



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:57 AM UTC

PDB ID : 6G50 / pdb_00006g50
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

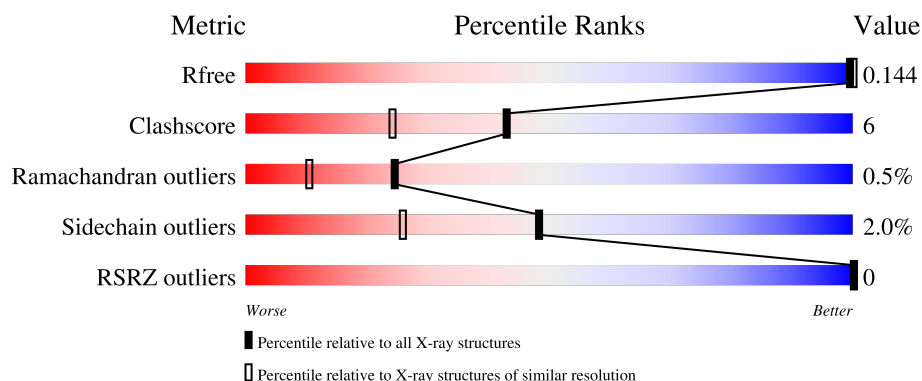
1 Overall quality at a glance

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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	B	467	
1	C	467	
1	D	467	

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 (CCD ID: CU) (formula: Cu).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: EDO) (formula: C₂H₆O₂).



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		

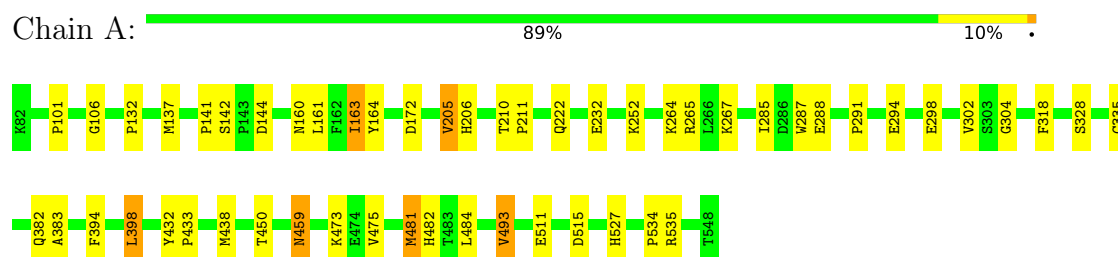
- Molecule 5 is water.

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		

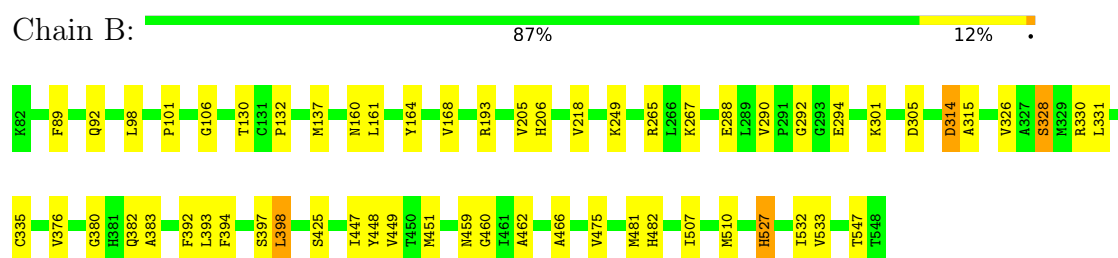
3 Residue-property plots

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.

