Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:12 AM EDT

PDB ID	:	1ZD1
Title	:	Human Sulfortransferase SULT4A1
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Deposited on	:	2005-04-13
Resolution	:	2.24 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

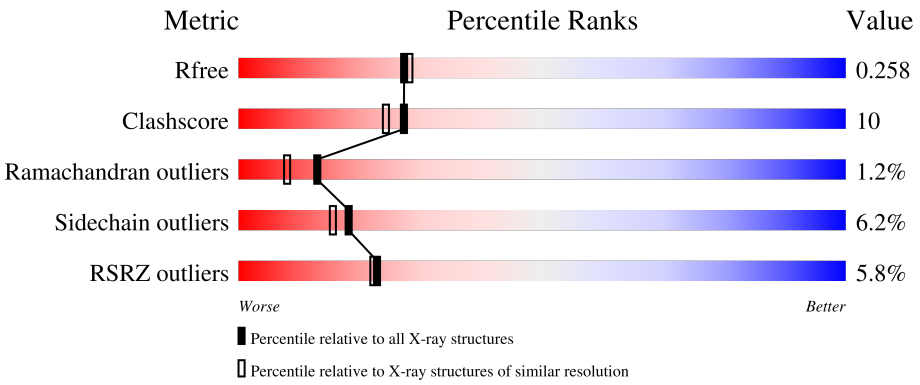
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.24 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}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	284	70% 15% • 12%
1	B	284	10% 58% 24% • 14%

2 Entry composition (i)

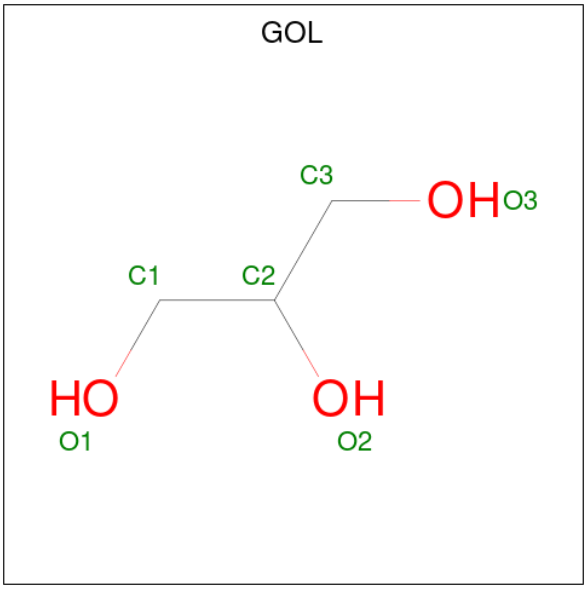
There are 3 unique types of molecules in this entry. The entry contains 4326 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sulfotransferase 4A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	2073	1339	346	373	15	0	0	0
1	B	245	2025	1310	340	360	15	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	146	146	146	0	0

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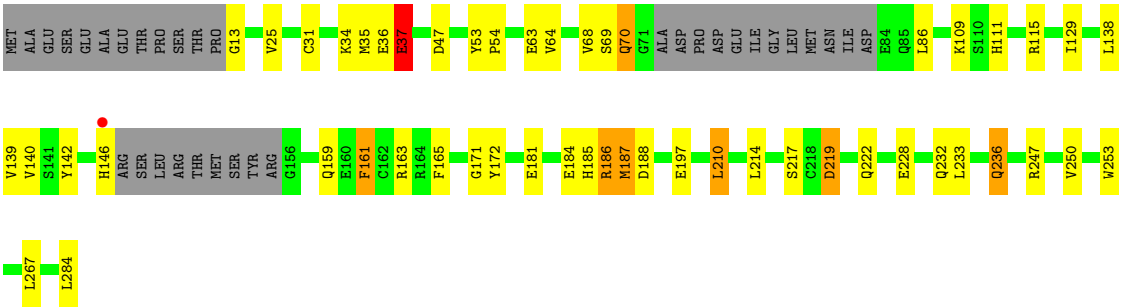
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	76	76	76	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

