



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 12:21 am BST

PDB ID : 3KZS  
Title : Crystal structure of glycosyl hydrolase family 5 (NP\_809925.1) from BACTEROIDES THETA IOTA MICRON VPI-5482 at 2.10 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2009-12-08  
Resolution : 2.10 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (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

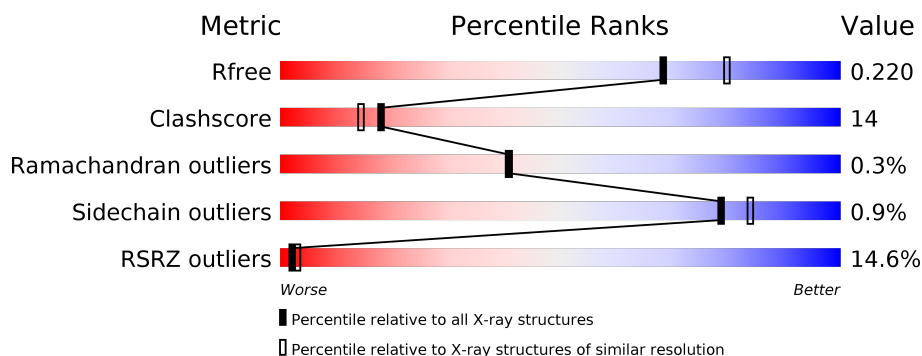
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	463	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	B	463	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	C	463	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>
1	D	463	<div> <div>50%</div> <div> <div>40%</div> <div>57%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MRD	B	485	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20249 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 glycosyl hydrolase family 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	Se	0	14	0
			3838	2459	649	712	3	15			
1	B	456	Total	C	N	O	S	Se	0	9	0
			3799	2434	643	704	3	15			
1	C	456	Total	C	N	O	S	Se	0	10	0
			3808	2440	645	705	3	15			
1	D	457	Total	C	N	O	S	Se	0	457	0
			7436	4756	1264	1380	6	30			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP Q8A905
B	0	GLY	-	leader sequence	UNP Q8A905
C	0	GLY	-	leader sequence	UNP Q8A905
D	0	GLY	-	leader sequence	UNP Q8A905

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



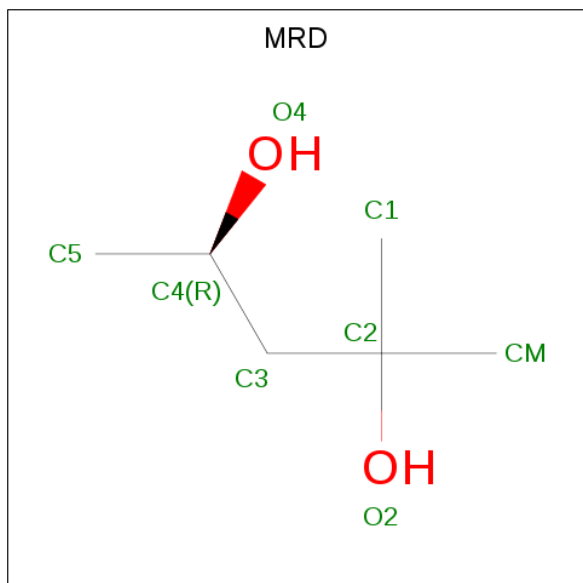
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

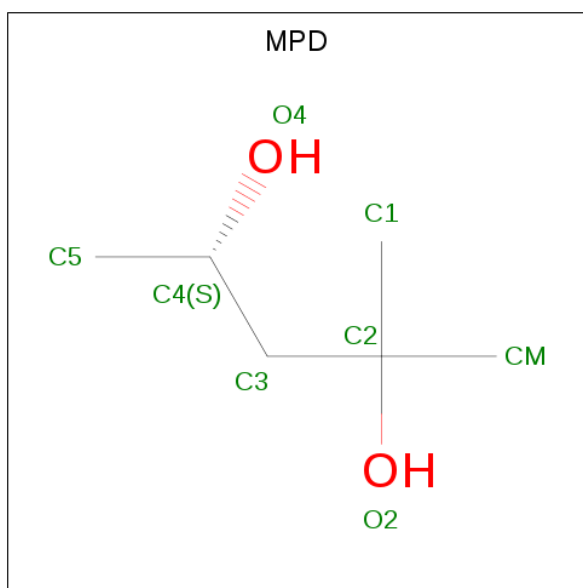
- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:

C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		

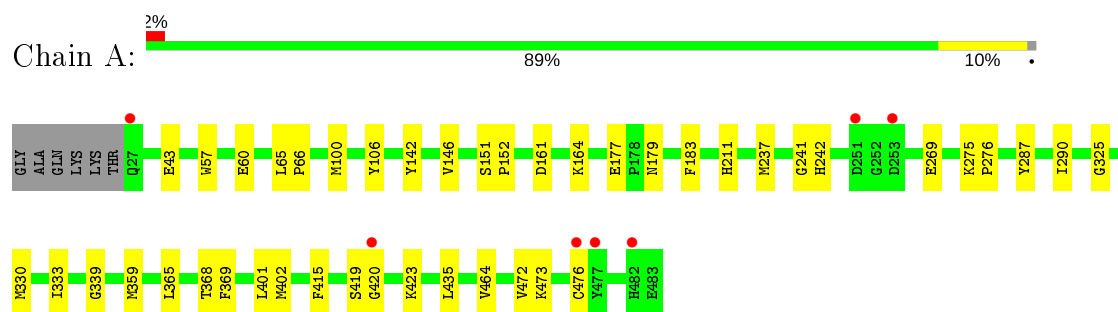
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	404	Total	O	0	0
			404	404		
5	B	352	Total	O	0	0
			352	352		
5	C	411	Total	O	0	0
			411	411		
5	D	41	Total	O	0	0
			41	41		

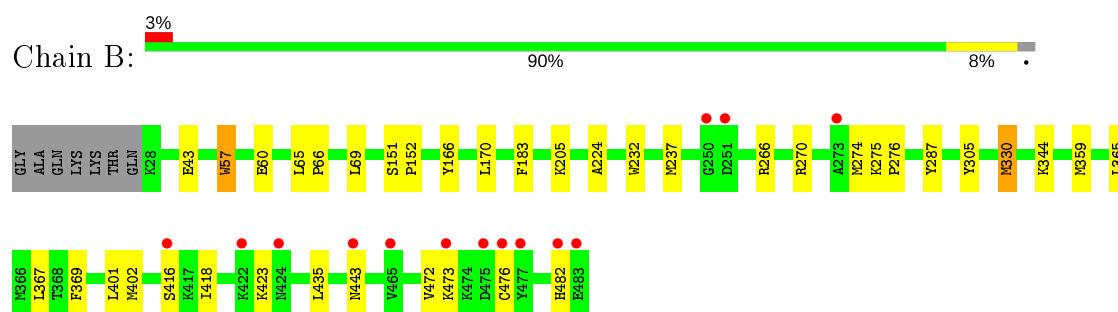
### 3 Residue-property plots [i](#)

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.

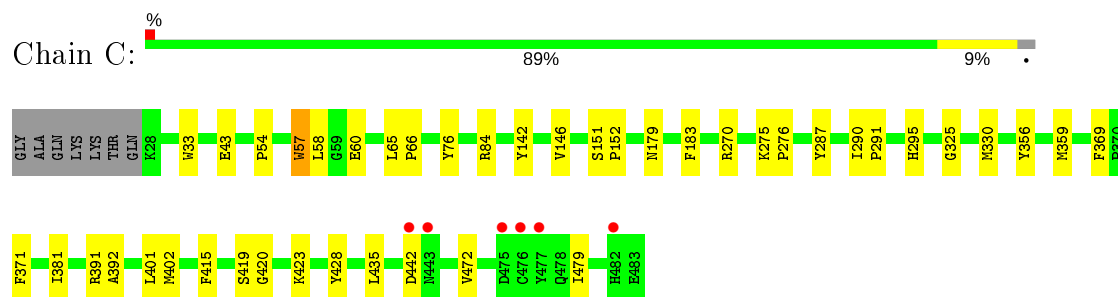
- Molecule 1: glycosyl hydrolase family 5



