Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 10:20 am BST

PDB ID	:	4ECL
Title	:	Crystal structure of the cytoplasmic domain of vancomycin resistance serine racemase VanTg
Authors	:	Stogios, P.J.; Wawrzak, Z.; Minasov, G.; Evdokimova, E.; Egorova, O.; Cosme, J.; Di Leo, R.; Krishnamoorthy, M.; Meziane-Cherif, D.; Courvalin, P.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2012-03-26
Resolution	:	2.02 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 following versions of software and data (see references (1)) were used in the production of this report:

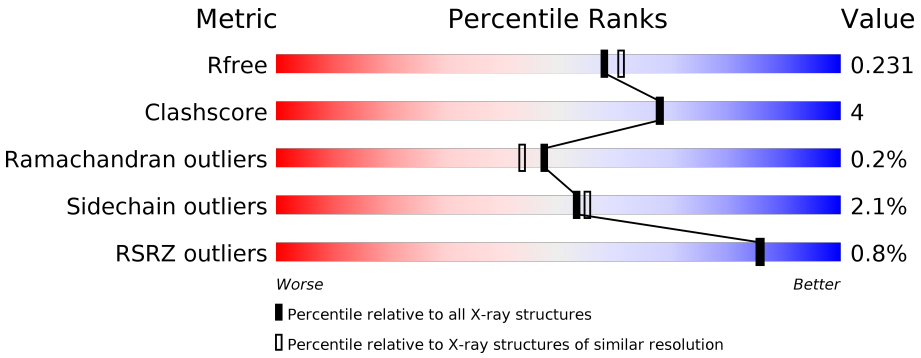
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 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	374	89% 9%
1	B	374	88% 11%
1	C	374	88% 11%
1	D	374	92% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12319 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.

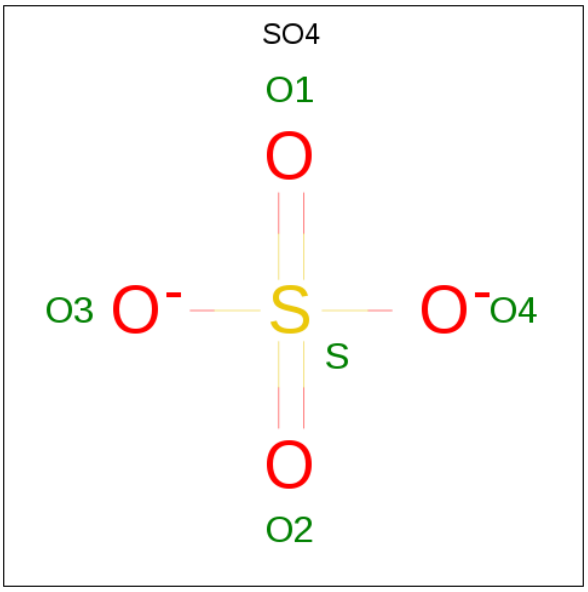
- Molecule 1 is a protein called Serine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	Se	0	0	0
			2889	1836	492	548	6	7			
1	B	369	Total	C	N	O	S	Se	0	3	0
			2892	1842	493	545	5	7			
1	C	370	Total	C	N	O	S	Se	0	7	0
			2920	1858	499	550	5	8			
1	D	369	Total	C	N	O	S	Se	0	4	0
			2890	1839	488	550	6	7			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cl	0	0
			2	2		
2	A	2	Total	Cl	0	0
			2	2		
2	D	3	Total	Cl	0	0
			3	3		
2	C	1	Total	Cl	0	0
			1	1		

- 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	B	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

- Molecule 4 is water.

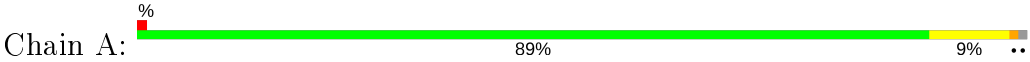
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	169	Total O 172 172	0	3
4	B	162	Total O 164 164	0	2
4	C	185	Total O 187 187	0	3
4	D	177	Total O 177 177	0	0

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 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.