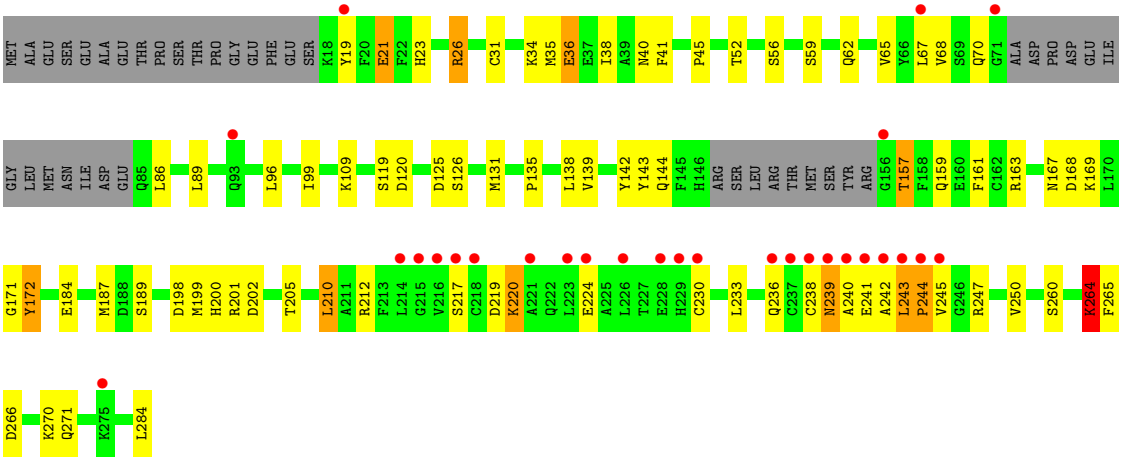
- Molecule 1: Sulfotransferase 4A1

Chain A:



- Molecule 1: Sulfotransferase 4A1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	98.94Å 74.19Å 85.83Å 90.00° 105.52° 90.00°	Depositor
Resolution (Å)	82.76 – 2.24 37.21 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.9 (82.76-2.24) 98.9 (37.21-2.24)	Depositor EDS
R_{merge}	0.87	Depositor
R_{sym}	0.87	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.262 0.185 , 0.258	Depositor DCC
R_{free} test set	1462 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.8	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	0.95	EDS
Total number of atoms	4326	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	1.29	10/2130 (0.5%)	1.12	11/2875 (0.4%)
1	B	1.08	2/2081 (0.1%)	0.99	3/2810 (0.1%)
All	All	1.19	12/4211 (0.3%)	1.05	14/5685 (0.2%)

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	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	GLU	CG-CD	7.38	1.63	1.51
1	A	161	PHE	CB-CG	-6.87	1.39	1.51
1	A	13	GLY	N-CA	6.85	1.56	1.46
1	B	264	LYS	CG-CD	5.73	1.72	1.52
1	A	37	GLU	CB-CG	5.55	1.62	1.52
1	A	250	VAL	CB-CG1	5.45	1.64	1.52
1	A	184	GLU	CG-CD	5.32	1.59	1.51
1	A	197	GLU	CD-OE1	5.13	1.31	1.25
1	A	36	GLU	CB-CG	5.10	1.61	1.52
1	A	181	GLU	CG-CD	5.07	1.59	1.51
1	B	36	GLU	CG-CD	5.07	1.59	1.51
1	A	165	PHE	CD2-CE2	5.05	1.49	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	ARG	NE-CZ-NH1	15.77	128.18	120.30
1	A	47	ASP	CB-CG-OD1	8.52	125.97	118.30
1	B	157	THR	N-CA-C	8.15	133.01	111.00
1	A	247	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	47	ASP	CB-CG-OD2	-7.84	111.25	118.30
1	B	266	ASP	CB-CG-OD2	7.36	124.93	118.30
1	A	186	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	109	LYS	CD-CE-NZ	-5.72	98.55	111.70
1	A	247	ARG	CD-NE-CZ	5.70	131.57	123.60
1	A	219	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	210	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	264	LYS	CA-CB-CG	5.27	124.99	113.40
1	A	139	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	A	187	MET	CG-SD-CE	5.04	108.27	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	244	PRO	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	2073	0	2013	33	0
1	B	2025	0	1978	49	0
2	B	6	0	8	0	0
3	A	146	0	0	4	0
3	B	76	0	0	8	1
All	All	4326	0	3999	82	1

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 10.

