Full wwPDB X-ray Structure Validation Report (i)

Apr 20, 2018 – 09:27 AM BST

PDB ID	:	6GC9
Title	:	Crystal structure of glutathione transferase Xi 1 from Trametes versicolor
Deposited on	:	2018-04-17
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

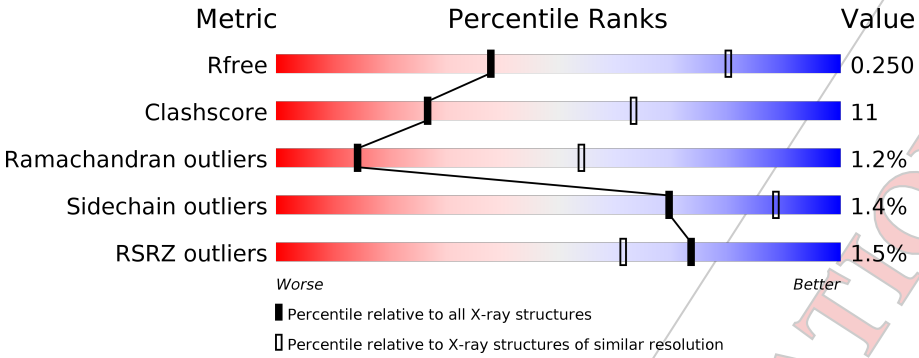
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031021
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

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 3.20 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	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

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	327	67% 24% • 8%
1	B	327	2% 65% 24% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4793 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 Glutathione transferase Xi 1 from Trametes versicolor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2429	1572	415	435	7			
1	B	292	Total	C	N	O	S	0	0	0
			2356	1526	398	425	7			

- Molecule 2 is water.

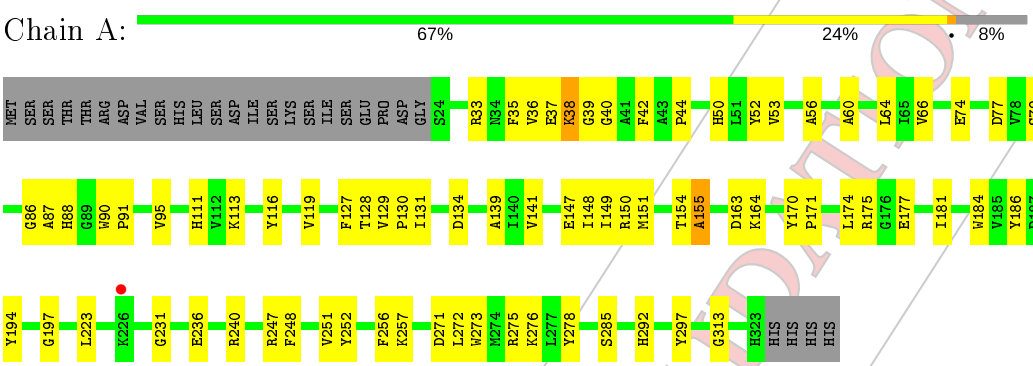
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	O	0	0
			5	5		
2	B	3	Total	O	0	0
			3	3		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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.

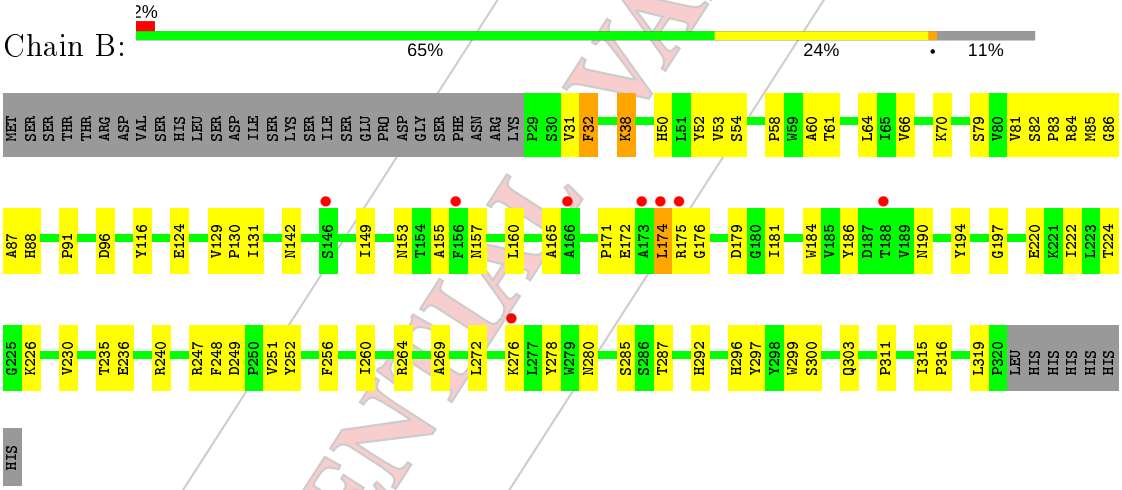
- Molecule 1: Glutathione transferase Xi 1 from Trametes versicolor

Chain A:



- Molecule 1: Glutathione transferase Xi 1 from Trametes versicolor

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	64.95Å 64.95Å 316.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.45 – 3.20 45.45 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.45-3.20) 100.0 (45.45-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.217 , 0.249 0.217 , 0.250	Depositor DCC
R_{free} test set	584 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	1.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.9	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	0.91	EDS
Total number of atoms	4793	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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

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	0.29	0/2505	0.44	0/3412
1	B	0.33	0/2429	0.47	0/3310
All	All	0.31	0/4934	0.46	0/6722

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	2429	0	2362	53	0
1	B	2356	0	2292	53	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
All	All	4793	0	4654	104	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 11.