- Molecule 1: glycosyl hydrolase family 5



- Molecule 1: glycosyl hydrolase family 5



- Molecule 1: glycosyl hydrolase family 5





S467	Y404	G339	A278	L212	P152	R84	GLY
S468		A340	M274	M213	V153	G85	ALA
K469	T407	Y341	K276	T214	S154	Y86	GLN
D470		G342	P276	F215	H155	N87	LYS
Y471	M411	A343	M277	H216	G156	V88	LYS
Y472	E412		K278	P217	E157	I89	THR
K473	V413	P346	P279	R218	M158	Q90	Q27
K474	D414	M347	V280	G219	N159	Y91	K28
D475	F415	Y348	I281	R220	V160	Q92	T29
C476	S416	D349	D282	T221	Q162	T93	Y30
Y477	K417	A350	G283	T222	Q162	L94	I31
Q478	I418	L351	E284	S223	A163	N95	P32
I479	S419	M352	P285	A224	K164	N96	W33
D480	G420	D353	I286	T225	A165	Y97	S34
T481	K421	P354	Y287	W226	Y166	P98	N35
H482	K422	G355	E288	F227	G167	S99	G36
E483	K423	Y356	E289	N228	K168	M100	K37
	N424	N357	I290	N229	F169	N101	L38
	A425	Q358	P291	A230	L170	I102	V39
	W426	M359	H292	P231	A171	Y103	V40
	W427	K360	G293	W232	E172	G104	S41
	Y428	Y361	L294	L233	R173	Q105	E42
	T429	L362	H295	D234	Y174	Y106	E43
	T430	K363	D296	F235	K175		G44
	K431	M364	E297	N236	D176		R45
	D432	L365	H298	M237	E177		Y46
	G433	M366	E299	F238	P178		L47
	K434	L367	L300		M179		K48
	L435	T368	L301	G241	I180		H49
	E436	F369	W302	H242	K115		E50
	Y437	P370	W302	R243	N116		M51
	L438	F371	Y305	R244	W182		G52
	G439	F372	D306	Y245	F183		T53
	E440	E373	V307	G246	G185		P54
	F441	R374	R308	Q247	G186		F55
	D442	V375	R309	R248	D187		F56
	R443	P376	Y310	F249	I188		W57
	G444	D377	A311	G250	R189		L58
	Y445	Q378	Y312	D251	G190		G59
	H446	S379	W313	G252	D127		E60
	K447	V380	S314	Y254	M129		T61
	F448	I381	V315	D253	V192		G62
	H449	A382	F316	P255	T194		W63
	H450	G383	F320	L256	A195		L64
	D451	Q384	G321	E257	E196		L65
	G453	N385		N259	W197		P66
	Y454	Y389	Y324	T260	E198		E67
	S455		G325	E261	A199		R68
	S456		H326	E262	L200		L69
	G457	I393	N327	D263	A201		N70
	D459	A394	S328	N264	T202		E73
	H460		I329	W265	S203		E76
	Y461	G397	M330	R266	L204		Y76
	L462	N398	Q331	R267	K205		E79
	T463	D399	F332	V268	C147		Q80
	V464	Y400	I333	E269	C147		C81
	W465	L401	V337	R270	D208		Q82
	D466	M402	G338	S271	K209		R83
		V403		M272	M210		
					S151		

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	261.33Å 261.33Å 183.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.18 – 2.10 85.18 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (85.18-2.10) 100.0 (85.18-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0053	Depositor
R, $R_{free}$	0.185 , 0.222 0.186 , 0.220	Depositor DCC
$R_{free}$ test set	6991 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, MPD, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.69	0/3982	0.48	0/5363
1	B	0.67	1/3929 (0.0%)	0.47	0/5295
1	C	0.68	0/3941	0.49	0/5310
1	D	0.41	0/7634	0.39	0/10294
All	All	0.59	1/19486 (0.0%)	0.45	0/26262