All (82) 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:142:TYR:CD2	1:A:161:PHE:HZ	1.72	1.08
1:A:142:TYR:CD2	1:A:161:PHE:CZ	2.47	1.02
1:B:19:TYR:CD2	1:B:26:ARG:HD3	2.08	0.89
1:B:238:CYS:HB3	1:B:242:ALA:HA	1.52	0.88
1:B:89:LEU:O	1:B:96:LEU:HD12	1.75	0.84
1:B:202:ASP:OD2	1:B:205:THR:OG1	1.95	0.84
1:B:220:LYS:O	1:B:224:GLU:HG3	1.84	0.78
1:B:31:CYS:HB3	1:B:35:MET:HE3	1.64	0.78
1:B:36:GLU:HB3	3:B:3062:HOH:O	1.87	0.74
1:A:186:ARG:HG3	1:A:187:MET:HE3	1.68	0.74
1:A:186:ARG:HG3	1:A:187:MET:CE	2.18	0.73
1:B:65:VAL:HG22	1:B:210:LEU:HD11	1.71	0.71
1:B:198:ASP:OD1	1:B:201:ARG:NH1	2.23	0.71
1:A:217:SER:HB3	3:A:428:HOH:O	1.89	0.70
1:A:142:TYR:CE2	1:A:161:PHE:HZ	2.09	0.69
1:B:89:LEU:O	1:B:96:LEU:CD1	2.40	0.69
1:B:62:GLN:HE22	1:B:109:LYS:HZ3	1.44	0.66
1:B:19:TYR:HB2	3:B:3051:HOH:O	1.96	0.65
1:B:187:MET:HB2	3:B:3011:HOH:O	1.96	0.65
1:A:146:HIS:HB2	3:A:349:HOH:O	1.96	0.65
1:B:171:GLY:HA3	3:B:3037:HOH:O	1.97	0.65
1:B:270:LYS:HE2	3:B:3048:HOH:O	1.98	0.63
1:B:36:GLU:H	1:B:36:GLU:CD	2.02	0.62
1:B:143:TYR:HD1	1:B:161:PHE:CD1	2.17	0.62
1:B:144:GLN:OE1	1:B:247:ARG:HG2	1.99	0.61
1:B:62:GLN:HE22	1:B:109:LYS:NZ	1.97	0.60
1:B:243:LEU:HD22	1:B:250:VAL:HB	1.83	0.60
1:B:200:HIS:CE1	1:B:244:PRO:HD3	2.36	0.60
1:A:185:HIS:HD2	1:A:188:ASP:OD2	1.85	0.59
1:B:52:THR:HG22	1:B:131:MET:HB2	1.85	0.59
1:B:56:SER:HB2	1:B:138:LEU:HG	1.83	0.59
1:A:37:GLU:H	1:A:37:GLU:CD	2.06	0.59
1:A:54:PRO:HG3	1:A:172:TYR:CD2	2.38	0.58
1:B:159:GLN:O	1:B:163:ARG:HG3	2.06	0.55
1:B:171:GLY:O	1:B:172:TYR:HB2	2.07	0.55
1:A:228:GLU:O	1:A:232:GLN:HG3	2.06	0.55
1:A:142:TYR:CE2	1:A:161:PHE:CZ	2.90	0.54
1:A:25:VAL:HG23	1:A:115:ARG:NH2	2.24	0.53
1:B:89:LEU:HG	1:B:96:LEU:HD11	1.90	0.53
1:A:236:GLN:HG2	3:A:378:HOH:O	2.08	0.52
1:B:239:ASN:C	1:B:241:GLU:H	2.12	0.52
1:A:171:GLY:O	1:A:172:TYR:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:HG23	1:B:89:LEU:CD2	2.39	0.52
1:A:140:VAL:HG21	1:A:253:TRP:HA	1.91	0.51
1:B:35:MET:HE2	1:B:38:ILE:HD12	1.92	0.51
1:A:186:ARG:HG3	1:A:187:MET:HE2	1.94	0.50
1:A:31:CYS:O	1:A:35:MET:HE3	2.12	0.50
1:A:111:HIS:HB2	1:A:172:TYR:CZ	2.47	0.50
1:A:63:GLU:HB3	1:A:233:LEU:HD21	1.94	0.50
1:A:69:SER:O	1:A:70:GLN:HB3	2.12	0.49
1:B:239:ASN:ND2	1:B:241:GLU:HB2	2.28	0.49
1:B:143:TYR:CD1	1:B:161:PHE:CD1	2.99	0.49
1:A:64:VAL:O	1:A:68:VAL:HG23	2.13	0.49
1:A:142:TYR:HD2	1:A:161:PHE:CZ	2.19	0.48
1:B:142:TYR:HE1	3:B:3071:HOH:O	1.97	0.48
1:B:167:ASN:O	1:B:168:ASP:HB2	2.13	0.47
1:A:185:HIS:CD2	1:A:188:ASP:OD2	2.67	0.46
1:B:68:VAL:HG11	1:B:210:LEU:HB3	1.98	0.46
1:A:159:GLN:HG2	3:A:350:HOH:O	2.16	0.46
1:A:159:GLN:O	1:A:163:ARG:HG3	2.16	0.46
1:B:62:GLN:NE2	1:B:109:LYS:NZ	2.63	0.46
1:B:21:GLU:HG3	3:B:3024:HOH:O	2.17	0.45
1:A:138:LEU:C	1:A:138:LEU:HD23	2.37	0.45
1:B:120:ASP:O	1:B:125:ASP:HB2	2.17	0.45
1:A:34:LYS:HG3	1:A:35:MET:HE2	1.99	0.44
1:B:86:LEU:HB2	1:B:109:LYS:CD	2.47	0.44
1:B:26:ARG:HE	1:B:26:ARG:HB2	1.53	0.44
1:A:219:ASP:OD1	1:A:222:GLN:HG3	2.18	0.44
1:B:135:PRO:HB2	1:B:265:PHE:HZ	1.82	0.43
1:B:67:LEU:HD23	1:B:230:CYS:SG	2.58	0.43
1:A:54:PRO:HG3	1:A:172:TYR:HD2	1.83	0.42
1:B:38:ILE:HG23	1:B:89:LEU:HD23	2.01	0.42
1:B:219:ASP:HA	3:B:3025:HOH:O	2.19	0.42
1:A:69:SER:O	1:A:70:GLN:CB	2.68	0.42
1:B:40:ASN:O	1:B:41:PHE:C	2.58	0.42
1:B:41:PHE:HZ	1:B:99:ILE:HG22	1.84	0.42
1:A:129:ILE:HD11	1:A:214:LEU:HD21	2.03	0.41
1:B:260:SER:O	1:B:264:LYS:HG3	2.19	0.41
1:A:53:TYR:CG	1:A:54:PRO:HD2	2.56	0.41
1:B:239:ASN:O	1:B:241:GLU:N	2.49	0.41
1:B:243:LEU:HD21	1:B:284:LEU:HB2	2.02	0.40
1:B:199:MET:O	1:B:199:MET:HG2	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3005:HOH:O	3:B:3065:HOH:O[4_556]	2.12	0.08