All (104) 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:81:VAL:HG11	1:A:90:TRP:HB3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:PRO:HG2	1:B:174:LEU:HD21	1.54	0.88
1:B:175:ARG:HG3	1:B:176:GLY:H	1.48	0.77
1:B:172:GLU:HB3	1:B:175:ARG:HD3	1.67	0.75
1:B:175:ARG:HG3	1:B:176:GLY:N	2.05	0.71
1:A:56:ALA:O	1:A:247:ARG:NH1	2.26	0.68
1:B:172:GLU:HA	1:B:175:ARG:HB3	1.77	0.65
1:B:84:ARG:NH2	1:B:96:ASP:OD1	2.30	0.64
1:A:50:HIS:ND1	1:A:77:ASP:OD1	2.30	0.64
1:A:150:ARG:NH2	1:A:236:GLU:OE2	2.31	0.63
1:B:31:VAL:HG12	1:B:32:PHE:H	1.63	0.63
1:A:186:TYR:HA	1:A:190:ASN:HB2	1.79	0.63
1:B:248:PHE:HA	1:B:252:TYR:HB2	1.80	0.62
1:B:82:SER:HB3	1:B:91:PRO:HG2	1.82	0.62
1:A:53:VAL:HA	1:A:129:VAL:CG1	2.31	0.61
1:A:38:LYS:O	1:A:40:GLY:N	2.34	0.60
1:B:66:VAL:HG21	1:B:149:ILE:HB	1.83	0.60
1:A:278:TYR:O	1:A:285:SER:OG	2.20	0.59
1:B:157:ASN:HA	1:B:160:LEU:HD12	1.84	0.58
1:A:52:TYR:HB2	1:A:131:ILE:HB	1.85	0.58
1:B:175:ARG:CG	1:B:176:GLY:H	2.15	0.57
1:B:52:TYR:HB2	1:B:131:ILE:HB	1.86	0.57
1:B:171:PRO:HG2	1:B:174:LEU:CD2	2.31	0.56
1:B:61:THR:HG23	1:B:287:THR:HG22	1.87	0.56
1:A:53:VAL:HG21	1:A:64:LEU:HD21	1.88	0.56
1:B:172:GLU:CB	1:B:175:ARG:HD3	2.34	0.55
1:A:171:PRO:HG2	1:A:174:LEU:HD13	1.88	0.54
1:B:264:ARG:HD3	1:B:319:LEU:HD11	1.89	0.54
1:B:86:GLY:O	1:B:88:HIS:N	2.40	0.54
1:B:53:VAL:HG11	1:B:64:LEU:HD21	1.89	0.53
1:B:220:GLU:OE1	1:B:269:ALA:HB3	2.09	0.53
1:B:83:PRO:HD3	1:B:292:HIS:CE1	2.44	0.53
1:A:236:GLU:O	1:A:240:ARG:HG3	2.08	0.53
1:A:272:LEU:O	1:A:276:LYS:HG3	2.10	0.52
1:A:116:TYR:CE1	1:A:131:ILE:HD11	2.45	0.52
1:A:194:TYR:OH	1:A:297:TYR:OH	2.23	0.52
1:B:50:HIS:NE2	1:B:79:SER:OG	2.27	0.51
1:A:50:HIS:NE2	1:A:79:SER:OG	2.32	0.51
1:B:186:TYR:HA	1:B:190:ASN:HB2	1.93	0.51
1:A:111:HIS:HB2	1:A:113:LYS:HG2	1.93	0.50
1:A:251:VAL:HG11	1:A:297:TYR:CG	2.46	0.50
1:A:257:LYS:HD3	1:B:311:PRO:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HG21	1:A:149:ILE:HB	1.94	0.49
1:B:236:GLU:O	1:B:240:ARG:HG3	2.12	0.49
1:B:53:VAL:HB	1:B:60:ALA:HB1	1.94	0.49
1:B:116:TYR:CE2	1:B:131:ILE:HD11	2.47	0.49
1:B:38:LYS:H	1:B:38:LYS:HD3	1.78	0.48
1:B:278:TYR:O	1:B:285:SER:OG	2.30	0.48
1:A:129:VAL:CG1	1:A:130:PRO:HA	2.44	0.48
1:A:86:GLY:O	1:A:88:HIS:N	2.46	0.48
1:A:129:VAL:HG13	1:A:130:PRO:HA	1.96	0.48
1:A:33:ARG:NH1	1:A:147:GLU:OE1	2.47	0.48
1:B:85:MET:O	1:B:300:SER:HB3	2.13	0.47
1:B:194:TYR:OH	1:B:297:TYR:OH	2.25	0.47
1:A:147:GLU:O	1:A:151:MET:HG3	2.15	0.47
1:A:174:LEU:HD21	1:A:231:GLY:HA3	1.97	0.47
1:A:154:THR:HG22	1:A:155:ALA:H	1.79	0.46
1:B:53:VAL:HG21	1:B:64:LEU:HD21	1.98	0.46
1:A:53:VAL:HB	1:A:60:ALA:HB1	1.97	0.46
1:A:223:LEU:HD13	1:A:273:TRP:CG	2.51	0.46
1:A:116:TYR:OH	1:A:128:THR:O	2.25	0.46
1:B:222:ILE:O	1:B:226:LYS:HD3	2.16	0.46
1:A:197:GLY:HA3	1:A:256:PHE:CD1	2.52	0.45
1:B:276:LYS:O	1:B:280:ASN:HB2	2.16	0.45
1:A:271:ASP:OD2	1:A:275:ARG:NH1	2.49	0.45
1:A:83:PRO:HD3	1:A:292:HIS:CE1	2.52	0.45
1:B:53:VAL:HG21	1:B:64:LEU:HD11	1.98	0.45
1:B:296:HIS:O	1:B:300:SER:OG	2.34	0.45
1:B:197:GLY:HA3	1:B:256:PHE:CD1	2.52	0.44
1:B:54:SER:HB2	1:B:81:VAL:HG22	1.99	0.44
1:A:177:GLU:O	1:A:181:ILE:HG22	2.16	0.44
1:A:272:LEU:HD13	1:A:276:LYS:HD2	1.99	0.44
1:A:81:VAL:HG13	1:A:91:PRO:O	2.17	0.44
1:A:148:ILE:HA	1:A:151:MET:HE2	2.00	0.44
1:B:249:ASP:OD2	1:B:264:ARG:HB2	2.18	0.43
1:B:287:THR:HG22	1:B:287:THR:O	2.19	0.43
1:A:119:VAL:HG21	1:A:139:ALA:HA	2.01	0.43
1:A:184:TRP:O	1:A:188:THR:OG1	2.30	0.43
1:A:271:ASP:O	1:A:275:ARG:HG3	2.19	0.42
1:A:313:GLY:O	1:B:260:ILE:HA	2.19	0.42
1:B:264:ARG:HE	1:B:264:ARG:HB2	1.42	0.42
1:A:36:VAL:HA	1:A:42:PHE:O	2.20	0.42
1:B:84:ARG:HD2	1:B:299:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:HB2	1:A:95:VAL:HG23	2.01	0.42
1:B:315:ILE:HA	1:B:316:PRO:HA	1.89	0.42
1:A:134:ASP:HB2	1:A:141:VAL:CG2	2.49	0.42
1:B:220:GLU:O	1:B:224:THR:HG23	2.19	0.42
1:A:163:ASP:OD1	1:A:164:LYS:N	2.53	0.41
1:B:174:LEU:HD13	1:B:230:VAL:HG12	2.02	0.41
1:A:37:GLU:O	1:A:44:PRO:HD3	2.20	0.41
1:B:129:VAL:HG13	1:B:130:PRO:HA	2.02	0.41
1:B:160:LEU:HB2	1:B:165:ALA:HB2	2.02	0.41
1:B:235:THR:OG1	1:B:236:GLU:N	2.53	0.41
1:B:70:LYS:HE3	1:B:153:ASN:O	2.20	0.41
1:A:170:TYR:CZ	1:A:175:ARG:HG2	2.56	0.41
1:A:113:LYS:HA	1:A:127:PHE:CD1	2.54	0.41
1:A:35:PHE:CD2	1:A:151:MET:HG2	2.56	0.41
1:B:181:ILE:HA	1:B:184:TRP:NE1	2.36	0.41
1:B:251:VAL:HG11	1:B:297:TYR:CG	2.56	0.41
1:A:170:TYR:CE1	1:A:175:ARG:HG2	2.56	0.41
1:B:58:PRO:HA	1:B:247:ARG:NH2	2.35	0.41
1:A:247:ARG:HG3	1:A:252:TYR:CE2	2.56	0.41
1:A:74:GLU:O	1:A:74:GLU:HG2	2.21	0.40
1:A:248:PHE:HA	1:A:252:TYR:HB2	2.03	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	298/327 (91%)	280 (94%)	14 (5%)	4 (1%)	13	52
1	B	290/327 (89%)	275 (95%)	12 (4%)	3 (1%)	17	58
All	All	588/654 (90%)	555 (94%)	26 (4%)	7 (1%)	14	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ALA
1	A	38	LYS
1	A	39	GLY
1	B	32	PHE
1	B	87	ALA
1	B	155	ALA
1	A	87	ALA

