



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:03 AM BST

PDB ID : 6G50  
Title : The structure of thiocyanate dehydrogenase from Thioalkalivibrio paradoxus as isolated.  
Authors : Polyakov, K.M.; Tsallagov, S.I.; Tikhkonova, T.V.; Popov, V.O.  
Deposited on : 2018-03-28  
Resolution : 1.65 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.

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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 : 2.13.1  
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) : 2.13.1

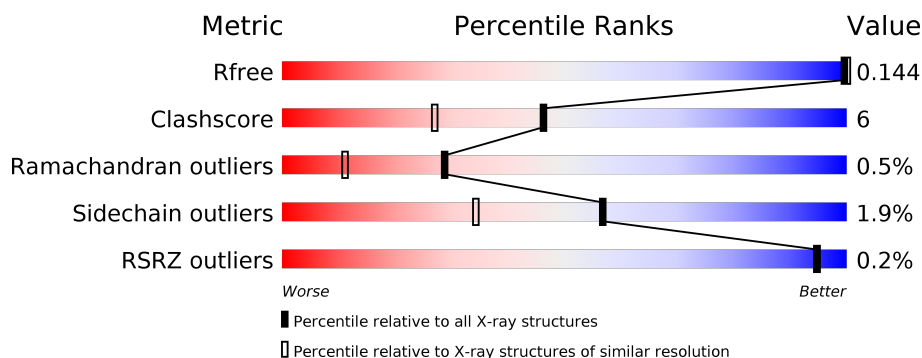
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	467	<div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	B	467	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	C	467	<div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	D	467	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16327 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	13	0
			3685	2350	615	700	20			
1	B	467	Total	C	N	O	S	0	10	0
			3664	2338	611	694	21			
1	C	467	Total	C	N	O	S	0	9	0
			3679	2349	613	697	20			
1	D	467	Total	C	N	O	S	0	17	0
			3694	2359	612	703	20			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Cu	0	0
			4	4		
2	A	3	Total	Cu	0	0
			3	3		
2	D	3	Total	Cu	0	0
			3	3		
2	C	3	Total	Cu	0	0
			3	3		

- Molecule 3 is SULFATE ION (three-letter code: 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		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	1
			10	8	2		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

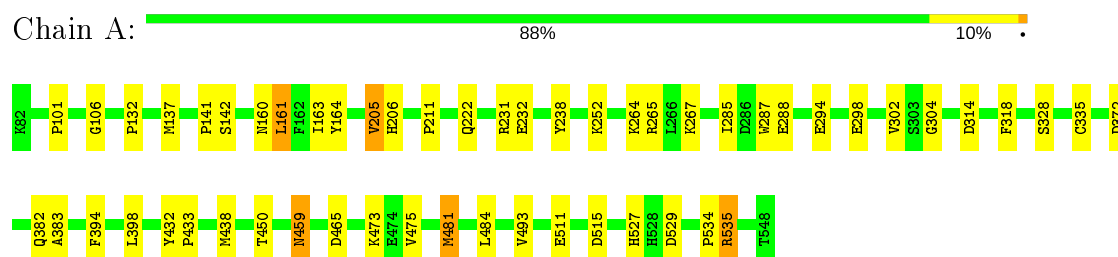
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	383	Total	O	0	0
			383	383		
5	B	356	Total	O	0	0
			356	356		
5	C	399	Total	O	0	0
			399	399		
5	D	393	Total	O	0	0
			393	393		

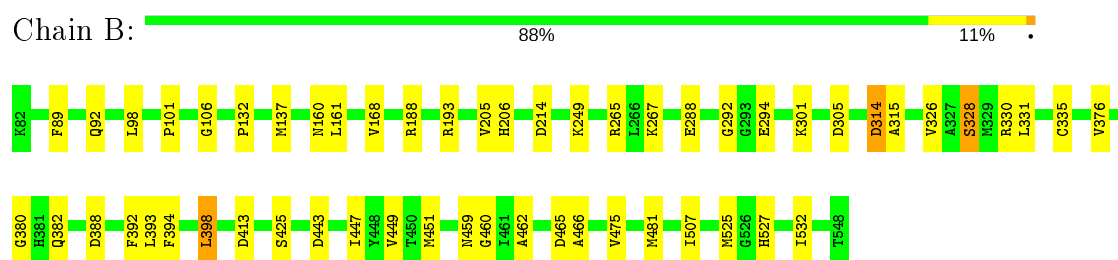
### 3 Residue-property plots

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.