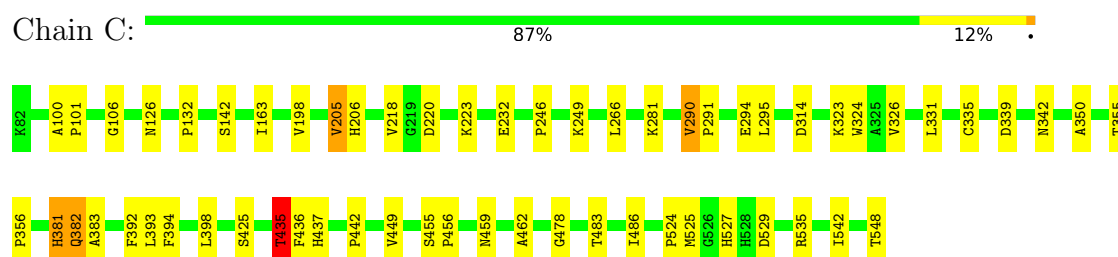
• Molecule 1: Uncharacterized protein



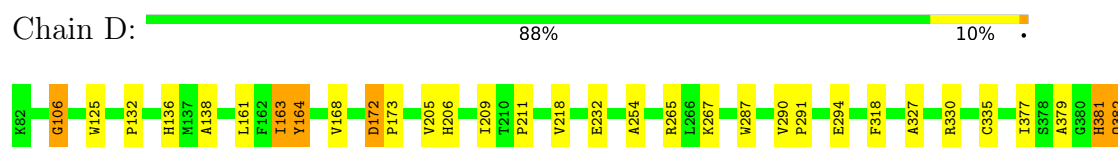
• Molecule 1: Uncharacterized protein



• Molecule 1: Uncharacterized protein



• Molecule 1: Uncharacterized protein



A383	
D388	
G389	
Q390	
S391	
F392	
L393	
F394	
M395	
L398	
M434	
T435	
F436	
H437	
I447	
T450	
M451	
W452	
M459	
D465	
E470	
M481	
H482	
H527	
V533	
T547	
T548	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.63Å 162.28Å 90.57Å 90.00° 119.51° 90.00°	Depositor
Resolution (Å)	45.31 – 1.65 45.31 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.3 (45.31-1.65) 97.3 (45.31-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EDO, CU, 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	1.07	0/3849	1.08	7/5249 (0.1%)
1	B	1.04	1/3824 (0.0%)	1.14	12/5214 (0.2%)
1	C	1.10	3/3824 (0.1%)	1.11	7/5214 (0.1%)
1	D	1.06	3/3882 (0.1%)	1.09	4/5297 (0.1%)
All	All	1.07	7/15379 (0.0%)	1.11	30/20974 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	435	THR	CA-C	-9.32	1.43	1.53
1	C	524	PRO	CA-C	6.53	1.58	1.53
1	C	455	SER	CA-C	6.43	1.59	1.53
1	B	218	VAL	C-O	6.08	1.30	1.24
1	D	172	ASP	CA-CB	5.58	1.59	1.53
1	D	106	GLY	N-CA	5.35	1.53	1.45
1	C	198	VAL	N-CA	5.27	1.52	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	VAL	CA-C-N	-10.13	110.50	120.52
1	B	290	VAL	C-N-CA	-10.13	110.50	120.52
1	B	383	ALA	N-CA-C	-7.01	103.61	112.93
1	A	482	HIS	N-CA-C	6.01	118.40	108.48
1	B	527	HIS	N-CA-C	6.00	119.06	110.24
1	D	254	ALA	N-CA-C	5.97	118.56	111.33
1	A	144	ASP	CA-C-N	5.96	125.84	119.28
1	A	144	ASP	C-N-CA	5.96	125.84	119.28
1	A	172	ASP	CA-C-N	-5.91	113.85	119.76
1	A	172	ASP	C-N-CA	-5.91	113.85	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	VAL	CA-C-N	-5.84	114.59	120.31
1	B	533	VAL	C-N-CA	-5.84	114.59	120.31
1	B	482	HIS	N-CA-C	5.82	118.08	108.48
1	C	355	THR	CA-C-N	-5.58	114.85	120.21
1	C	355	THR	C-N-CA	-5.58	114.85	120.21
1	C	331	LEU	CA-C-N	-5.48	115.25	120.83
1	C	331	LEU	C-N-CA	-5.48	115.25	120.83
1	B	481	MET	CA-CB-CG	-5.34	103.42	114.10
1	D	382	GLN	N-CA-C	-5.29	101.92	109.86
1	D	164	TYR	N-CA-C	-5.24	102.40	109.95
1	C	425	SER	CA-C-N	5.21	124.87	119.56
1	C	425	SER	C-N-CA	5.21	124.87	119.56
1	B	130	THR	CA-C-N	-5.15	117.58	122.37
1	B	130	THR	C-N-CA	-5.15	117.58	122.37
1	B	397	SER	N-CA-C	5.12	117.79	109.24
1	C	435	THR	N-CA-CB	5.08	117.54	109.71
1	A	210	THR	CA-C-N	-5.08	114.59	119.87
1	A	210	THR	C-N-CA	-5.08	114.59	119.87
1	D	533	VAL	N-CA-CB	5.04	118.27	111.21
1	B	164	TYR	N-CA-C	-5.01	102.74	109.95