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	245/284 (86%)	238 (97%)	6 (2%)	1 (0%)	34 35
1	B	239/284 (84%)	213 (89%)	21 (9%)	5 (2%)	7 2
All	All	484/568 (85%)	451 (93%)	27 (6%)	6 (1%)	13 8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	B	157	THR
1	B	245	VAL
1	B	126	SER
1	B	240	ALA
1	B	172	TYR

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	229/258 (89%)	223 (97%)	6 (3%)	46 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	224/258 (87%)	202 (90%)	22 (10%)	8 4
All	All	453/516 (88%)	425 (94%)	28 (6%)	18 15

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	86	LEU
1	A	210	LEU
1	A	236	GLN
1	A	267	LEU
1	A	284	LEU
1	B	21	GLU
1	B	23	HIS
1	B	26	ARG
1	B	34	LYS
1	B	45	PRO
1	B	59	SER
1	B	70	GLN
1	B	119	SER
1	B	139	VAL
1	B	169	LYS
1	B	184	GLU
1	B	189	SER
1	B	210	LEU
1	B	212	ARG
1	B	217	SER
1	B	220	LYS
1	B	233	LEU
1	B	236	GLN
1	B	239	ASN
1	B	243	LEU
1	B	264	LYS
1	B	271	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	185	HIS
1	B	62	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	GOL	B	3000	-	5,5,5	0.85	0	5,5,5	0.68	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	GOL	B	3000	-	-	0/4/4/4	-

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.

No monomer is involved in short contacts.

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	251/284 (88%)	-0.34	1 (0%) 92 93	17, 27, 45, 62	0
1	B	245/284 (86%)	0.42	28 (11%) 5 4	20, 43, 78, 95	0
All	All	496/568 (87%)	0.03	29 (5%) 23 22	17, 34, 73, 95	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	ALA	6.7
1	B	218	CYS	6.1
1	B	241	GLU	5.5
1	B	275	LYS	5.4
1	B	238	CYS	4.8
1	B	237	CYS	3.9
1	B	239	ASN	3.9
1	B	156	GLY	3.7
1	B	67	LEU	3.5
1	B	221	ALA	3.4
1	B	236	GLN	3.4
1	B	226	LEU	3.1
1	B	216	VAL	3.0
1	B	71	GLY	3.0
1	B	245	VAL	2.9
1	B	217	SER	2.8
1	B	229	HIS	2.8
1	B	223	LEU	2.7
1	B	230	CYS	2.7
1	B	243	LEU	2.7
1	B	214	LEU	2.5
1	B	19	TYR	2.5
1	A	146	HIS	2.5
1	B	224	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	242	ALA	2.2
1	B	228	GLU	2.2
1	B	215	GLY	2.2
1	B	244	PRO	2.1
1	B	93	GLN	2.1

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 monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
2	GOL	B	3000	6/6	0.76	0.31	54,58,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.