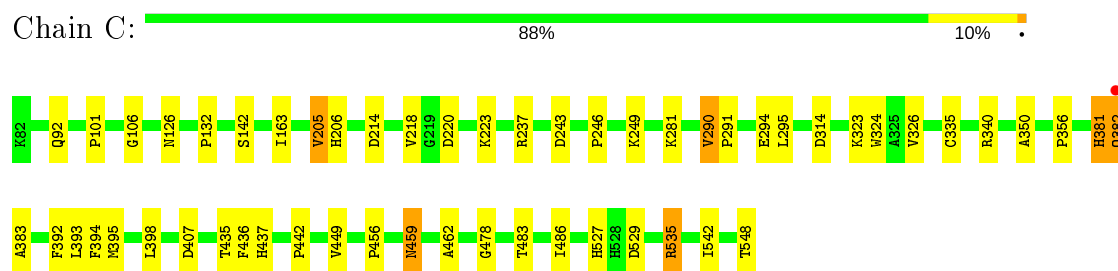
- Molecule 1: Uncharacterized protein



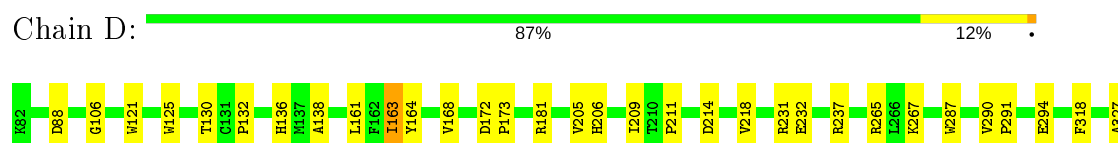
- Molecule 1: Uncharacterized protein

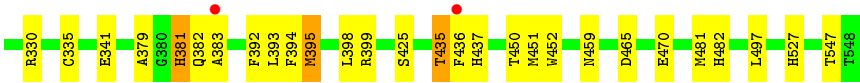


- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.63Å 162.28Å 90.57Å 90.00° 119.51° 90.00°	Depositor
Resolution (Å)	45.31 – 1.65 45.28 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.3 (45.31-1.65) 97.3 (45.28-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.143 , 0.207 0.152 , 0.144	Depositor DCC
$R_{free}$ test set	12651 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 28.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.047 for l,k,-h-l 0.047 for -h-l,k,h 0.047 for -h-l,-k,l 0.047 for h,-k,-h-l 0.457 for l,-k,h	Xtriage
Reported twinning fraction	0.551 for H, K, L 0.449 for L, -K, H	Depositor
Outliers	0 of 265481 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16327	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% 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: SO4, CU, EDO