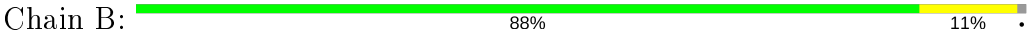
- Molecule 1: Serine racemase

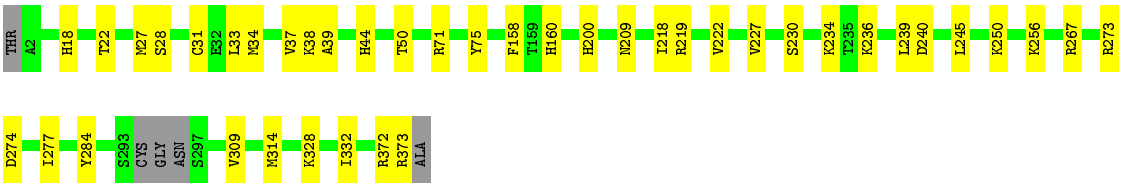
Chain A:



- Molecule 1: Serine racemase

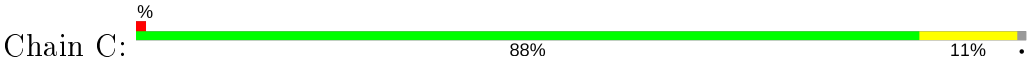
Chain B:

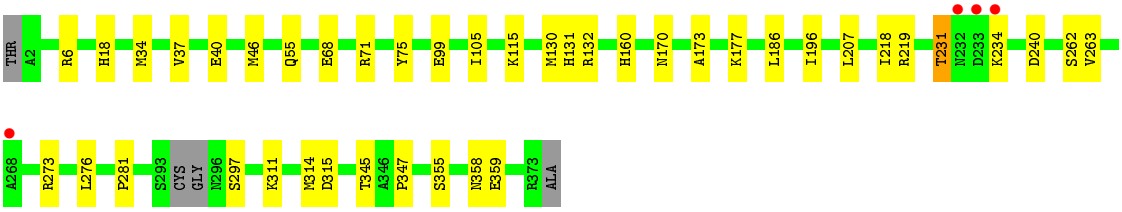




- Molecule 1: Serine racemase

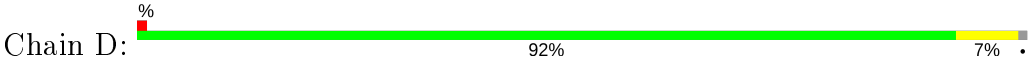
Chain C:

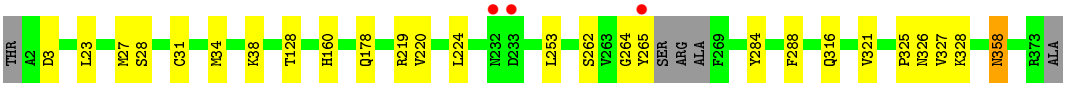




- Molecule 1: Serine racemase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.68Å 82.34Å 117.47Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	19.91 – 2.02 19.91 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.91-2.02) 90.7 (19.91-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.02Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.181 , 0.233 0.184 , 0.231	Depositor DCC
R_{free} test set	1990 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	1.595	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.010 for -k,-h,-l 0.009 for k,h,-l 0.135 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12319	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.44% 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: SO4, CL

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	0.35	0/2927	0.52	0/3943
1	B	0.35	0/2935	0.54	0/3951
1	C	0.35	0/2975	0.52	0/4004
1	D	0.36	0/2933	0.52	0/3951
All	All	0.35	0/11770	0.53	0/15849

There are no bond length outliers.

There are no bond angle outliers.

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	2889	0	2965	33	0
1	B	2892	0	2984	29	0
1	C	2920	0	3019	24	0
1	D	2890	0	2966	18	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	3	0	0	0	0
3	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	172	0	0	2	0
4	B	164	0	0	1	0
4	C	187	0	0	2	0
4	D	177	0	0	1	0
All	All	12319	0	11934	89	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 4.

