



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:28 PM GMT

PDB ID : 1XA0  
Title : Crystal Structure of MCSG Target APC35536 from *Bacillus stearothermophilus*  
Authors : Brunzelle, J.S.; Sommerhalter, M.; Minasov, G.; Shuvalova, L.; Collart, F.R.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2004-08-24  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

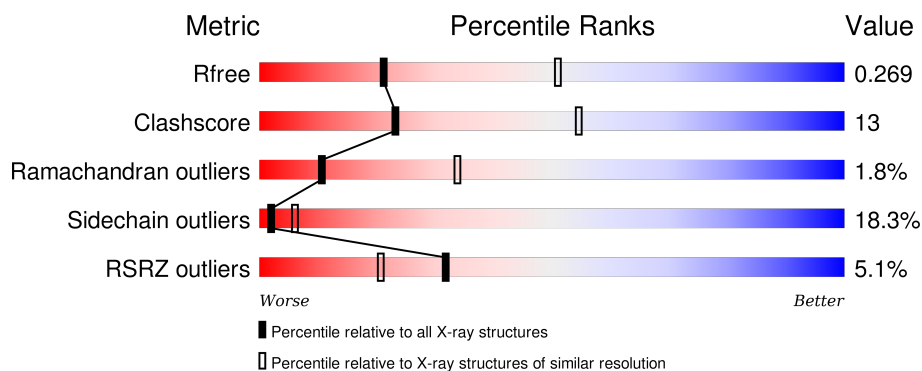
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	328	<div> <div>3%</div> <div>67%</div> <div>25%</div> <div>5%</div> <div>.</div> </div>
1	B	328	<div> <div>7%</div> <div>59%</div> <div>28%</div> <div>8%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

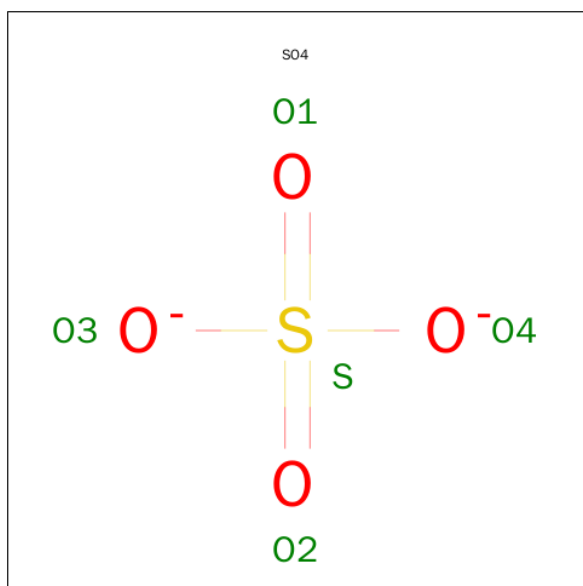
There are 4 unique types of molecules in this entry. The entry contains 4867 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative NADPH Dependent oxidoreductases.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	Se	0	0	0
			2415	1533	427	448	1	6			
1	B	317	Total	C	N	O	S	Se	0	0	0
			2388	1518	419	445	1	5			

- 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	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0

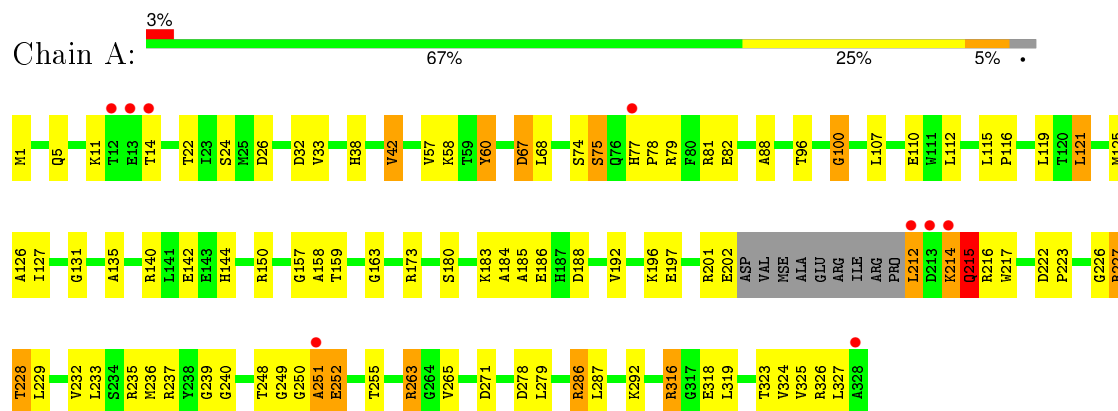
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total 29	O 29	0	0
4	B	19	Total 19	O 19	0	0