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	260/286 (91%)	260 (100%)	0	100	100
1	B	252/286 (88%)	245 (97%)	7 (3%)	47	77
All	All	512/572 (90%)	505 (99%)	7 (1%)	69	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	LYS
1	B	124	GLU
1	B	142	ASN
1	B	174	LEU
1	B	179	ASP
1	B	272	LEU
1	B	303	GLN

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

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)

There are no ligands in this entry.

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	300/327 (91%)	-0.03	1 (0%)	93	92	32, 49, 71, 100	0
1	B	292/327 (89%)	0.35	8 (2%)	54	40	34, 59, 90, 128	0
All	All	592/654 (90%)	0.16	9 (1%)	73	61	32, 54, 85, 128	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	SER	3.4
1	B	174	LEU	3.3
1	B	175	ARG	2.9
1	B	166	ALA	2.8
1	B	156	PHE	2.7
1	B	173	ALA	2.5
1	A	226	LYS	2.2
1	B	188	THR	2.2
1	B	276	LYS	2.2

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

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

Full wwPDB X-ray Structure Validation Report (i)

Apr 18, 2018 – 04:55 PM BST

PDB ID	:	6GCA
Title	:	Crystal structure of glutathione transferase Xi 3 from Trametes versicolor
Deposited on	:	2018-04-17
Resolution	:	2.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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
Xtriage (Phenix)	:	1.13
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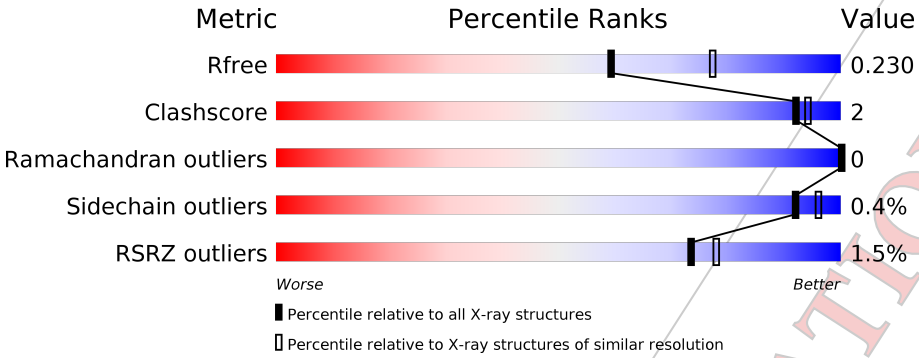
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

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 2.28 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	6121 (2.30-2.26)
Clashscore	122126	6842 (2.30-2.26)
Ramachandran outliers	120053	6755 (2.30-2.26)
Sidechain outliers	120020	6755 (2.30-2.26)
RSRZ outliers	108989	5992 (2.30-2.26)

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	325	2% 88% 7%
1	B	325	% 86% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9938 atoms, of which 4746 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 Glutathione transferase Xi 3 from Trametes versicolor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	301	Total	C	H	N	O	S	0	0	0
			4853	1595	2405	409	441	3			
1	B	293	Total	C	H	N	O	S	0	0	0
			4730	1559	2341	398	429	3			

- Molecule 2 is water.