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	330	MSE	CB-CG	-5.14	1.37	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3838	0	3621	33	0
1	B	3799	0	3573	29	0
1	C	3808	0	3586	29	0
1	D	7436	0	6920	394	0
2	A	30	0	0	0	0
2	B	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	25	0	0	1	0
3	A	24	0	42	5	0
3	B	24	0	42	7	0
3	C	16	0	28	4	0
4	C	16	0	28	5	0
5	A	404	0	0	2	0
5	B	352	0	0	0	0
5	C	411	0	0	2	0
5	D	41	0	0	6	0
All	All	20249	0	17840	498	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 14.

The worst 5 of 498 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)
3:A:485:MRD:C5	3:A:485:MRD:HMC2	1.50	1.40
3:A:485:MRD:H5C3	3:A:485:MRD:CM	1.51	1.36
1:D:42[A]:GLU:OE1	1:D:43[A]:GLU:N	1.63	1.32
1:D:65[A]:LEU:HD13	1:D:69[A]:LEU:HD12	1.31	1.12
1:D:65[A]:LEU:CD1	1:D:69[A]:LEU:HD12	1.81	1.10

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	469/463 (101%)	452 (96%)	17 (4%)	0	100	100
1	B	463/463 (100%)	444 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	464/463 (100%)	444 (96%)	20 (4%)	0	100	100
1	D	910/463 (196%)	834 (92%)	66 (7%)	10 (1%)	14	9
All	All	2306/1852 (124%)	2174 (94%)	122 (5%)	10 (0%)	41	32

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	41[A]	SER
1	D	41[B]	SER
1	D	295[A]	HIS
1	D	295[B]	HIS
1	D	478[A]	GLN

### 5.3.2 Protein sidechains ⓘ

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	401/380 (106%)	398 (99%)	3 (1%)	84	88
1	B	395/380 (104%)	392 (99%)	3 (1%)	81	86
1	C	396/380 (104%)	392 (99%)	4 (1%)	76	82
1	D	758/380 (200%)	750 (99%)	8 (1%)	73	79
All	All	1950/1520 (128%)	1932 (99%)	18 (1%)	78	84

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	60	GLU
1	C	330	MSE
1	D	129[A]	MSE
1	C	43	GLU
1	C	57	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	295	HIS
1	B	116	ASN
1	C	116	ASN
1	C	298	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

26 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	SO4	A	6	-	4,4,4	0.12	0	6,6,6	0.11	0
2	SO4	C	1	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	A	5	-	4,4,4	0.18	0	6,6,6	0.08	0
2	SO4	A	15	-	4,4,4	1.34	0	6,6,6	0.33	0
3	MRD	C	484	-	7,7,7	0.26	0	9,10,10	0.32	0
4	MPD	C	17	-	7,7,7	0.39	0	9,10,10	0.29	0
3	MRD	C	20	-	7,7,7	0.54	0	9,10,10	0.25	0
2	SO4	A	9	-	4,4,4	0.18	0	6,6,6	0.14	0
3	MRD	B	485	-	7,7,7	0.34	0	9,10,10	0.20	0
3	MRD	A	485	-	7,7,7	0.46	0	9,10,10	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	16	-	4,4,4	0.19	0	6,6,6	0.10	0
2	SO4	A	12	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	13	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	C	4	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	C	11	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	B	7	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SO4	C	14	-	4,4,4	0.17	0	6,6,6	0.09	0
4	MPD	C	485	-	7,7,7	0.42	0	9,10,10	0.16	0
3	MRD	A	19	-	7,7,7	0.47	0	9,10,10	0.17	0
2	SO4	C	8	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	B	10	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	B	2	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	A	3	-	4,4,4	0.17	0	6,6,6	0.13	0
3	MRD	B	18	-	7,7,7	0.46	0	9,10,10	0.32	0
3	MRD	A	484	-	7,7,7	0.41	0	9,10,10	0.15	0
3	MRD	B	484	-	7,7,7	0.35	0	9,10,10	0.25	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
3	MRD	A	485	-	-	5/5/5/5	-
3	MRD	A	19	-	-	2/5/5/5	-
3	MRD	B	485	-	-	3/5/5/5	-
4	MPD	C	485	-	-	4/5/5/5	-
3	MRD	C	484	-	-	2/5/5/5	-
4	MPD	C	17	-	-	4/5/5/5	-
3	MRD	C	20	-	-	0/5/5/5	-
3	MRD	B	18	-	-	2/5/5/5	-
3	MRD	A	484	-	-	0/5/5/5	-
3	MRD	B	484	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	484	MRD	C2-C3-C4-O4
4	C	17	MPD	CM-C2-C3-C4
4	C	17	MPD	C2-C3-C4-O4
3	A	485	MRD	CM-C2-C3-C4
3	A	485	MRD	C2-C3-C4-O4