All (89) 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:314:MSE:HE2	1:B:38:LYS:HG3	1.49	0.92
1:A:314:MSE:HE3	1:B:39:ALA:HB3	1.54	0.88
1:D:358:ASN:H	1:D:358:ASN:HD22	1.39	0.69
1:A:358:ASN:HD22	1:A:358:ASN:H	1.39	0.69
3:B:403:SO4:O3	4:B:656:HOH:O	2.11	0.68
3:A:403:SO4:O1	4:A:638:HOH:O	2.12	0.67
1:A:40:GLU:OE2	1:A:71:ARG:NH2	2.27	0.64
1:B:27:MSE:HG2	1:B:218:ILE:HD12	1.80	0.62
1:C:132:ARG:HD3	1:D:316:GLN:HE21	1.64	0.61
1:B:71:ARG:NH2	1:B:75:TYR:OH	2.30	0.60
1:D:321:VAL:HG21	1:D:327:VAL:HG11	1.86	0.58
1:C:55:GLN:NE2	4:C:659:HOH:O	2.26	0.57
1:D:358:ASN:H	1:D:358:ASN:ND2	2.02	0.57
1:C:18:HIS:HE1	1:C:240:ASP:O	1.87	0.56
1:A:39:ALA:CB	1:B:314:MSE:HE3	2.35	0.56
1:C:358:ASN:HD22	1:C:358:ASN:H	1.52	0.56
1:C:231:THR:HG22	1:C:347:PRO:HB2	1.87	0.56
1:C:355:SER:OG	1:C:359:GLU:OE1	2.21	0.56
1:C:311:LYS:NZ	4:C:507:HOH:O	2.38	0.56
1:D:34:MSE:CE	1:D:219:ARG:HG2	2.36	0.56
1:D:34:MSE:HE2	1:D:219:ARG:HG2	1.88	0.55
1:D:23:LEU:HD13	1:D:220[A]:VAL:HG21	1.89	0.55
1:D:27:MSE:HG2	1:D:31:CYS:HB3	1.88	0.55
1:B:222[A]:VAL:HG22	1:B:227:VAL:HG23	1.88	0.55
1:C:71[A]:ARG:NE	1:C:75:TYR:OH	2.37	0.55
1:C:314:MSE:SE	1:D:38:LYS:HE3	2.58	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:MSE:CE	1:B:38:LYS:HG3	2.30	0.54
1:B:34:MSE:CE	1:B:219:ARG:HG2	2.39	0.53
1:A:268:ALA:HB1	1:A:294:CYS:SG	2.48	0.53
1:B:160:HIS:HD2	1:B:219:ARG:HH21	1.57	0.52
1:B:18:HIS:HE1	1:B:240:ASP:O	1.94	0.51
1:C:46:MSE:HE1	1:C:68:GLU:HG2	1.92	0.51
1:A:266:SER:C	1:A:268:ALA:H	2.13	0.51
1:A:267:ARG:H	1:A:267:ARG:HE	1.57	0.51
1:A:290:ARG:NH1	4:A:658:HOH:O	2.44	0.51
1:A:358:ASN:N	1:A:358:ASN:HD22	2.09	0.50
1:A:174:PHE:HA	1:A:177:LYS:HE3	1.94	0.50
1:A:38:LYS:HG3	1:B:314:MSE:HE1	1.91	0.50
1:B:37:VAL:HG11	1:B:50:THR:HG22	1.94	0.49
1:B:273:ARG:HG3	1:B:274:ASP:O	2.13	0.49
1:A:39:ALA:HB3	1:B:314:MSE:HE3	1.93	0.49
1:A:200:HIS:HB3	1:A:217:TYR:HB2	1.96	0.48
1:D:316:GLN:NE2	4:D:501:HOH:O	2.45	0.47
1:A:47:TYR:HD1	1:A:75:TYR:CG	2.33	0.47
1:A:314:MSE:CE	1:B:39:ALA:HB3	2.36	0.46
1:A:171:ASP:OD2	1:B:267:ARG:NH2	2.49	0.46
1:C:131:HIS:HD2	1:D:262:SER:O	1.98	0.46
1:C:345:THR:HB	1:C:347:PRO:HD2	1.97	0.46
1:B:209:ASN:O	1:B:236:LYS:HD2	2.16	0.46