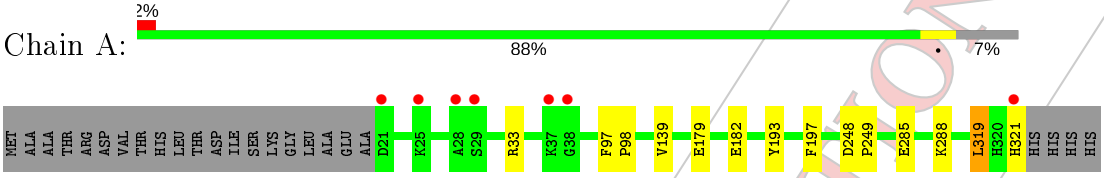
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	169	Total	O	0	0
			169	169		
2	B	186	Total	O	0	0
			186	186		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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.

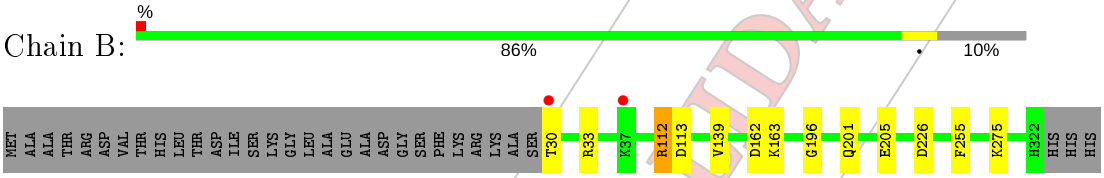
- Molecule 1: Glutathione transferase Xi 3 from Trametes versicolor

Chain A:



- Molecule 1: Glutathione transferase Xi 3 from Trametes versicolor

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	146.37Å 57.46Å 94.56Å 90.00° 107.32° 90.00°	Depositor
Resolution (Å)	36.43 – 2.28 48.68 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.2 (36.43-2.28) 98.2 (48.68-2.28)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.164 , 0.231 0.166 , 0.230	Depositor DCC
R_{free} test set	1657 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9938	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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

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	0.58	0/2522	0.65	0/3434
1	B	0.56	0/2463	0.65	0/3358
All	All	0.57	0/4985	0.65	0/6792

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	2448	2405	2404	9	0
1	B	2389	2341	2341	7	0
2	A	169	0	0	1	0
2	B	186	0	0	1	0
All	All	5192	4746	4745	16	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 2.

All (16) 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:33:ARG:NH1	1:A:139:VAL:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:O	1:A:182:GLU:HG2	2.06	0.55
1:A:319:LEU:C	1:A:321:HIS:H	2.12	0.53
1:B:226:ASP:OD1	1:B:275:LYS:NZ	2.38	0.51
1:A:285:GLU:O	1:A:288:LYS:NZ	2.44	0.50
1:A:33:ARG:NH2	2:A:402:HOH:O	2.34	0.50
1:B:112:ARG:HG3	1:B:113:ASP:N	2.26	0.48
1:B:162:ASP:OD1	1:B:163:LYS:N	2.48	0.47
1:B:33:ARG:NH1	1:B:139:VAL:O	2.50	0.45
1:A:319:LEU:O	1:A:319:LEU:HD23	2.17	0.45
1:B:30:THR:HG21	2:B:416:HOH:O	2.16	0.45
1:A:97:PHE:CD1	1:A:98:PRO:HD2	2.53	0.43
1:A:193:TYR:O	1:A:197:PHE:HB2	2.21	0.40
1:B:201:GLN:O	1:B:205:GLU:HG3	2.22	0.40
1:B:196:GLY:HA3	1:B:255:PHE:CG	2.57	0.40
1:A:248:ASP:HB2	1:A:249:PRO:HD3	2.03	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	299/325 (92%)	292 (98%)	7 (2%)	0	100	100
1	B	291/325 (90%)	282 (97%)	9 (3%)	0	100	100
All	All	590/650 (91%)	574 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	260/279 (93%)	259 (100%)	1 (0%)	92	96
1	B	254/279 (91%)	253 (100%)	1 (0%)	92	96
All	All	514/558 (92%)	512 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	LEU
1	B	112	ARG

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

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)

There are no ligands in this entry.

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	301/325 (92%)	-0.22	7 (2%)	60	66	16, 24, 44, 79	0
1	B	293/325 (90%)	-0.35	2 (0%)	87	90	17, 24, 38, 66	0
All	All	594/650 (91%)	-0.28	9 (1%)	73	78	16, 24, 42, 79	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	LYS	3.2
1	A	321	HIS	3.2
1	B	30	THR	3.2
1	A	28	ALA	3.0
1	A	37	LYS	3.0
1	A	25	LYS	2.8
1	A	21	ASP	2.3
1	A	38	GLY	2.1
1	A	29	SER	2.0

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

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

Full wwPDB X-ray Structure Validation Report (i)

Apr 18, 2018 – 04:58 PM BST

PDB ID	:	6GCB
Title	:	Crystal structure of glutathione transferase Xi 3 from Trametes versicolor in complex with glutathione
Deposited on	:	2018-04-17
Resolution	:	1.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

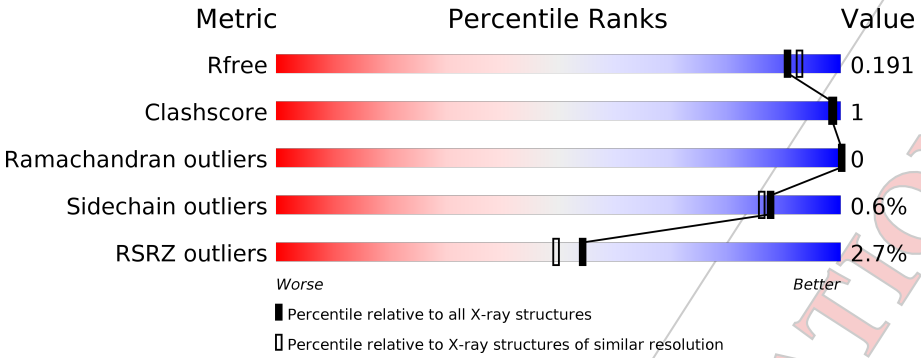
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031021
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