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	0.85	1/3849 (0.0%)	0.95	6/5249 (0.1%)
1	B	0.83	0/3824	0.98	8/5214 (0.2%)
1	C	0.86	0/3824	0.97	7/5214 (0.1%)
1	D	0.83	1/3882 (0.0%)	0.96	9/5297 (0.2%)
All	All	0.84	2/15379 (0.0%)	0.96	30/20974 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	TYR	CG-CD1	5.17	1.45	1.39
1	D	121	TRP	CE3-CZ3	5.01	1.47	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	C	214	ASP	CB-CG-OD1	7.47	125.02	118.30
1	C	535	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	529	ASP	CB-CG-OD1	6.75	124.37	118.30
1	D	435	THR	CA-CB-CG2	-6.58	103.19	112.40
1	D	237	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	C	407	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	237	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	388	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	214	ASP	CB-CG-OD1	6.28	123.95	118.30
1	D	231	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	161	LEU	CB-CG-CD2	-6.07	100.68	111.00
1	A	231	ARG	NE-CZ-NH1	-6.01	117.29	120.30
1	B	481	MET	CA-CB-CG	-5.81	103.42	113.30
1	B	443	ASP	CB-CG-OD1	5.78	123.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	C	340	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	535	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	465	ASP	CB-CG-OD1	5.60	123.34	118.30
1	D	88	ASP	CB-CG-OD1	5.55	123.29	118.30
1	B	413	ASP	CB-CG-OD1	5.53	123.28	118.30
1	D	399	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	372	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	535	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	D	214	ASP	CB-CG-OD1	5.35	123.11	118.30
1	C	407	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	D	181	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	465	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	237	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	88	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	3685	0	3544	38	0
1	B	3664	0	3540	34	0
1	C	3679	0	3545	47	0
1	D	3694	0	3542	65	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	25	0	0	0	0
3	D	10	0	0	0	0
4	C	8	0	12	0	0
4	D	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	383	0	0	4	0
5	B	356	0	0	0	0
5	C	399	0	0	10	0
5	D	393	0	0	15	0
All	All	16327	0	14195	181	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 6.

