



# Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2025 – 02:20 AM EDT

PDB ID : 2ZXL / pdb\_00002zxl  
Title : Crystal structure of red chlorophyll catabolite reductase from *Arabidopsis thaliana*  
Authors : Sugishima, M.; Kitamori, Y.; Fukuyama, K.  
Deposited on : 2008-12-29  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

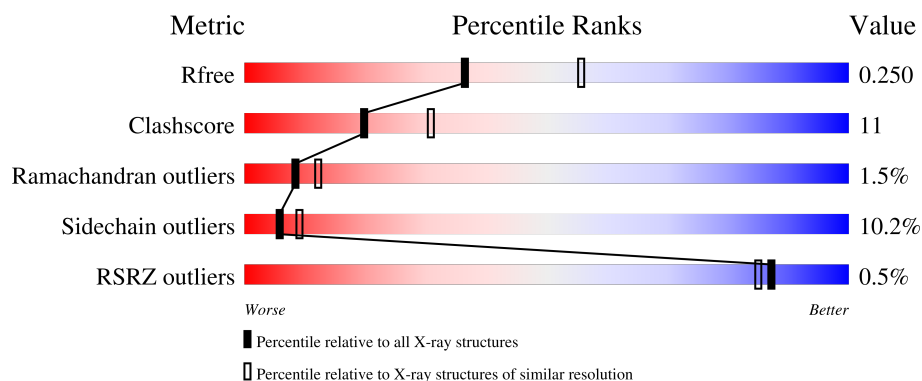
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	285	
1	B	285	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4466 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 Red chlorophyll catabolite reductase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2192	1381	379	422	10			
1	B	278	Total	C	N	O	S	0	0	0
			2160	1361	371	418	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	GLY	-	expression tag	UNP Q8LDU4
A	36	PRO	-	expression tag	UNP Q8LDU4
A	37	LEU	-	expression tag	UNP Q8LDU4
A	38	GLY	-	expression tag	UNP Q8LDU4
A	39	SER	-	expression tag	UNP Q8LDU4
B	35	GLY	-	expression tag	UNP Q8LDU4
B	36	PRO	-	expression tag	UNP Q8LDU4
B	37	LEU	-	expression tag	UNP Q8LDU4
B	38	GLY	-	expression tag	UNP Q8LDU4
B	39	SER	-	expression tag	UNP Q8LDU4

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

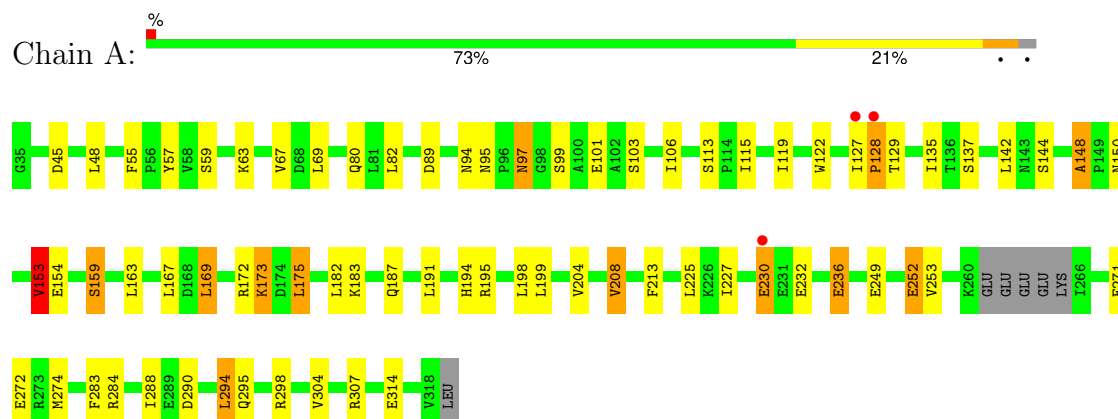
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	45	Total	O	0	0
			45	45		