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 1.79 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	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

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	325	3% 88% · 10%
1	B	325	2% 88% · 10%

2 Entry composition

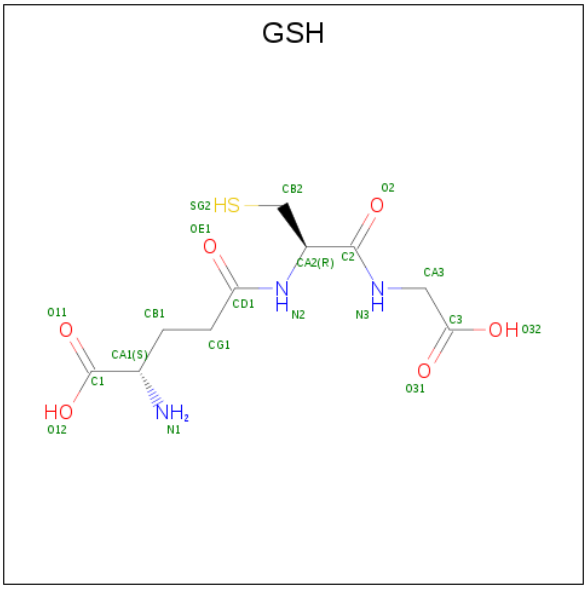
There are 3 unique types of molecules in this entry. The entry contains 9981 atoms, of which 4703 are hydrogens and 0 are deuteriums.

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 Glutathione transferase Xi 3 from Trametes versicolor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	293	Total	C	H	N	O	S	0	0	0
			4722	1553	2343	393	430	3			
1	B	291	Total	C	H	N	O	S	0	1	0
			4698	1546	2330	390	429	3			

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			35	10	15	3	6	1		
2	B	1	Total	C	H	N	O	S	0	0
			35	10	15	3	6	1		

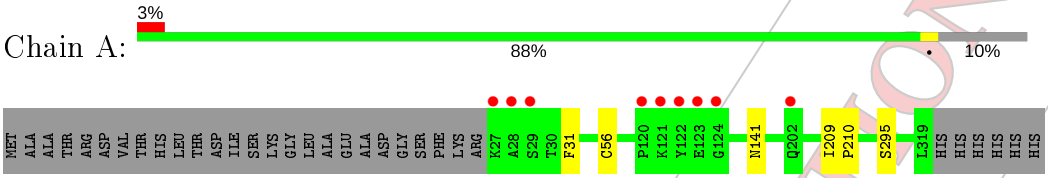
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	241	Total O 241 241	0	0
3	B	250	Total O 250 250	0	0

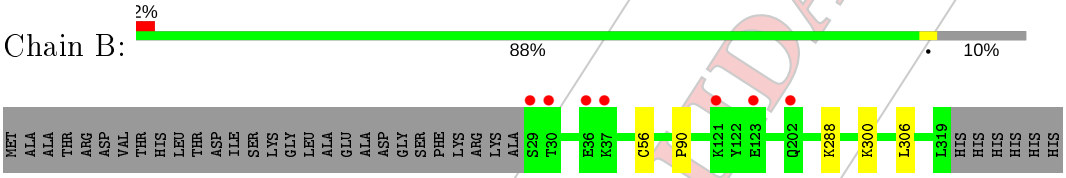
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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: Glutathione transferase Xi 3 from Trametes versicolor



- Molecule 1: Glutathione transferase Xi 3 from Trametes versicolor



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	72.37Å 72.37Å 316.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.69 – 1.79 48.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.69-1.79) 97.1 (48.69-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.161 , 0.189 0.162 , 0.191	Depositor DCC
R_{free} test set	3947 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	12.7	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.46 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9981	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: GSH

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	0.47	0/2450	0.61	0/3339
1	B	0.46	0/2442	0.59	0/3330
All	All	0.46	0/4892	0.60	0/6669

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	2379	2343	2343	3	0
1	B	2368	2330	2330	3	0
2	A	20	15	15	1	0
2	B	20	15	15	2	0
3	A	241	0	0	0	0
3	B	250	0	0	0	0
All	All	5278	4703	4703	6	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 1.

All (6) 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:B:56:CYS:HG	2:B:401:GSH:HSG	1.22	0.77
1:B:300:LYS:HG2	1:B:306:LEU:HD21	1.79	0.62
1:B:56:CYS:SG	2:B:401:GSH:SG2	2.88	0.61
1:A:56:CYS:SG	2:A:401:GSH:SG2	2.96	0.51
1:A:209:ILE:HB	1:A:210:PRO:HD3	2.00	0.44
1:A:31:PHE:O	1:A:141:ASN:HA	2.20	0.42

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	291/325 (90%)	287 (99%)	4 (1%)	0	100	100
1	B	290/325 (89%)	287 (99%)	3 (1%)	0	100	100
All	All	581/650 (89%)	574 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	253/279 (91%)	252 (100%)	1 (0%)	92	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	253/279 (91%)	251 (99%)	2 (1%)	83 80
All	All	506/558 (91%)	503 (99%)	3 (1%)	87 86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	SER
1	B	90	PRO
1	B	288	LYS

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

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)

2 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	GSH	A	401	-	11,19,19	2.27	3 (27%)	15,24,24	1.37	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GSH	B	401	-	11,19,19	2.33	2 (18%)	15,24,24	1.35	2 (13%)