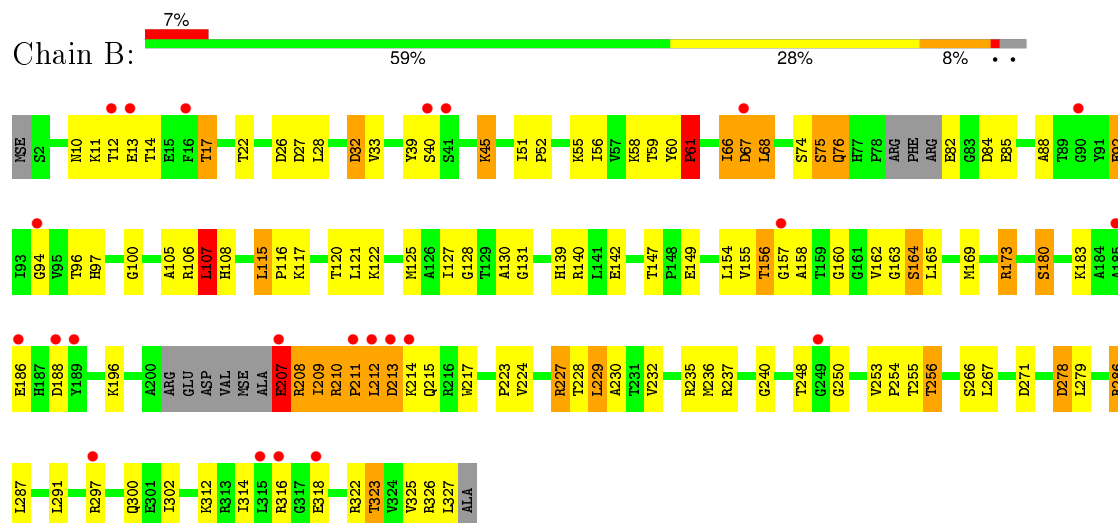
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Putative NADPH Dependent oxidoreductases



#### • Molecule 1: Putative NADPH Dependent oxidoreductases



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.24Å 156.24Å 68.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.13 – 2.74	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.80) 99.9 (29.13-2.74)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.18 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.212 , 0.269 0.216 , 0.269	Depositor DCC
$R_{free}$ test set	2172 reflections (11.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.2	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 22742 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4867	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: DTY, SO4, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.75	2/2441 (0.1%)	0.85	8/3298 (0.2%)
1	B	0.59	3/2413 (0.1%)	0.87	13/3264 (0.4%)
All	All	0.68	5/4854 (0.1%)	0.86	21/6562 (0.3%)

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	A	0	6
1	B	0	3
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	GLU	CD-OE1	19.71	1.47	1.25
1	A	82	GLU	CD-OE2	16.41	1.43	1.25
1	B	45	LYS	CB-CG	7.08	1.71	1.52
1	B	85	GLU	CD-OE1	5.64	1.31	1.25
1	B	45	LYS	CG-CD	5.43	1.71	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	GLU	CG-CD-OE1	8.51	135.32	118.30
1	B	207	GLU	CG-CD-OE2	-7.53	103.24	118.30
1	B	61	PRO	O-C-N	-6.60	112.13	122.70
1	B	107	LEU	CA-CB-CG	5.97	129.04	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	GLY	O-C-N	-5.94	113.11	123.20
1	A	158	ALA	O-C-N	-5.92	113.23	122.70
1	B	84	ASP	CB-CG-OD2	5.88	123.60	118.30
1	A	26	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	32	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	188	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	67	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	222	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	26	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	271	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	32	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	278	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	228	THR	O-C-N	-5.17	114.44	122.70
1	B	27	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	271	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	67	ASP	CB-CG-OD2	5.03	122.82	118.30
1	B	207	GLU	CB-CG-CD	5.00	127.71	114.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLY	Mainchain
1	A	215	GLN	Mainchain
1	A	226	GLY	Mainchain
1	A	227	ARG	Sidechain
1	A	228	THR	Mainchain
1	A	60	DTY	Mainchain
1	B	209	ILE	Peptide
1	B	210	ARG	Peptide
1	B	61	PRO	Mainchain