All (181) 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:C:436[A]:PHE:HB2	5:C:725:HOH:O	1.38	1.24
1:C:436[B]:PHE:CD2	5:C:725:HOH:O	1.65	1.22
1:D:381[B]:HIS:NE2	1:D:436[B]:PHE:HA	1.55	1.20
1:C:381[B]:HIS:NE2	1:C:436[B]:PHE:HB2	1.57	1.17
1:D:436[B]:PHE:CD2	5:D:862:HOH:O	1.96	1.17
1:B:449[A]:VAL:HG23	1:B:451[A]:MET:CE	1.75	1.16
1:B:449[A]:VAL:HG23	1:B:451[A]:MET:HE2	1.19	1.14
1:D:436[B]:PHE:HD2	5:D:862:HOH:O	1.31	1.11
1:C:436[B]:PHE:HD2	5:C:725:HOH:O	0.96	1.10
1:C:381[B]:HIS:NE2	1:C:436[B]:PHE:CB	2.15	1.09
1:D:435:THR:HG22	1:D:451:MET:HE2	1.27	1.07
1:A:163[B]:ILE:HD11	1:A:287:TRP:CD1	1.93	1.03
1:D:382:GLN:HB3	1:D:395[B]:MET:CG	1.89	1.02
1:B:449[A]:VAL:CG2	1:B:451[A]:MET:CE	2.45	0.93
1:D:450:THR:HG21	1:D:482[A]:HIS:O	1.68	0.93
1:D:437:HIS:CD2	1:D:482[B]:HIS:O	2.23	0.92
1:D:381[B]:HIS:CD2	1:D:382:GLN:N	2.39	0.91
1:A:265:ARG:HD2	1:A:267:LYS:HE2	1.51	0.90
1:A:314[A]:ASP:OD1	5:A:701:HOH:O	1.88	0.90
1:D:381[B]:HIS:NE2	1:D:436[B]:PHE:CA	2.36	0.89
1:D:437:HIS:HE1	5:D:740:HOH:O	1.57	0.88
1:D:435:THR:HG22	1:D:451:MET:CE	2.04	0.87
1:D:382:GLN:HB3	1:D:395[B]:MET:HG2	1.57	0.85
1:D:435:THR:CG2	1:D:451:MET:HE2	2.07	0.85
1:D:382:GLN:HB3	1:D:395[B]:MET:HG3	1.59	0.83
1:D:437:HIS:CE1	5:D:740:HOH:O	2.32	0.81
1:D:435:THR:CG2	1:D:451:MET:CE	2.58	0.81
1:D:382:GLN:CB	1:D:395[B]:MET:HG3	2.11	0.80
1:C:381[B]:HIS:CD2	1:C:382:GLN:N	2.48	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:SER:HB3	1:A:382[B]:GLN:HB3	1.63	0.79
1:D:130[B]:THR:O	5:D:701:HOH:O	2.05	0.75
1:D:290:VAL:HG22	1:D:291:PRO:CD	2.17	0.75
1:D:164:TYR:HE2	5:D:927:HOH:O	1.70	0.74
1:A:328:SER:HB3	1:A:382[A]:GLN:HB2	1.68	0.74
1:C:381[B]:HIS:O	1:C:382:GLN:O	2.06	0.74
1:D:232[A]:GLU:HG2	5:D:817:HOH:O	1.88	0.72
1:D:232[B]:GLU:HG3	5:D:817:HOH:O	1.90	0.72
1:B:161:LEU:HG	1:B:168:VAL:HG11	1.71	0.71
1:D:381[B]:HIS:NE2	1:D:436[B]:PHE:CB	2.53	0.71
1:C:449:VAL:CG2	1:C:462:ALA:HB3	2.20	0.70
1:A:328:SER:HB3	1:A:382[A]:GLN:CB	2.22	0.69
1:A:484:LEU:HD22	1:A:493:VAL:CG1	2.22	0.69
1:C:449:VAL:HG23	1:C:462:ALA:HB3	1.73	0.69
1:D:294:GLU:CD	1:D:294:GLU:H	1.97	0.68
1:A:163[B]:ILE:CD1	1:A:287:TRP:CD1	2.76	0.67
1:A:450:THR:HB	1:A:481:MET:HG2	1.77	0.66
1:D:381[B]:HIS:CE1	1:D:436[B]:PHE:HA	2.27	0.66
1:B:449[A]:VAL:CG2	1:B:451[A]:MET:HE3	2.25	0.66
1:D:381[B]:HIS:CE1	1:D:436[B]:PHE:HB3	2.30	0.66
1:B:314:ASP:OD2	1:B:328:SER:HB3	1.97	0.65
1:D:435:THR:HG21	1:D:451:MET:HE1	1.79	0.64
1:D:106:GLY:HA2	1:D:132:PRO:O	1.97	0.64
1:C:381[B]:HIS:NE2	1:C:436[B]:PHE:HB3	2.11	0.62
1:C:381[B]:HIS:CD2	1:C:436[B]:PHE:HB2	2.32	0.60
1:D:290:VAL:HG22	1:D:291:PRO:HD3	1.82	0.59
1:C:381[B]:HIS:CG	1:C:382:GLN:N	2.54	0.59
1:D:382:GLN:CB	1:D:395[B]:MET:CG	2.68	0.59
1:A:232:GLU:HG2	5:A:747:HOH:O	2.02	0.59
1:C:205:VAL:HG23	1:C:220:ASP:HA	1.84	0.59
1:A:287:TRP:HD1	1:A:288:GLU:O	1.86	0.59