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	SO4	1	0
3	C	484	MRD	3	0
4	C	17	MPD	2	0
3	C	20	MRD	1	0
3	B	485	MRD	6	0
3	A	485	MRD	5	0
4	C	485	MPD	3	0
3	B	18	MRD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	442/463 (95%)	-0.07	7 (1%) 72 75	11, 20, 38, 55	0
1	B	441/463 (95%)	0.01	14 (3%) 47 54	14, 24, 42, 60	0
1	C	441/463 (95%)	-0.15	6 (1%) 75 78	13, 20, 36, 57	0
1	D	442/463 (95%)	2.24	230 (52%) 0 0	26, 32, 42, 59	0
All	All	1766/1852 (95%)	0.51	257 (14%) 2 3	11, 25, 41, 60	0

The worst 5 of 257 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	477[A]	TYR	7.2
1	D	470[A]	ASP	7.0
1	A	476	CYS	6.8
1	D	464[A]	VAL	6.1
1	D	184[A]	ILE	5.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MRD	C	484	8/8	0.62	0.35	74,76,77,78	0
2	SO4	A	15	5/5	0.63	0.22	22,22,26,36	0
2	SO4	B	13	5/5	0.77	0.27	83,83,84,84	0
2	SO4	A	6	5/5	0.78	0.20	74,74,75,76	0
4	MPD	C	485	8/8	0.80	0.34	38,44,46,46	0
3	MRD	B	485	8/8	0.84	0.30	51,53,55,57	0
4	MPD	C	17	8/8	0.86	0.21	47,47,48,49	0
2	SO4	A	12	5/5	0.87	0.18	67,67,69,69	0
2	SO4	B	7	5/5	0.88	0.15	74,74,75,76	0
3	MRD	B	18	8/8	0.89	0.22	48,49,51,53	0
3	MRD	A	485	8/8	0.90	0.18	45,46,48,48	0
3	MRD	C	20	8/8	0.90	0.14	29,34,37,39	0
3	MRD	A	19	8/8	0.91	0.19	37,41,44,46	0
3	MRD	B	484	8/8	0.92	0.11	34,36,38,41	0
3	MRD	A	484	8/8	0.93	0.15	32,35,40,42	0
2	SO4	A	3	5/5	0.94	0.15	54,55,56,57	0
2	SO4	C	8	5/5	0.94	0.14	63,64,65,65	0
2	SO4	A	5	5/5	0.96	0.13	50,51,53,55	0
2	SO4	B	16	5/5	0.96	0.13	56,57,58,59	0
2	SO4	C	14	5/5	0.97	0.15	57,58,59,60	0
2	SO4	A	9	5/5	0.97	0.10	43,44,44,45	0
2	SO4	C	11	5/5	0.98	0.11	36,37,38,38	0
2	SO4	C	1	5/5	0.98	0.13	44,45,47,47	0
2	SO4	B	10	5/5	0.98	0.14	38,39,40,41	0
2	SO4	B	2	5/5	0.98	0.12	46,47,49,49	0
2	SO4	C	4	5/5	0.99	0.15	41,42,46,46	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.