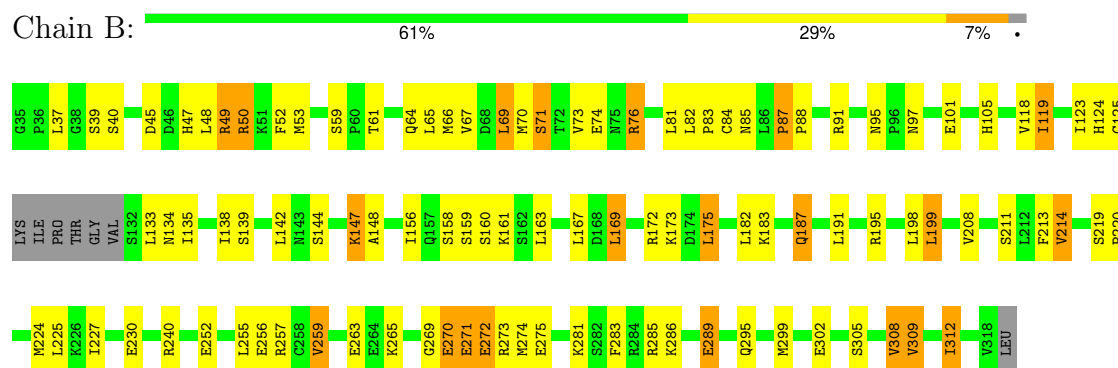
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Red chlorophyll catabolite reductase, chloroplastic



- Molecule 1: Red chlorophyll catabolite reductase, chloroplastic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.29Å 68.14Å 83.27Å 90.00° 95.32° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.40) 97.4 (20.00-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.16 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.216 , 0.298 0.244 , 0.250	Depositor DCC
$R_{free}$ test set	1146 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 20.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.70	0/2237	1.03	5/3030 (0.2%)
1	B	0.67	0/2203	1.02	5/2987 (0.2%)
All	All	0.68	0/4440	1.03	10/6017 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	308	VAL	N-CA-C	7.61	118.06	111.90
1	B	87	PRO	CA-C-N	6.20	125.93	119.05
1	B	87	PRO	C-N-CA	6.20	125.93	119.05
1	B	272	GLU	N-CA-C	-5.92	105.16	112.38
1	A	148	ALA	CA-C-N	5.47	125.47	119.89
1	A	148	ALA	C-N-CA	5.47	125.47	119.89
1	A	59	SER	CA-C-N	5.40	124.86	119.24
1	A	59	SER	C-N-CA	5.40	124.86	119.24
1	A	153	VAL	CB-CA-C	-5.24	102.68	110.33
1	B	289	GLU	N-CA-C	5.14	116.89	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	271	GLU	Peptide

