	0	5,5,5	0.40	0
5	SO4	B	393	-	4,4,4	0.19	0	6,6,6	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	394	-	-	0/0/0/0	0/0/0/0
9	DLU	A	398	8	-	0/9/35/35	0/3/4/4
5	SO4	A	399	-	-	0/0/0/0	0/0/0/0
6	GOL	A	801	-	-	0/4/4/4	0/0/0/0
6	GOL	A	802	-	-	0/4/4/4	0/0/0/0
6	GOL	A	803	-	-	0/4/4/4	0/0/0/0
6	GOL	A	805	-	-	0/4/4/4	0/0/0/0
5	SO4	B	393	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	398	DLU	CAO-CBB	-2.72	1.47	1.51
9	A	398	DLU	OAQ-CAL	2.50	1.50	1.44



All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	398	DLU	CAO-NBD-CAK	-3.37	115.77	118.21
9	A	398	DLU	CAA-CBA-CAM	-2.67	107.50	112.71
9	A	398	DLU	CAH-CAI-CAV	-2.50	118.10	121.40
9	A	398	DLU	CAN-CAV-CAI	-2.02	116.47	121.00
9	A	398	DLU	CAL-OAQ-CBB	-2.01	107.81	110.84
9	A	398	DLU	CAW-CAY-CAS	2.55	123.66	120.32
9	A	398	DLU	CBA-NBC-CAS	2.87	123.31	118.25
9	A	398	DLU	CAO-NBD-CAY	3.42	122.82	118.68
9	A	398	DLU	CAY-CAS-NBC	3.94	118.64	113.06
9	A	398	DLU	OAQ-CAL-CAM	6.30	123.06	110.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	398	DLU	2	0
5	A	399	SO4	1	0
6	A	801	GOL	1	0
5	B	393	SO4	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

### 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	368/395 (93%)	0.13	12 (3%) 46 50	36, 52, 94, 125	0
1	B	181/395 (45%)	0.17	19 (10%) 6 5	45, 60, 139, 147	0
2	C	19/19 (100%)	-0.24	0 100 100	42, 56, 68, 73	0
3	D	17/17 (100%)	-0.37	0 100 100	51, 53, 69, 98	0
All	All	585/826 (70%)	0.12	31 (5%) 26 28	36, 55, 113, 147	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	LEU	7.1
1	B	279	ALA	4.1
1	B	295	LEU	4.0
1	B	292	LEU	4.0
1	B	260	VAL	3.8
1	B	280	ASN	3.8
1	A	358	LEU	3.7
1	B	289	GLU	3.7
1	A	17	GLN	3.6
1	B	298	ILE	3.4
1	B	288	ARG	3.4
1	B	296	GLN	3.3
1	A	19	HIS	3.2
1	A	9	ASP	3.2
1	B	297	GLU	3.2
1	A	15	LEU	3.1
1	B	116	ASP	3.1
1	B	294	LEU	3.0
1	A	16	LEU	2.9
1	B	237	GLY	2.8
1	B	281	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	299	ARG	2.7
1	B	286	LEU	2.5
1	A	20	TYR	2.4
1	B	212	TYR	2.3
1	A	153	THR	2.2
1	A	14	GLN	2.1
1	B	283	THR	2.1
1	B	282	ASP	2.1
1	A	29	THR	2.1
1	A	21	ILE	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	801	6/6	0.84	0.19	72,76,76,77	0
6	GOL	A	805	6/6	0.88	0.16	85,88,89,90	0
6	GOL	A	803	6/6	0.88	0.25	73,75,76,79	0
7	NH4	A	395	1/1	0.89	0.53	37,37,37,37	0
6	GOL	A	802	6/6	0.91	0.16	86,88,89,89	0
5	SO4	A	394	5/5	0.96	0.14	82,82,83,84	0
9	DLU	A	398	30/30	0.96	0.12	39,45,48,50	0
5	SO4	A	399	5/5	0.96	0.17	76,76,76,78	0
5	SO4	B	393	5/5	0.96	0.16	105,106,106,106	0
8	MG	A	397	1/1	0.98	0.10	46,46,46,46	0
8	MG	A	396	1/1	0.99	0.08	41,41,41,41	0
4	ZN	A	393	1/1	1.00	0.13	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.