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	GSH	A	401	-	-	0/18/24/24	0/0/0/0
2	GSH	B	401	-	-	0/18/24/24	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GSH	CB2-CA2	-2.57	1.50	1.53
2	A	401	GSH	C2-N3	4.52	1.42	1.33
2	A	401	GSH	CD1-N2	4.78	1.44	1.34
2	B	401	GSH	CD1-N2	4.85	1.44	1.34
2	B	401	GSH	C2-N3	5.40	1.44	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	GSH	CA2-CB2-SG2	-2.76	110.93	114.15
2	B	401	GSH	CB2-CA2-C2	-2.62	104.02	109.64
2	A	401	GSH	CA3-N3-C2	-2.48	119.09	122.40
2	A	401	GSH	CB1-CG1-CD1	-2.29	108.06	113.16
2	A	401	GSH	CA2-CB2-SG2	-2.18	111.60	114.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GSH	1	0
2	B	401	GSH	2	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	293/325 (90%)	0.04	9 (3%) 49 43	8, 12, 25, 49	0
1	B	291/325 (89%)	0.19	7 (2%) 59 54	8, 13, 26, 43	0
All	All	584/650 (89%)	0.11	16 (2%) 54 49	8, 12, 25, 49	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	LYS	6.9
1	B	30	THR	4.0
1	A	123	GLU	3.7
1	A	28	ALA	3.6
1	A	121	LYS	3.5
1	B	202	GLN	3.4
1	B	121	LYS	3.1
1	B	29	SER	3.1
1	B	123	GLU	3.0
1	A	122	TYR	2.8
1	A	29	SER	2.8
1	B	37	LYS	2.6
1	B	36	GLU	2.2
1	A	202	GLN	2.2
1	A	120	PRO	2.1
1	A	124	GLY	2.0

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 (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^{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	GSH	A	401	20/20	0.98	0.10	8,13,19,21	0
2	GSH	B	401	20/20	0.98	0.09	9,12,21,22	0

6.5 Other polymers (i)

There are no such residues in this entry.

Full wwPDB X-ray Structure Validation Report (i)

Apr 20, 2018 – 09:35 AM BST

PDB ID	:	6GCC
Title	:	Crystal structure of glutathione transferase Xi 3 mutant C56S from Trametes versicolor in complex with dextran-sulfate
Deposited on	:	2018-04-17
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

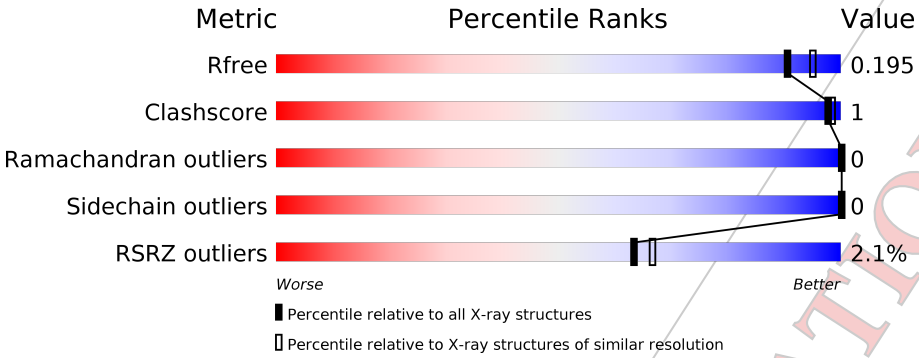
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031021
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

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 1.90 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	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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	325	2% 87% • 10%
1	B	325	2% 87% • 11%

2 Entry composition

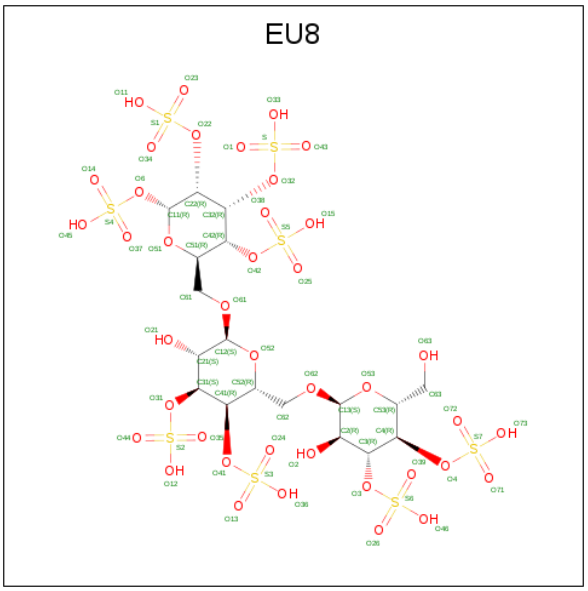
There are 3 unique types of molecules in this entry. The entry contains 10290 atoms, of which 4699 are hydrogens and 0 are deuteriums.

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 Glutathione transferase Xi 3 mutant C56S.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	H	N	O	S	0	0	0
			4690	1544	2325	390	429	2			
1	B	290	Total	C	H	N	O	S	0	1	0
			4688	1543	2326	389	428	2			

- Molecule 2 is [(2 {R},3 {R},4 {R},5 {R},6 {R})-2-[[(2 {S},3 {S},4 {S},5 {R},6 {R})-6-[[(2 {S},3 {R},4 {R},5 {R},6 {R})-6-(hydroxymethyl)-3-oxidanyl-4,5-disulfooxy-oxan-2-yl]oxymethyl]-3-oxidanyl-4,5-disulfooxy-oxan-2-yl]oxymethyl]-3,5,6-trisulfooxy-oxan-4-yl] hydrogen sulfate (three-letter code: EU8) (formula: $C_{18}H_{32}O_{40}S_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	0	0
			90	18	24	40	8		
2	B	1	Total	C	H	O	S	0	0
			90	18	24	40	8		

- Molecule 3 is water.