## 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	2415	0	2462	52	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2388	0	2429	83	1
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
4	A	29	0	0	1	0
4	B	19	0	0	3	0
All	All	4867	0	4891	130	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (130) 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:213:ASP:HB3	1:B:235:ARG:HD3	1.39	1.02
1:B:157:GLY:CA	1:B:223:PRO:HG2	2.01	0.89
1:B:314:ILE:HD11	4:B:348:HOH:O	1.73	0.88
1:A:67:ASP:HB3	1:A:125:MSE:HE1	1.57	0.87
1:A:67:ASP:HB3	1:A:125:MSE:CE	2.09	0.82
1:B:40:SER:HA	1:B:125:MSE:HE3	1.63	0.78
1:B:208:ARG:CG	1:B:208:ARG:HH11	1.97	0.77
1:B:158:ALA:HB2	1:B:180:SER:O	1.84	0.77
1:B:154:LEU:HD22	1:B:217:TRP:CZ2	2.20	0.76
1:B:213:ASP:HB3	1:B:235:ARG:CD	2.16	0.75
1:B:157:GLY:HA2	1:B:223:PRO:HG2	1.69	0.75
1:B:66:ILE:CG2	1:B:94:GLY:HA3	2.16	0.74
1:A:215:GLN:HG3	1:A:215:GLN:O	1.89	0.71
1:B:68:LEU:HD23	1:B:100:GLY:HA3	1.73	0.71
1:B:92:GLU:O	1:B:97:HIS:HB3	1.91	0.70
1:A:251:ALA:HB1	1:B:230:ALA:O	1.92	0.70
1:B:67:ASP:C	1:B:125:MSE:HE1	2.13	0.69
1:B:40:SER:HA	1:B:125:MSE:CE	2.23	0.68
1:A:127:ILE:HG23	1:A:131:GLY:HA3	1.75	0.68
1:B:162:VAL:CG1	1:B:223:PRO:HB3	2.23	0.68
1:A:188:ASP:O	1:A:192:VAL:HG23	1.92	0.68
1:A:68:LEU:HD21	1:A:100:GLY:HA2	1.75	0.67
1:B:66:ILE:HG23	1:B:94:GLY:HA3	1.77	0.67
1:B:157:GLY:HA3	1:B:223:PRO:HG2	1.77	0.66
1:A:214:LYS:O	1:A:215:GLN:HB3	1.94	0.66
1:A:236:MSE:HE1	1:A:240:GLY:HA3	1.78	0.66
1:B:139:HIS:HD2	1:B:286:ARG:HE	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:HD21	1:B:100:GLY:HA2	1.77	0.65
1:A:67:ASP:CB	1:A:125:MSE:HE1	2.25	0.65
1:A:77:HIS:N	1:A:78:PRO:HD3	2.11	0.65
1:A:316:ARG:HE	1:B:211:PRO:HD3	1.63	0.64
1:A:251:ALA:HB3	1:B:207:GLU:OE1	1.98	0.63
1:A:236:MSE:CE	1:A:240:GLY:HA3	2.29	0.63
1:A:232:VAL:O	1:A:236:MSE:HG2	2.00	0.62
1:B:209:ILE:O	1:B:209:ILE:HG12	2.00	0.62
1:B:154:LEU:HD22	1:B:217:TRP:CE2	2.35	0.62
1:B:162:VAL:HG12	1:B:223:PRO:HB3	1.81	0.62
1:A:115:LEU:HD22	1:A:121:LEU:HD13	1.81	0.62
1:B:208:ARG:NH1	1:B:208:ARG:CG	2.57	0.61
1:B:208:ARG:HG2	1:B:208:ARG:HH11	1.63	0.61
1:B:68:LEU:HB2	1:B:88:ALA:HB3	1.83	0.60
1:A:215:GLN:HE21	1:A:237:ARG:HD3	1.66	0.59
1:A:157:GLY:HA3	1:A:223:PRO:HG2	1.85	0.59
1:B:66:ILE:HG22	1:B:94:GLY:HA3	1.83	0.59
1:B:312:LYS:HG2	1:B:316:ARG:HH21	1.67	0.59
1:B:130:ALA:HA	1:B:162:VAL:HG23	1.85	0.58
1:A:215:GLN:NE2	1:A:237:ARG:HD3	2.20	0.57
1:A:215:GLN:HB2	1:A:237:ARG:HA	1.87	0.57
1:B:68:LEU:HD12	1:B:107:LEU:HD21	1.87	0.56
1:A:157:GLY:O	1:A:163:GLY:HA3	2.05	0.56
1:B:154:LEU:HD22	1:B:217:TRP:CH2	2.41	0.56
1:B:229:LEU:HB3	1:B:255:THR:HG21	1.86	0.56
1:B:236:MSE:CE	1:B:240:GLY:HA3	2.36	0.56
1:B:68:LEU:CD2	1:B:100:GLY:CA	2.84	0.55
1:B:67:ASP:HB3	1:B:125:MSE:HE1	1.87	0.55
1:A:125:MSE:HE3	1:A:125:MSE:HA	1.89	0.55
1:B:229:LEU:HB3	1:B:255:THR:CG2	2.37	0.54
1:B:162:VAL:HG11	1:B:223:PRO:HB3	1.88	0.54
1:A:263:ARG:HB2	1:A:265:VAL:HG23	1.90	0.54
1:A:60:DTY:HB3	4:A:359:HOH:O	2.08	0.54
1:B:10:ASN:HB3	1:B:17:THR:HG23	1.90	0.53
1:B:68:LEU:CD2	1:B:100:GLY:HA3	2.37	0.53