1:D:161:LEU:HG	1:D:168[B]:VAL:HG11	1.85	0.58
1:A:106:GLY:HA2	1:A:132:PRO:O	2.03	0.58
1:D:290:VAL:HG22	1:D:291:PRO:HD2	1.85	0.58
1:B:292:GLY:HA2	1:B:398:LEU:HD21	1.85	0.58
1:C:381[B]:HIS:CE1	1:C:436[B]:PHE:HB3	2.39	0.57
1:D:381[B]:HIS:CG	1:D:382:GLN:N	2.64	0.57
1:D:163[B]:ILE:HD11	1:D:287:TRP:HB2	1.87	0.57
1:C:435:THR:HB	5:C:727:HOH:O	2.05	0.57
1:A:287:TRP:CZ2	1:A:302:VAL:HA	2.40	0.56
1:D:381[B]:HIS:CE1	1:D:436[B]:PHE:CB	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:HIS:HE1	5:D:740:HOH:O	1.87	0.56
1:B:89:PHE:O	1:B:92:GLN:HG2	2.06	0.56
1:C:281:LYS:HE3	5:C:921:HOH:O	2.05	0.56
1:B:314:ASP:CG	1:B:328:SER:HB3	2.27	0.55
1:C:381[B]:HIS:O	1:C:382:GLN:C	2.44	0.55
1:A:473:LYS:HD2	5:A:788:HOH:O	2.07	0.55
1:B:168:VAL:HG13	1:C:126:ASN:O	2.07	0.55
1:B:206:HIS:HB2	1:B:315:ALA:HB2	1.89	0.55
1:A:205:VAL:HG12	1:A:206:HIS:N	2.22	0.54
1:A:101:PRO:HD3	1:A:137:MET:HG2	1.89	0.54
1:D:436[B]:PHE:H	1:D:436[B]:PHE:HD2	1.54	0.54
1:B:449[A]:VAL:HG21	1:B:451[A]:MET:HE3	1.88	0.54
1:D:161:LEU:CD2	1:D:168[B]:VAL:HG11	2.39	0.53
1:A:160:ASN:HD21	1:A:222:GLN:HE22	1.55	0.53
1:A:294:GLU:O	1:A:298:GLU:HG3	2.09	0.53
1:A:484:LEU:HD22	1:A:493:VAL:HG13	1.91	0.52
1:A:163[B]:ILE:HD11	1:A:287:TRP:CG	2.43	0.52
1:A:383:ALA:HB1	1:A:438:MET:SD	2.49	0.52
1:D:437:HIS:HD2	1:D:482[B]:HIS:O	1.85	0.52
1:D:265:ARG:HD2	1:D:267:LYS:HE2	1.91	0.51
1:C:326:VAL:HG11	1:C:392:PHE:CZ	2.45	0.51
1:D:138:ALA:HB1	1:D:209:ILE:HG12	1.93	0.51
1:D:161:LEU:CG	1:D:168[B]:VAL:HG11	2.41	0.51
1:B:314:ASP:OD1	1:B:328:SER:HB3	2.11	0.50
1:B:265:ARG:HD2	1:B:267:LYS:HE3	1.92	0.50
1:C:290:VAL:HG12	1:C:291:PRO:HD3	1.92	0.50
1:D:383:ALA:HB2	1:D:394:PHE:HD1	1.77	0.50
1:C:246:PRO:HG2	1:C:249:LYS:HD3	1.94	0.50
1:D:436[B]:PHE:CE2	5:D:862:HOH:O	2.41	0.50
1:B:160:ASN:OD1	1:B:288:GLU:HG2	2.11	0.50
1:A:473:LYS:HE2	1:A:475:VAL:CG1	2.42	0.49
1:A:141:PRO:HA	1:A:534:PRO:O	2.13	0.49
1:C:442:PRO:HD2	5:C:1028:HOH:O	2.12	0.49
1:D:383:ALA:HA	1:D:393:LEU:O	2.12	0.49
1:D:436[B]:PHE:CE2	1:D:452:TRP:HB2	2.47	0.49
1:C:459:ASN:HB2	1:C:478:GLY:O	2.13	0.48
1:D:206:HIS:O	1:D:218:VAL:HA	2.13	0.48
1:B:98:LEU:HA	1:B:532[B]:ILE:HD13	1.95	0.48
1:A:459:ASN:HD22	1:A:459:ASN:N	2.12	0.48
1:D:330:ARG:NH2	5:D:707:HOH:O	2.46	0.48
1:D:465:ASP:HB3	1:D:470:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASN:HD21	1:A:222:GLN:NE2	2.11	0.48
1:C:381[B]:HIS:CE1	1:C:436[B]:PHE:CB	2.90	0.48
1:A:205:VAL:HG12	1:A:206:HIS:H	1.79	0.48
1:B:447:ILE:HG13	1:B:466:ALA:HB2	1.95	0.47
1:D:382:GLN:HB2	1:D:395[B]:MET:HG3	1.90	0.47
1:B:460:GLY:HA3	1:B:475:VAL:O	2.15	0.46
1:C:106:GLY:HA2	1:C:132:PRO:O	2.14	0.46
1:A:335:CYS:SG	1:A:394:PHE:CD1	3.08	0.46
1:C:435:THR:CB	5:C:727:HOH:O	2.63	0.46
1:C:323:LYS:HD3	1:C:324:TRP:CZ2	2.51	0.46
1:C:437:HIS:ND1	1:C:483:THR:HG22	2.30	0.46