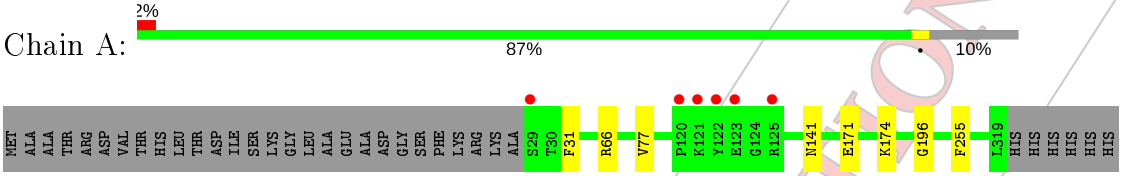
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	373	Total O 373 373	0	0
3	B	359	Total O 359 359	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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.

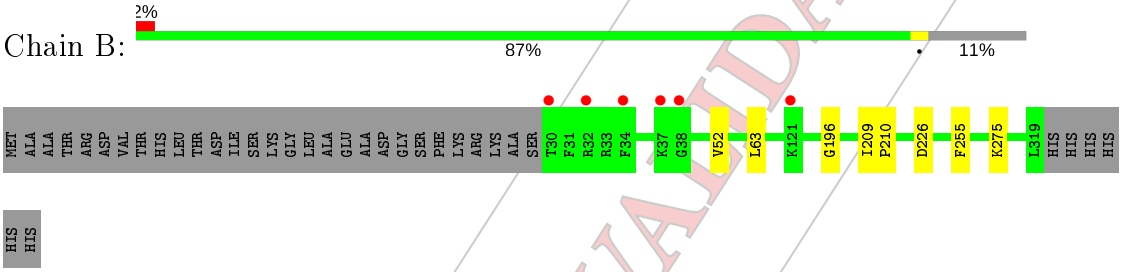
- Molecule 1: Glutathione transferase Xi 3 mutant C56S

Chain A:



- Molecule 1: Glutathione transferase Xi 3 mutant C56S

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	72.26Å 72.26Å 317.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.01 – 1.90 46.01 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.01-1.90) 97.0 (46.01-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.160 , 0.193 0.163 , 0.195	Depositor DCC
R_{free} test set	3357 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10290	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: EU8

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	0.56	0/2436	0.64	0/3321
1	B	0.54	0/2436	0.63	0/3322
All	All	0.55	0/4872	0.64	0/6643

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	2365	2325	2325	4	0
1	B	2362	2326	2325	4	0
2	A	66	24	0	0	0
2	B	66	24	0	0	0
3	A	373	0	0	0	0
3	B	359	0	0	0	0
All	All	5591	4699	4650	8	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 1.

All (8) 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:171:GLU:HA	1:A:174:LYS:HE2	1.82	0.61
1:B:52:VAL:HG21	1:B:63:LEU:HD21	1.98	0.45
1:B:209:ILE:HB	1:B:210:PRO:HD3	2.01	0.43
1:A:196:GLY:HA3	1:A:255:PHE:CD1	2.55	0.42
1:B:196:GLY:HA3	1:B:255:PHE:CD1	2.55	0.41
1:A:66:ARG:CZ	1:A:77:VAL:HG23	2.51	0.41
1:B:226:ASP:OD1	1:B:275:LYS:NZ	2.53	0.40
1:A:31:PHE:O	1:A:141:ASN:HA	2.21	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	289/325 (89%)	283 (98%)	6 (2%)	0	100	100
1	B	289/325 (89%)	286 (99%)	3 (1%)	0	100	100
All	All	578/650 (89%)	569 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	252/279 (90%)	252 (100%)	0	100	100
1	B	252/279 (90%)	252 (100%)	0	100	100
All	All	504/558 (90%)	504 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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)

2 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	EU8	A	400	-	67,68,68	1.70	16 (23%)	79,109,109	2.42	29 (36%)
2	EU8	B	400	-	67,68,68	1.79	16 (23%)	79,109,109	2.78	33 (41%)

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	EU8	A	400	-	-	1/50/112/112	0/3/3/3
2	EU8	B	400	-	-	1/50/112/112	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	EU8	O22-C22	-3.98	1.38	1.46
2	B	400	EU8	O4-C4	-3.33	1.39	1.46
2	B	400	EU8	O41-C41	-3.30	1.39	1.46
2	A	400	EU8	O22-C22	-3.26	1.39	1.46
2	B	400	EU8	O31-C31	-3.15	1.39	1.46
2	A	400	EU8	O31-C31	-3.01	1.40	1.46
2	A	400	EU8	O42-C42	-2.94	1.40	1.46
2	A	400	EU8	O3-C3	-2.93	1.40	1.46
2	B	400	EU8	O42-C42	-2.76	1.40	1.46
2	B	400	EU8	O3-C3	-2.66	1.40	1.46
2	A	400	EU8	O4-C4	-2.63	1.40	1.46
2	A	400	EU8	O41-C41	-2.58	1.41	1.46
2	A	400	EU8	O32-C32	-2.20	1.41	1.46
2	B	400	EU8	O32-C32	-2.18	1.41	1.46
2	A	400	EU8	C22-C32	2.20	1.56	1.52
2	B	400	EU8	C22-C32	2.47	1.57	1.52
2	A	400	EU8	O4-S7	2.98	1.65	1.56
2	B	400	EU8	O4-S7	3.09	1.65	1.56
2	B	400	EU8	O31-S2	3.12	1.65	1.56
2	A	400	EU8	O31-S2	3.15	1.65	1.56
2	A	400	EU8	O3-S6	3.15	1.65	1.56
2	B	400	EU8	O41-S3	3.33	1.66	1.56
2	B	400	EU8	O3-S6	3.44	1.66	1.56
2	B	400	EU8	O22-S1	3.50	1.66	1.56
2	A	400	EU8	O22-S1	3.51	1.66	1.56
2	A	400	EU8	O41-S3	3.76	1.67	1.56
2	A	400	EU8	O32-S	3.82	1.67	1.56
2	B	400	EU8	O32-S	4.02	1.67	1.56
2	A	400	EU8	O42-S5	4.07	1.68	1.56
2	B	400	EU8	O42-S5	4.26	1.68	1.56
2	A	400	EU8	O6-S4	4.58	1.69	1.56
2	B	400	EU8	O6-S4	4.93	1.70	1.56