1:B:127:ILE:HG23	1:B:131:GLY:HA3	1.91	0.53
1:A:159:THR:HG21	1:A:186:GLU:HG3	1.92	0.52
1:A:33:VAL:HA	1:A:75:SER:CB	2.40	0.52
1:A:67:ASP:HB3	1:A:125:MSE:SE	2.60	0.51
1:B:208:ARG:NH1	1:B:208:ARG:HG3	2.26	0.51
1:B:286:ARG:HG2	1:B:291:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:O	1:A:79:ARG:HB2	2.11	0.51
1:A:316:ARG:NE	1:B:211:PRO:HD3	2.24	0.50
1:B:314:ILE:CD1	4:B:348:HOH:O	2.41	0.50
1:B:68:LEU:HD21	1:B:100:GLY:CA	2.41	0.49
1:B:97:HIS:HA	4:B:339:HOH:O	2.12	0.48
1:A:250:GLY:O	1:A:251:ALA:C	2.51	0.48
1:A:212:LEU:HD13	1:A:216:ARG:HG3	1.95	0.48
1:A:33:VAL:HA	1:A:75:SER:HB2	1.96	0.48
1:B:228:THR:O	1:B:232:VAL:HG23	2.13	0.48
1:A:142:GLU:OE1	1:A:286:ARG:NH2	2.46	0.48
1:B:39:TYR:HA	1:B:325:VAL:O	2.14	0.48
1:B:156:THR:HG22	1:B:223:PRO:HD2	1.95	0.47
1:B:127:ILE:HD13	1:B:287:LEU:HD22	1.96	0.47
1:B:155:VAL:HG12	1:B:156:THR:N	2.29	0.47
1:A:252:GLU:HG2	1:B:256:THR:CG2	2.45	0.47
1:A:217:TRP:CZ3	1:A:235:ARG:HB2	2.49	0.47
1:B:107:LEU:N	1:B:107:LEU:HD12	2.30	0.47
1:B:157:GLY:HA3	1:B:163:GLY:HA3	1.97	0.46
1:A:144:HIS:O	1:A:144:HIS:ND1	2.48	0.46
1:B:33:VAL:HG22	1:B:75:SER:HB2	1.97	0.46
1:A:33:VAL:HG11	1:A:112:LEU:HD11	1.98	0.45
1:A:135:ALA:HB2	1:A:287:LEU:HD21	1.98	0.45
1:B:227:ARG:HH11	1:B:227:ARG:HD2	1.62	0.45
1:B:130:ALA:O	1:B:162:VAL:HG22	2.17	0.45
1:B:67:ASP:CB	1:B:125:MSE:HE1	2.47	0.45
1:A:215:GLN:HE21	1:A:237:ARG:CD	2.30	0.45
1:A:184:ALA:O	1:A:185:ALA:HB3	2.16	0.45
1:A:68:LEU:HB2	1:A:88:ALA:HB3	1.99	0.45
1:B:68:LEU:HD11	1:B:105:ALA:HB3	1.99	0.44
1:B:59:THR:HG22	1:B:60:DTY:N	2.33	0.44
1:B:67:ASP:HB3	1:B:125:MSE:CE	2.48	0.44
1:B:92:GLU:HB3	1:B:97:HIS:HB2	2.00	0.44
1:B:28:LEU:HD22	1:B:106:ARG:H	1.83	0.43
1:A:286:ARG:NH1	1:A:286:ARG:HG2	2.33	0.43
1:A:42:VAL:HG13	1:A:323:THR:HB	1.99	0.43
1:B:59:THR:CG2	1:B:60:DTY:N	2.82	0.43
1:B:212:LEU:H	1:B:212:LEU:HG	1.49	0.42
1:B:60:DTY:HA	1:B:61:PRO:HD3	1.78	0.42
1:B:300:GLN:HB3	1:B:323:THR:HG23	2.01	0.42
1:B:108:HIS:N	1:B:108:HIS:CD2	2.88	0.42
1:B:253:VAL:HA	1:B:254:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:SER:CA	1:B:125:MSE:HE3	2.41	0.42
1:B:142:GLU:CD	1:B:173:ARG:HH21	2.24	0.42
1:B:128:GLY:HA3	1:B:322:ARG:NH2	2.35	0.41
1:A:126:ALA:HA	1:A:324:VAL:CG1	2.50	0.41
1:A:116:PRO:HG2	1:A:119:LEU:HD12	2.02	0.41
1:A:74:SER:O	1:A:75:SER:HB3	2.20	0.41
1:B:160:GLY:O	1:B:164:SER:HB2	2.20	0.41
1:A:125:MSE:HE3	1:A:125:MSE:CA	2.50	0.41
1:B:120:THR:HG22	1:B:122:LYS:H	1.85	0.41
1:B:32:ASP:O	1:B:76:GLN:NE2	2.51	0.41
1:A:229:LEU:HD12	1:A:229:LEU:HA	1.89	0.41
1:B:154:LEU:HG	1:B:154:LEU:O	2.19	0.41
1:B:212:LEU:O	1:B:214:LYS:HB2	2.21	0.41
1:A:67:ASP:CB	1:A:125:MSE:CE	2.91	0.41
1:B:208:ARG:HG2	1:B:208:ARG:H	1.67	0.41
1:B:165:LEU:HB3	1:B:169:MSE:HE3	2.03	0.41
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.86	0.40
1:B:115:LEU:HA	1:B:116:PRO:HD2	1.91	0.40
1:B:68:LEU:N	1:B:125:MSE:HE1	2.36	0.40
1:A:77:HIS:N	1:A:78:PRO:CD	2.81	0.40
1:A:119:LEU:HD23	1:A:292:LYS:HE3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:HIS:CD2	1:B:326:ARG:NH1[5_445]	2.07	0.13