1:B:101:PRO:HD3	1:B:137:MET:HG2	1.98	0.46
1:D:382:GLN:O	1:D:394:PHE:HA	2.15	0.46
1:C:383:ALA:HA	1:C:393:LEU:O	2.16	0.45
1:D:381[B]:HIS:CD2	1:D:382:GLN:CA	2.99	0.45
1:B:330:ARG:HA	1:B:380:GLY:O	2.16	0.45
1:C:314[B]:ASP:OD2	1:C:381[B]:HIS:HB2	2.17	0.45
1:B:449[A]:VAL:CG2	1:B:462:ALA:HB3	2.47	0.45
1:C:290:VAL:HG12	1:C:291:PRO:CD	2.47	0.44
1:B:382:GLN:HA	1:B:394:PHE:CD1	2.52	0.44
1:C:486:ILE:HG21	1:C:542:ILE:HD12	2.00	0.44
1:A:211:PRO:HD3	1:A:318:PHE:CB	2.47	0.44
1:D:211:PRO:HD3	1:D:318:PHE:HB3	1.99	0.44
1:C:206:HIS:O	1:C:218:VAL:HA	2.18	0.43
1:A:161:LEU:HD13	1:D:125:TRP:CH2	2.53	0.43
1:A:511:GLU:O	1:A:515:ASP:HA	2.18	0.43
1:B:301:LYS:HA	1:B:301:LYS:HD3	1.83	0.43
1:C:436[B]:PHE:CE2	5:C:778:HOH:O	0.78	0.43
1:B:267:LYS:HD2	1:D:172:ASP:HB2	2.00	0.43
1:C:435:THR:CG2	1:C:449:VAL:HB	2.49	0.43
1:A:264[A]:LYS:HE3	5:A:758:HOH:O	2.18	0.43
1:C:335:CYS:SG	1:C:394:PHE:CD1	3.11	0.43
1:A:163[B]:ILE:HD11	1:A:287:TRP:NE1	2.31	0.43
1:D:383:ALA:HB1	1:D:392:PHE:CZ	2.54	0.43
1:D:173:PRO:HA	5:D:701:HOH:O	2.19	0.42
1:D:290:VAL:HG21	5:D:1018:HOH:O	2.19	0.42
1:C:294:GLU:HG2	1:C:295:LEU:N	2.34	0.42
1:C:382:GLN:NE2	1:C:548:THR:OG1	2.52	0.42
1:B:382:GLN:HA	1:B:394:PHE:HD1	1.85	0.42
1:C:436[B]:PHE:HE2	5:C:778:HOH:O	0.54	0.42
1:B:98:LEU:CD2	1:B:507[A]:ILE:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLU:CD	1:B:330:ARG:HH21	2.22	0.42
1:D:381[A]:HIS:HE1	5:D:1039:HOH:O	2.02	0.42
1:A:142:SER:O	1:A:535:ARG:HA	2.20	0.41
1:C:350:ALA:HB3	1:C:356:PRO:O	2.19	0.41
1:B:314:ASP:OD1	1:B:315:ALA:N	2.53	0.41
1:B:326:VAL:CG1	1:B:335:CYS:HB3	2.50	0.41
1:D:382:GLN:HE22	1:D:547:THR:HB	1.86	0.41
1:B:525[B]:MET:HE2	1:B:525[B]:MET:HB3	1.71	0.41
1:C:381[B]:HIS:CE1	5:C:1014:HOH:O	2.73	0.41
1:D:327:ALA:O	1:D:335:CYS:HA	2.21	0.41
1:A:285:ILE:HA	1:A:304:GLY:HA3	2.02	0.41
1:B:328:SER:OG	1:B:394:PHE:HE1	2.04	0.41
1:D:294:GLU:HG2	1:D:379:ALA:CB	2.51	0.41
1:B:392:PHE:C	1:B:393:LEU:HD12	2.41	0.41
1:B:106:GLY:HA2	1:B:132:PRO:O	2.21	0.41
1:C:101:PRO:HD2	1:C:529:ASP:O	2.22	0.40
1:A:211:PRO:HD3	1:A:318:PHE:HB3	2.03	0.40
1:B:331:LEU:O	1:B:376:VAL:HG11	2.20	0.40
1:C:142:SER:O	1:C:535:ARG:HA	2.20	0.40
1:A:432:TYR:HB3	1:A:433:PRO:HA	2.02	0.40
1:D:164:TYR:CE2	5:D:927:HOH:O	2.58	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	478/467 (102%)	456 (95%)	20 (4%)	2 (0%)	34	16
1	B	475/467 (102%)	446 (94%)	28 (6%)	1 (0%)	47	28
1	C	474/467 (102%)	447 (94%)	22 (5%)	5 (1%)	14	2
1	D	482/467 (103%)	455 (94%)	23 (5%)	4 (1%)	19	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1909/1868 (102%)	1804 (94%)	93 (5%)	12 (1%)	29	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	381[A]	HIS
1	C	381[B]	HIS
1	C	382	GLN
1	D	205	VAL
1	B	205	VAL
1	D	398	LEU
1	A	205	VAL
1	A	398	LEU
1	C	398	LEU
1	D	381[A]	HIS
1	D	381[B]	HIS
1	C	205	VAL