## 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	2192	0	2144	38	0
1	B	2160	0	2090	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	57	0	0	1	0
4	B	45	0	0	0	0
All	All	4466	0	4234	97	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 (97) 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:47:HIS:HA	1:B:50:ARG:NH1	1.78	0.97
1:B:271:GLU:HG2	1:B:273:ARG:HB2	1.53	0.90
1:A:195:ARG:NH1	1:B:208:VAL:HG11	1.97	0.79
1:B:308:VAL:O	1:B:312:ILE:HG12	1.88	0.73
1:A:213:PHE:HZ	1:A:283:PHE:HA	1.54	0.71
1:B:40:SER:HB2	1:B:50:ARG:HH22	1.54	0.71
1:A:55:PHE:HB2	1:A:63:LYS:HB2	1.73	0.69
1:B:271:GLU:HB3	1:B:274:MET:HB2	1.74	0.69
1:B:183:LYS:HA	1:B:187:GLN:HG3	1.78	0.65
1:A:194:HIS:HE1	1:A:249:GLU:OE2	1.79	0.64
1:B:125:CYS:SG	1:B:299:MET:HG3	2.38	0.64
1:B:73:VAL:HG11	1:B:118:VAL:HG11	1.82	0.61
1:B:66:MET:HE1	1:B:138:ILE:HG13	1.81	0.61
1:B:211:SER:HB3	1:B:214:VAL:HG13	1.83	0.60
1:B:47:HIS:HA	1:B:50:ARG:HH12	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:HIS:CD2	1:B:134:ASN:HD21	2.20	0.60
1:A:106:ILE:HG12	1:A:119:ILE:HG13	1.85	0.58
1:A:230:GLU:H	1:A:230:GLU:CD	2.11	0.58
1:A:57:TYR:OH	1:A:101:GLU:OE2	2.17	0.58
1:B:270:GLU:O	1:B:271:GLU:HG3	2.04	0.58
1:A:97:ASN:HD22	1:A:97:ASN:C	2.12	0.58
1:B:124:HIS:HD2	1:B:134:ASN:HD21	1.53	0.57
1:B:61:THR:HG21	1:B:240:ARG:HB2	1.88	0.56
1:A:295:GLN:HG2	1:A:298:ARG:HH22	1.72	0.55
1:A:169:LEU:HD22	1:A:191:LEU:HD11	1.88	0.55
1:A:208:VAL:HG21	1:B:195:ARG:NH2	2.22	0.55
1:B:124:HIS:HD2	1:B:134:ASN:ND2	2.06	0.54
1:B:135:ILE:HG12	1:B:156:ILE:HG12	1.89	0.54
1:B:147:LYS:NZ	1:B:272:GLU:OE2	2.41	0.54
1:B:271:GLU:HB3	1:B:274:MET:CB	2.37	0.53
1:B:175:LEU:HG	1:B:182:LEU:HD13	1.91	0.53
1:A:213:PHE:CZ	1:A:283:PHE:HA	2.39	0.51
1:B:119:ILE:HG23	1:B:139:SER:HB2	1.92	0.51
1:B:255:LEU:HA	1:B:259:VAL:HG13	1.93	0.51
1:B:69:LEU:HB3	1:B:138:ILE:CD1	2.41	0.50
1:A:199:LEU:HD13	1:A:225:LEU:HD22	1.92	0.50
1:A:252:GLU:HG3	4:A:358:HOH:O	2.11	0.50
1:B:173:LYS:NZ	1:B:275:GLU:OE1	2.45	0.50
1:B:169:LEU:HD22	1:B:191:LEU:HD11	1.93	0.49
1:B:69:LEU:HB3	1:B:138:ILE:HD12	1.94	0.49
1:A:153:VAL:HG13	1:A:167:LEU:HD13	1.94	0.49
1:B:125:CYS:SG	1:B:299:MET:CG	3.01	0.49
1:A:232:GLU:O	1:A:236:GLU:HB2	2.13	0.49
1:B:281:LYS:HG2	1:B:285:ARG:HH11	1.77	0.49
1:B:52:PHE:HE2	1:B:70:MET:HG2	1.77	0.48
1:B:305:SER:O	1:B:309:VAL:HG13	2.13	0.48
1:A:175:LEU:HG	1:A:182:LEU:HD13	1.96	0.48
1:A:183:LYS:HA	1:A:187:GLN:HB2	1.95	0.48
1:B:48:LEU:HD11	1:B:88:PRO:HB3	1.96	0.48
1:B:271:GLU:OE1	1:B:274:MET:HE3	2.14	0.47
1:A:94:ASN:O	1:A:304:VAL:HG21	2.15	0.47
1:A:150:ASN:O	1:A:169:LEU:HA	2.15	0.47
1:B:148:ALA:O	1:B:172:ARG:HD3	2.14	0.47
1:B:199:LEU:HD13	1:B:225:LEU:HD22	1.96	0.47
1:B:124:HIS:CD2	1:B:134:ASN:ND2	2.82	0.47
1:B:76:ARG:HH11	1:B:252:GLU:CD	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLN:O	1:B:299:MET:HB2	2.16	0.46
1:B:147:LYS:NZ	1:B:173:LYS:HD2	2.30	0.46
1:A:80:GLN:NE2	1:A:113:SER:OG	2.47	0.46
1:A:122:TRP:HA	1:A:135:ILE:O	2.15	0.46
1:A:290:ASP:O	1:A:294:LEU:HB2	2.15	0.45
1:A:128:PRO:HB2	1:A:129:THR:H	1.67	0.45
1:B:213:PHE:HZ	1:B:283:PHE:HA	1.81	0.45
1:B:50:ARG:HB3	1:B:50:ARG:CZ	2.46	0.45
1:B:219:SER:HB2	1:B:220:PRO:HD2	1.99	0.45
1:B:224:MET:HB2	1:B:224:MET:HE2	1.83	0.45
1:B:74:GLU:OE2	1:B:105:HIS:NE2	2.49	0.44
1:B:160:SER:O	1:B:161:LYS:CB	2.65	0.44
1:A:284:ARG:O	1:A:288:ILE:HG12	2.18	0.44
1:B:269:GLY:O	1:B:270:GLU:C	2.61	0.44
1:B:163:LEU:HD23	1:B:227:ILE:HD12	1.99	0.44
1:B:53:MET:HE3	1:B:67:VAL:HG22	2.00	0.44
1:B:142:LEU:HD12	1:B:148:ALA:O	2.18	0.44
1:B:87:PRO:O	1:B:91:ARG:HG3	2.18	0.43
1:B:95:ASN:OD1	1:B:97:ASN:ND2	2.51	0.43
1:A:63:LYS:O	1:A:67:VAL:HG23	2.17	0.43
1:B:49:ARG:NH2	1:B:74:GLU:OE1	2.51	0.43
1:A:148:ALA:O	1:A:172:ARG:HD3	2.18	0.43
1:A:271:GLU:HA	1:A:274:MET:HE2	2.01	0.43
1:B:87:PRO:HA	1:B:88:PRO:HD3	1.79	0.43
1:A:95:ASN:CG	1:A:97:ASN:ND2	2.76	0.43
1:A:103:SER:HB3	1:A:122:TRP:CE2	2.54	0.42
1:A:173:LYS:HE3	1:A:272:GLU:OE2	2.19	0.42
1:A:45:ASP:O	1:A:48:LEU:HG	2.20	0.42
1:B:83:PRO:O	1:B:85:ASN:N	2.52	0.42
1:A:89:ASP:OD2	1:A:307:ARG:CD	2.68	0.41
1:A:137:SER:HB2	1:A:154:GLU:HG2	2.03	0.41
1:A:142:LEU:HD12	1:A:148:ALA:O	2.20	0.41
1:B:308:VAL:HG22	1:B:312:ILE:HD11	2.02	0.41
1:B:101:GLU:OE1	1:B:124:HIS:ND1	2.49	0.41
1:B:285:ARG:HG2	1:B:289:GLU:CD	2.46	0.41
1:B:76:ARG:NH2	1:B:256:GLU:OE2	2.54	0.41
1:B:67:VAL:O	1:B:71:SER:HB3	2.21	0.40
1:A:80:GLN:NE2	1:A:115:ILE:HD12	2.36	0.40
1:B:45:ASP:O	1:B:49:ARG:HB3	2.21	0.40
1:A:97:ASN:ND2	1:A:99:SER:H	2.19	0.40
1:A:204:VAL:HG22	1:A:227:ILE:HG12	2.04	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	275/285 (96%)	262 (95%)	10 (4%)	3 (1%)	12	18
1	B	274/285 (96%)	252 (92%)	17 (6%)	5 (2%)	7	9
All	All	549/570 (96%)	514 (94%)	27 (5%)	8 (2%)	8	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	PRO
1	B	263	GLU
1	B	270	GLU
1	A	159	SER
1	B	84	CYS
1	A	127	ILE
1	B	302	GLU
1	B	159	SER