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	314/328 (96%)	286 (91%)	23 (7%)	5 (2%)	12	38
1	B	310/328 (94%)	280 (90%)	24 (8%)	6 (2%)	10	32
All	All	624/656 (95%)	566 (91%)	47 (8%)	11 (2%)	11	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	211	PRO
1	B	213	ASP
1	A	215	GLN
1	A	251	ALA
1	B	210	ARG
1	A	75	SER
1	A	248	THR
1	B	14	THR
1	A	249	GLY
1	B	250	GLY
1	B	52	PRO

### 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	250/251 (100%)	211 (84%)	39 (16%)	3	9
1	B	248/251 (99%)	196 (79%)	52 (21%)	1	4
All	All	498/502 (99%)	407 (82%)	91 (18%)	2	6

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	5	GLN
1	A	11	LYS
1	A	14	THR
1	A	22	THR

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Mol	Chain	Res	Type
1	A	24	SER
1	A	42	VAL
1	A	57	VAL
1	A	58	LYS
1	A	81	ARG
1	A	96	THR
1	A	107	LEU
1	A	110	GLU
1	A	121	LEU
1	A	140	ARG
1	A	150	ARG
1	A	173	ARG
1	A	180	SER
1	A	183	LYS
1	A	196	LYS
1	A	197	GLU
1	A	201	ARG
1	A	202	GLU
1	A	212	LEU
1	A	214	LYS
1	A	227	ARG
1	A	233	LEU
1	A	252	GLU
1	A	255	THR
1	A	263	ARG
1	A	278	ASP
1	A	279	LEU
1	A	286	ARG
1	A	316	ARG
1	A	318	GLU
1	A	319	LEU
1	A	325	VAL
1	A	326	ARG
1	A	327	LEU
1	B	11	LYS
1	B	12	THR
1	B	13	GLU
1	B	17	THR
1	B	22	THR
1	B	45	LYS
1	B	51	ILE
1	B	55	LYS