### 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	405/392 (103%)	401 (99%)	4 (1%)	76	62
1	B	402/392 (103%)	393 (98%)	9 (2%)	52	27
1	C	401/392 (102%)	392 (98%)	9 (2%)	52	27
1	D	408/392 (104%)	398 (98%)	10 (2%)	47	22
All	All	1616/1568 (103%)	1584 (98%)	32 (2%)	57	32

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	LYS
1	A	459	ASN
1	A	481	MET

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Mol	Chain	Res	Type
1	A	527	HIS
1	B	193	ARG
1	B	249	LYS
1	B	305	ASP
1	B	314	ASP
1	B	328	SER
1	B	398	LEU
1	B	425	SER
1	B	459	ASN
1	B	527	HIS
1	C	92	GLN
1	C	163	ILE
1	C	223	LYS
1	C	243	ASP
1	C	290	VAL
1	C	395	MET
1	C	456	PRO
1	C	459	ASN
1	C	527	HIS
1	D	163[A]	ILE
1	D	163[B]	ILE
1	D	341	GLU
1	D	395[A]	MET
1	D	395[B]	MET
1	D	425	SER
1	D	459	ASN
1	D	481	MET
1	D	497	LEU
1	D	527	HIS

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

Mol	Chain	Res	Type
1	A	222	GLN
1	A	278	GLN
1	B	382	GLN
1	C	126	ASN
1	C	360	GLN
1	C	382	GLN
1	C	434	ASN
1	D	278	GLN
1	D	342	ASN