### 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	248/264 (94%)	230 (93%)	18 (7%)	11	20
1	B	241/264 (91%)	209 (87%)	32 (13%)	3	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	489/528 (93%)	439 (90%)	50 (10%)	<b>6</b> <b>9</b>

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	82	LEU
1	A	97	ASN
1	A	144	SER
1	A	153	VAL
1	A	159	SER
1	A	163	LEU
1	A	169	LEU
1	A	173	LYS
1	A	175	LEU
1	A	198	LEU
1	A	208	VAL
1	A	230	GLU
1	A	236	GLU
1	A	252	GLU
1	A	253	VAL
1	A	294	LEU
1	A	314	GLU
1	B	37	LEU
1	B	39	SER
1	B	49	ARG
1	B	50	ARG
1	B	59	SER
1	B	64	GLN
1	B	65	LEU
1	B	69	LEU
1	B	71	SER
1	B	76	ARG
1	B	81	LEU
1	B	82	LEU
1	B	119	ILE
1	B	123	ILE
1	B	133	LEU
1	B	144	SER
1	B	147	LYS
1	B	158	SER
1	B	167	LEU

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Mol	Chain	Res	Type
1	B	169	LEU
1	B	175	LEU
1	B	187	GLN
1	B	198	LEU
1	B	199	LEU
1	B	214	VAL
1	B	230	GLU
1	B	257	ARG
1	B	259	VAL
1	B	265	LYS
1	B	286	LYS
1	B	309	VAL
1	B	312	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	85	ASN
1	A	97	ASN
1	A	105	HIS
1	A	187	GLN
1	A	194	HIS
1	B	75	ASN
1	B	97	ASN
1	B	134	ASN
1	B	157	GLN
1	B	242	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	3	-	4,4,4	0.23	0	6,6,6	0.27	0
3	SO4	A	4	-	4,4,4	0.21	0	6,6,6	0.49	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.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	279/285 (97%)	-0.15	3 (1%) 77 75	19, 31, 40, 47	0
1	B	278/285 (97%)	-0.05	0 100 100	18, 32, 43, 52	0
All	All	557/570 (97%)	-0.10	3 (0%) 87 85	18, 31, 41, 52	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	ILE	2.7
1	A	128	PRO	2.5
1	A	230	GLU	2.3

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	A	1	1/1	0.50	0.30	65,65,65,65	0
3	SO4	B	3	5/5	0.76	0.13	82,82,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	B	2	1/1	0.84	0.18	57,57,57,57	0
3	SO4	A	4	5/5	0.93	0.11	47,48,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.