1:C:34:MSE:CE	1:C:219:ARG:HG2	2.46	0.45
1:A:38:LYS:HG3	1:B:314:MSE:CE	2.46	0.45
1:D:128:THR:O	1:D:178:GLN:HG2	2.17	0.45
1:D:220[A]:VAL:HG22	1:D:224:LEU:H	1.82	0.45
1:A:97:LYS:HE2	1:A:97:LYS:HB3	1.89	0.45
1:B:158:PHE:HB2	1:B:200:HIS:O	2.17	0.45
1:A:266:SER:C	1:A:268:ALA:N	2.70	0.44
1:B:284:TYR:CE1	1:B:314:MSE:HG3	2.53	0.44
1:C:6:ARG:HG3	1:C:281:PRO:HB2	1.99	0.44
1:C:105:ILE:HD12	1:D:253:LEU:HD12	1.99	0.44
1:C:130[B]:MSE:SE	1:D:264:GLY:HA2	2.68	0.44
1:B:34:MSE:HE2	1:B:219:ARG:HG2	2.00	0.44
1:A:13:LEU:HD13	1:A:52:TYR:CD1	2.53	0.44
1:A:231:THR:HA	1:A:232:ASN:HA	1.67	0.43
1:A:253:LEU:HG	1:A:254:ILE:N	2.33	0.43
1:C:37:VAL:O	1:C:46:MSE:HE2	2.19	0.43
1:C:130[B]:MSE:HE3	1:C:132:ARG:HD2	2.01	0.43
1:A:140:LYS:HD2	1:A:188:TRP:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLU:OE2	1:C:71[A]:ARG:NH2	2.32	0.42
1:C:207:LEU:HB2	1:C:218:ILE:HD13	2.02	0.42
1:A:104:LEU:HB2	1:A:124:ILE:HA	2.02	0.42
1:C:186:LEU:HD13	1:C:196:ILE:HG21	2.00	0.42
1:A:314:MSE:HE3	1:B:39:ALA:CB	2.36	0.42
1:B:31:CYS:SG	1:B:218:ILE:HG13	2.60	0.42
1:A:355:SER:OG	1:A:356:ILE:N	2.51	0.42
1:B:250:LYS:HE2	1:B:332:ILE:HG12	2.01	0.42
1:B:44:HIS:CD2	1:B:245:LEU:HB2	2.54	0.41
1:B:22:THR:HG22	1:B:239:LEU:HD13	2.02	0.41
1:B:277:ILE:HD12	1:B:309:VAL:HG21	2.02	0.41
1:C:132:ARG:HD3	1:D:316:GLN:NE2	2.32	0.41
1:D:325:PRO:HA	1:D:326:ASN:HA	1.58	0.41
1:C:173:ALA:O	1:C:177:LYS:HG2	2.20	0.41
1:D:284:TYR:HA	1:D:288:PHE:O	2.21	0.41
1:A:39:ALA:HB2	1:B:314:MSE:HE3	2.01	0.41
1:C:262:SER:OG	1:C:263:VAL:N	2.53	0.41
1:A:236:LYS:HD3	1:A:236:LYS:HA	1.87	0.41
1:A:265:TYR:O	1:A:265:TYR:CG	2.74	0.41
1:A:229:SER:HA	1:A:357:THR:HB	2.02	0.41
1:B:27:MSE:HE1	1:B:33:LEU:HA	2.03	0.41
1:A:264:GLY:O	1:A:266:SER:N	2.54	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	370/374 (99%)	357 (96%)	10 (3%)	3 (1%)	19 12
1	B	368/374 (98%)	357 (97%)	11 (3%)	0	100 100
1	C	373/374 (100%)	364 (98%)	9 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	369/374 (99%)	353 (96%)	16 (4%)	0	100 100
All	All	1480/1496 (99%)	1431 (97%)	46 (3%)	3 (0%)	47 43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	TYR
1	A	229	SER
1	A	267	ARG