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	EU8	C61-C51-C42	-4.80	101.23	113.31
2	A	400	EU8	C61-C51-C42	-4.35	102.37	113.31
2	B	400	EU8	C2-C3-C4	-4.26	101.99	111.67
2	A	400	EU8	C13-C2-C3	-4.13	102.90	110.08
2	B	400	EU8	C62-C52-C41	-4.01	103.23	113.31
2	B	400	EU8	C13-C2-C3	-3.95	103.23	110.08
2	A	400	EU8	O4-C4-C3	-3.91	99.85	108.46
2	B	400	EU8	O37-S4-O14	-3.78	95.91	112.25
2	B	400	EU8	C31-O31-S2	-3.58	112.08	118.97
2	A	400	EU8	C2-C3-C4	-3.24	104.32	111.67
2	A	400	EU8	C62-C52-C41	-3.23	105.18	113.31
2	A	400	EU8	O37-S4-O14	-3.10	98.86	112.25
2	B	400	EU8	O51-C11-C22	-2.75	104.02	109.50
2	B	400	EU8	O45-S4-O14	-2.68	99.29	108.79
2	A	400	EU8	O52-C12-C21	-2.40	105.20	110.34
2	B	400	EU8	O22-C22-C32	-2.35	103.28	108.46
2	B	400	EU8	O36-S3-O13	-2.33	100.52	108.79
2	A	400	EU8	O1-S-O43	-2.32	102.24	112.25
2	A	400	EU8	O36-S3-O13	-2.27	100.74	108.79
2	A	400	EU8	O25-S5-O38	-2.26	102.51	112.25
2	B	400	EU8	O13-S3-O24	-2.24	102.56	112.25
2	B	400	EU8	O53-C13-O62	-2.24	104.66	109.96
2	B	400	EU8	O25-S5-O38	-2.09	103.20	112.25
2	B	400	EU8	O4-C4-C3	-2.07	103.91	108.46
2	B	400	EU8	O1-S-O43	-2.03	103.47	112.25
2	A	400	EU8	O12-S2-O35	-2.03	101.60	108.79
2	A	400	EU8	O13-S3-O24	-2.02	103.52	112.25
2	A	400	EU8	C32-O32-S	-2.00	115.12	118.97
2	B	400	EU8	O2-C2-C3	2.24	115.98	109.93
2	A	400	EU8	O42-C42-C32	2.26	113.43	108.46
2	A	400	EU8	O22-C22-C11	2.28	110.73	107.58
2	B	400	EU8	O51-C11-O6	2.34	114.37	107.99
2	A	400	EU8	O51-C11-O6	2.47	114.72	107.99
2	A	400	EU8	C31-C41-C52	2.79	116.46	110.55
2	B	400	EU8	C61-O61-C12	2.98	119.77	113.80
2	A	400	EU8	C61-O61-C12	2.98	119.78	113.80
2	B	400	EU8	O42-C42-C32	3.00	115.06	108.46
2	A	400	EU8	O2-C2-C13	3.05	117.55	110.06
2	B	400	EU8	O52-C52-C41	3.07	116.28	109.76
2	A	400	EU8	C41-O41-S3	3.18	125.08	118.97
2	B	400	EU8	C31-C41-C52	3.19	117.30	110.55
2	A	400	EU8	O52-C52-C41	3.26	116.69	109.76
2	B	400	EU8	O22-C22-C11	3.27	112.11	107.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	EU8	C11-C22-C32	3.31	117.48	110.75
2	B	400	EU8	O2-C2-C13	3.73	119.22	110.06
2	B	400	EU8	C22-C32-C42	3.91	119.03	110.43
2	A	400	EU8	O62-C62-C52	4.03	116.92	109.14
2	A	400	EU8	C22-C32-C42	4.18	119.64	110.43
2	A	400	EU8	O62-C13-C2	4.37	115.30	108.24
2	B	400	EU8	O52-C52-C62	4.52	115.66	106.64
2	A	400	EU8	O52-C52-C62	4.68	115.99	106.64
2	B	400	EU8	C41-O41-S3	4.88	128.35	118.97
2	B	400	EU8	O62-C62-C52	5.18	119.15	109.14
2	A	400	EU8	C4-O4-S7	5.53	129.61	118.97
2	B	400	EU8	O51-C51-C61	5.75	118.13	106.64
2	A	400	EU8	O51-C51-C61	5.77	118.17	106.64
2	B	400	EU8	C3-O3-S6	5.98	130.47	118.97
2	A	400	EU8	O6-C11-C22	6.12	118.19	107.19
2	A	400	EU8	C3-O3-S6	6.24	130.97	118.97
2	B	400	EU8	O62-C13-C2	6.83	119.28	108.24
2	B	400	EU8	C4-O4-S7	6.85	132.16	118.97
2	B	400	EU8	O6-C11-C22	8.54	122.55	107.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	EU8	S7-O4-C4-C53
2	A	400	EU8	S7-O4-C4-C53

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

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	291/325 (89%)	-0.26	6 (2%) 63 66	13, 18, 32, 54	0
1	B	290/325 (89%)	-0.14	6 (2%) 63 66	13, 19, 34, 50	0
All	All	581/650 (89%)	-0.20	12 (2%) 63 66	13, 19, 33, 54	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	LYS	5.0
1	A	123	GLU	3.5
1	A	29	SER	3.5
1	B	30	THR	3.2
1	B	32	ARG	2.8
1	B	34	PHE	2.5
1	B	37	LYS	2.5
1	B	38	GLY	2.4
1	A	122	TYR	2.2
1	A	125	ARG	2.2
1	B	121	LYS	2.2
1	A	120	PRO	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 (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^{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	EU8	A	400	66/66	0.92	0.19	25,44,67,83	0
2	EU8	B	400	66/66	0.93	0.15	23,41,62,84	0

6.5 Other polymers (i)

There are no such residues in this entry.