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Mol	Chain	Res	Type
1	B	56	ILE
1	B	58	LYS
1	B	66	ILE
1	B	68	LEU
1	B	74	SER
1	B	75	SER
1	B	76	GLN
1	B	82	GLU
1	B	92	GLU
1	B	96	THR
1	B	107	LEU
1	B	115	LEU
1	B	117	LYS
1	B	121	LEU
1	B	140	ARG
1	B	147	THR
1	B	149	GLU
1	B	156	THR
1	B	164	SER
1	B	173	ARG
1	B	180	SER
1	B	183	LYS
1	B	186	GLU
1	B	196	LYS
1	B	207	GLU
1	B	208	ARG
1	B	212	LEU
1	B	215	GLN
1	B	224	VAL
1	B	227	ARG
1	B	229	LEU
1	B	237	ARG
1	B	248	THR
1	B	256	THR
1	B	266	SER
1	B	267	LEU
1	B	278	ASP
1	B	279	LEU
1	B	286	ARG
1	B	297	ARG
1	B	302	ILE
1	B	318	GLU

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Mol	Chain	Res	Type
1	B	323	THR
1	B	327	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	76	GLN
1	A	187	HIS
1	A	215	GLN
1	A	300	GLN
1	B	10	ASN
1	B	43	ASN
1	B	108	HIS
1	B	139	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	DTY	A	60	1	11,12,13	0.58	0	12,15,17	1.07	1 (8%)
1	DTY	B	60	1	11,12,13	0.60	0	12,15,17	1.03	1 (8%)

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
1	DTY	A	60	1	-	0/4/6/8	0/1/1/1
1	DTY	B	60	1	-	0/4/6/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	DTY	O-C-CA	-2.78	118.25	125.49
1	B	60	DTY	CG-CB-CA	-2.58	108.37	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	60	DTY	1	0
1	B	60	DTY	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z  > 2$
2	SO4	A	329	-	4,4,4	0.17	0	6,6,6	0.27	0
2	SO4	A	330	-	4,4,4	0.09	0	6,6,6	0.21	0
2	SO4	B	329	-	4,4,4	0.21	0	6,6,6	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	329	-	-	0/0/0/0	0/0/0/0
2	SO4	A	330	-	-	0/0/0/0	0/0/0/0
2	SO4	B	329	-	-	0/0/0/0	0/0/0/0

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 ⓘ

### 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<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	312/328 (95%)	-0.12	9 (2%) 55 43	21, 33, 48, 86	0
1	B	311/328 (94%)	0.33	23 (7%) 17 9	21, 35, 49, 57	0
All	All	623/656 (94%)	0.10	32 (5%) 32 21	21, 34, 49, 86	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	ALA	6.0
1	B	315	LEU	5.1
1	B	213	ASP	4.5
1	B	212	LEU	4.3
1	B	249	GLY	3.9
1	B	214	LYS	3.8
1	A	213	ASP	3.8
1	A	77	HIS	3.7
1	B	13	GLU	3.6
1	A	214	LYS	3.4
1	B	316	ARG	3.0
1	B	185	ALA	3.0
1	B	318	GLU	2.9
1	B	12	THR	2.8
1	B	189	TYR	2.8
1	B	67	ASP	2.7
1	B	211	PRO	2.6
1	B	41	SER	2.5
1	A	251	ALA	2.5
1	B	90	GLY	2.4
1	A	14	THR	2.4
1	B	40	SER	2.4
1	A	13	GLU	2.4
1	A	12	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	207	GLU	2.3
1	B	94	GLY	2.3
1	B	186	GLU	2.2
1	B	297	ARG	2.2
1	A	212	LEU	2.1
1	B	188	ASP	2.1
1	B	157	GLY	2.0
1	B	16	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	DTY	A	60	12/13	0.84	0.30	-	36,38,39,40	0
1	DTY	B	60	12/13	0.76	0.36	-	44,46,47,47	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	330	5/5	0.86	0.21	0.24	105,105,106,107	0
2	SO4	B	329	5/5	0.90	0.19	-1.14	106,106,107,107	0
2	SO4	A	329	5/5	0.98	0.13	-1.30	68,68,69,69	0
3	CL	A	331	1/1	0.91	0.51	-	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.