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	317/311 (102%)	313 (99%)	4 (1%)	69 72
1	B	318/311 (102%)	311 (98%)	7 (2%)	52 53
1	C	323/311 (104%)	312 (97%)	11 (3%)	37 35
1	D	319/311 (103%)	313 (98%)	6 (2%)	57 59
All	All	1277/1244 (103%)	1249 (98%)	28 (2%)	53 53

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

Mol	Chain	Res	Type
1	A	138	GLU
1	A	267	ARG
1	A	315	ASP
1	A	358	ASN
1	B	28	SER
1	B	230	SER
1	B	234	LYS
1	B	256	LYS
1	B	328	LYS
1	B	372	ARG
1	B	373	ARG

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Mol	Chain	Res	Type
1	C	99	GLU
1	C	115	LYS
1	C	160	HIS
1	C	170[A]	ASN
1	C	170[B]	ASN
1	C	231	THR
1	C	234	LYS
1	C	273	ARG
1	C	276	LEU
1	C	297	SER
1	C	315	ASP
1	D	3	ASP
1	D	28	SER
1	D	160	HIS
1	D	265	TYR
1	D	328	LYS
1	D	358	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	ASN
1	B	18	HIS
1	B	24	GLN
1	C	18	HIS
1	C	102	GLN
1	C	358	ASN
1	D	316	GLN
1	D	358	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)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	SO4	B	403	-	4,4,4	0.21	0	6,6,6	0.13	0
3	SO4	A	403	-	4,4,4	0.18	0	6,6,6	0.17	0
3	SO4	D	404	-	4,4,4	0.16	0	6,6,6	0.21	0
3	SO4	C	402	-	4,4,4	0.11	0	6,6,6	0.40	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	SO4	1	0
3	A	403	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^{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	365/374 (97%)	-0.55	5 (1%) 75 74	19, 32, 59, 103	0
1	B	362/374 (96%)	-0.59	0 100 100	20, 33, 59, 100	0
1	C	363/374 (97%)	-0.49	4 (1%) 80 80	17, 32, 58, 103	0
1	D	362/374 (96%)	-0.59	3 (0%) 86 85	17, 29, 62, 101	0
All	All	1452/1496 (97%)	-0.55	12 (0%) 86 85	17, 32, 60, 103	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	233	ASP	5.3
1	D	232	ASN	3.7
1	A	232	ASN	3.3
1	A	231	THR	2.9
1	D	265	TYR	2.8
1	C	233	ASP	2.7
1	A	267	ARG	2.7
1	A	268	ALA	2.6
1	A	229	SER	2.5
1	C	232	ASN	2.4
1	C	234	LYS	2.1
1	C	268	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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^{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	B-factors(Å^2)	Q<0.9
2	CL	D	403	1/1	0.98	0.07	39,39,39,39	0
2	CL	D	402	1/1	0.98	0.07	36,36,36,36	0
2	CL	B	402	1/1	0.99	0.18	13,13,13,13	1
2	CL	A	402	1/1	0.99	0.13	20,20,20,20	1
2	CL	A	401	1/1	0.99	0.08	24,24,24,24	1
3	SO4	B	403	5/5	0.99	0.07	22,22,26,27	5
3	SO4	A	403	5/5	0.99	0.09	23,26,31,35	0
3	SO4	D	404	5/5	0.99	0.08	24,26,31,34	0
2	CL	B	401	1/1	0.99	0.09	33,33,33,33	1
3	SO4	C	402	5/5	0.99	0.08	23,26,30,30	0
2	CL	D	401	1/1	0.99	0.08	53,53,53,53	0
2	CL	C	401	1/1	0.99	0.08	33,33,33,33	1

6.5 Other polymers

There are no such residues in this entry.