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Mol	Chain	Res	Type
1	D	382	GLN
1	D	437	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 13 are monoatomic - leaving 13 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	C	606[B]	-	4,4,4	0.28	0	6,6,6	0.28	0
3	SO4	D	605	-	4,4,4	0.40	0	6,6,6	0.30	0
3	SO4	B	605	2	4,4,4	0.54	0	6,6,6	0.52	0
3	SO4	C	605	-	4,4,4	0.25	0	6,6,6	0.89	0
4	EDO	C	608	-	3,3,3	0.53	0	2,2,2	0.21	0
4	EDO	C	609	-	3,3,3	0.67	0	2,2,2	0.23	0
4	EDO	D	607	-	3,3,3	0.71	0	2,2,2	0.46	0
3	SO4	C	607	-	4,4,4	0.41	0	6,6,6	0.53	0
4	EDO	D	606	-	3,3,3	0.64	0	2,2,2	0.24	0
3	SO4	D	604	2	4,4,4	0.85	0	6,6,6	0.37	0
3	SO4	C	604	-	4,4,4	0.34	0	6,6,6	0.42	0
3	SO4	A	604	-	4,4,4	0.51	0	6,6,6	1.46	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	C	606[A]	-	4,4,4	0.67	0	6,6,6	0.45	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
4	EDO	C	609	-	-	0/1/1/1	-
4	EDO	C	608	-	-	0/1/1/1	-
4	EDO	D	607	-	-	0/1/1/1	-
4	EDO	D	606	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	SO4	O3-S-O1	2.60	122.86	109.31

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 [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	467/467 (100%)	-0.79	0 <a href="#">100</a> <a href="#">100</a>	11, 18, 28, 44	0
1	B	467/467 (100%)	-0.80	0 <a href="#">100</a> <a href="#">100</a>	11, 18, 27, 49	0
1	C	467/467 (100%)	-0.82	1 (0%) <a href="#">95</a> <a href="#">95</a>	12, 17, 26, 42	0
1	D	467/467 (100%)	-0.82	2 (0%) <a href="#">92</a> <a href="#">93</a>	11, 17, 26, 43	0
All	All	1868/1868 (100%)	-0.81	3 (0%) <a href="#">95</a> <a href="#">95</a>	11, 18, 27, 49	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	383	ALA	2.5
1	C	382	GLN	2.5
1	D	436[A]	PHE	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( $\text{\AA}^2$ )	Q<0.9
2	CU	B	603	1/1	0.93	0.17	35,35,35,35	1
2	CU	B	602	1/1	0.94	0.14	15,15,15,15	1
2	CU	A	602	1/1	0.94	0.10	27,27,27,27	1
3	SO4	B	605	5/5	0.94	0.10	25,26,27,29	0
3	SO4	A	604	5/5	0.95	0.09	26,27,32,32	0
2	CU	B	601	1/1	0.96	0.10	21,21,21,21	1
3	SO4	D	604	5/5	0.97	0.08	27,27,30,33	0
3	SO4	C	606[A]	5/5	0.97	0.09	19,19,20,23	5
3	SO4	C	606[B]	5/5	0.97	0.09	19,20,20,21	5
2	CU	D	602	1/1	0.97	0.10	15,15,15,15	1
2	CU	B	604	1/1	0.98	0.05	25,25,25,25	1
2	CU	A	601	1/1	0.98	0.07	20,20,20,20	1
2	CU	D	601	1/1	0.98	0.05	22,22,22,22	1
2	CU	D	603	1/1	0.99	0.14	30,30,30,30	1
2	CU	C	603	1/1	0.99	0.07	25,25,25,25	1
2	CU	A	603	1/1	0.99	0.06	33,33,33,33	1
3	SO4	C	605	5/5	0.99	0.04	23,23,26,28	0
4	EDO	C	608	4/4	0.99	0.04	20,21,21,21	0
2	CU	C	602	1/1	0.99	0.06	29,29,29,29	1
3	SO4	C	607	5/5	0.99	0.14	31,31,35,37	0
4	EDO	D	607	4/4	0.99	0.03	17,17,18,19	0
3	SO4	D	605	5/5	0.99	0.07	29,30,31,36	0
4	EDO	D	606	4/4	0.99	0.04	17,19,20,20	0
4	EDO	C	609	4/4	0.99	0.05	18,19,19,20	0
3	SO4	C	604	5/5	0.99	0.04	23,24,27,28	0
2	CU	C	601	1/1	0.99	0.08	19,19,19,19	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.