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	3685	0	3544	37	0
1	B	3664	0	3540	38	0
1	C	3679	0	3545	43	0
1	D	3694	0	3542	64	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
5	A	383	0	0	3	0
5	B	356	0	0	0	0
5	C	399	0	0	4	0
5	D	393	0	0	11	0
All	All	16327	0	14195	179	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 (179) 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: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:B:449[A]:VAL:HG23	1:B:451[A]:MET:CE	1.75	1.16
1:C:381[B]:HIS:NE2	1:C:436[B]:PHE:CB	2.15	1.09
1:B:449[A]:VAL:HG23	1:B:451[A]:MET:HE3	1.27	1.06
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:D:435:THR:CG2	1:D:451:MET:HE1	1.98	0.94
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:435:THR:HG21	1:D:451:MET:HE1	1.51	0.91
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:D:381[B]:HIS:NE2	1:D:436[B]:PHE:CA	2.36	0.89
1:B:449[A]:VAL:CG2	1:B:451[A]:MET:HE3	2.01	0.89
1:D:435:THR:HG22	1:D:451:MET:CE	2.04	0.88
1:D:437:HIS:HE1	5:D:740:HOH:O	1.57	0.88
1:D:382:GLN:HB3	1:D:395[B]:MET:HG2	1.57	0.85
1:D:382:GLN:HB3	1:D:395[B]:MET:HG3	1.59	0.83
1:D:435:THR:HG22	1:D:451:MET:HE2	1.60	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381[B]:HIS:CD2	1:C:382:GLN:N	2.48	0.80
1:A:328:SER:HB3	1:A:382[B]:GLN:HB3	1.63	0.79
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:294:GLU:CD	1:D:294:GLU:H	1.97	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:B:449[A]:VAL:HG23	1:B:451[A]:MET:HE2	1.73	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: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:106:GLY:HA2	1:D:132:PRO:O	1.97	0.64
1:B:448:TYR:HE2	1:B:510:MET:HE2	1.63	0.63
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:B:314:ASP:CG	1:B:328:SER:HB3	2.27	0.60
1:C:381[B]:HIS:O	1:C:382:GLN:C	2.44	0.59
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381[B]:HIS:CE1	1:D:436[B]:PHE:CB	2.88	0.56
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: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: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:B:451[A]:MET:HE3	1:B:462:ALA:HB3	1.91	0.52
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:381[B]:HIS:CG	1:D:382:GLN:N	2.64	0.51
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: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
1:A:160:ASN:HD21	1:A:222:GLN:NE2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:294:GLU:CD	1:B:330:ARG:HH21	2.22	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:B:448:TYR:CE2	1:B:510:MET:HE2	2.47	0.45
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:B:392:PHE:C	1:B:393:LEU:HD12	2.41	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:100:ALA:O	1:C:525:MET:HE1	2.18	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: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:D:434:ASN:C	1:D:435:THR:HG23	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:GLN:HA	1:B:394:PHE:HD1	1.85	0.42
1:B:449[A]:VAL:HG21	1:B:451[A]:MET:CE	2.45	0.42
1:D:294:GLU:CD	1:D:294:GLU:N	2.73	0.42
1:B:98:LEU:CD2	1:B:507[A]:ILE:HD13	2.50	0.42
1:C:339:ASP:CG	1:C:342:ASN:HB2	2.44	0.42
1:B:328:SER:HB2	1:B:382:GLN:CD	2.45	0.42
1:D:381[A]:HIS:HE1	5:D:1039:HOH:O	2.02	0.42
1:D:388:ASP:CG	1:D:390:GLN:HG2	2.45	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: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: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%)	30 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	475/467 (102%)	446 (94%)	28 (6%)	1 (0%)	43	27
1	C	474/467 (102%)	447 (94%)	22 (5%)	5 (1%)	11	2
1	D	482/467 (103%)	455 (94%)	23 (5%)	4 (1%)	16	4
All	All	1909/1868 (102%)	1804 (94%)	93 (5%)	12 (1%)	24	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 ⓘ

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%)	396 (98%)	9 (2%)	45	23
1	B	402/392 (103%)	392 (98%)	10 (2%)	42	18
1	C	401/392 (102%)	393 (98%)	8 (2%)	48	26
1	D	408/392 (104%)	401 (98%)	7 (2%)	53	32
All	All	1616/1568 (103%)	1582 (98%)	34 (2%)	48	24

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163[A]	ILE
1	A	163[B]	ILE
1	A	252	LYS
1	A	291	PRO
1	A	398	LEU
1	A	459	ASN
1	A	481	MET
1	A	493	VAL
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	B	547	THR
1	C	163	ILE
1	C	223	LYS
1	C	232	GLU
1	C	266	LEU
1	C	290	VAL
1	C	435	THR
1	C	456	PRO
1	C	527	HIS
1	D	163[A]	ILE
1	D	163[B]	ILE
1	D	377	ILE
1	D	447	ILE
1	D	459	ASN
1	D	481	MET
1	D	527	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	342	ASN
1	A	390	GLN
1	A	530	ASN
1	B	382	GLN

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Mol	Chain	Res	Type
1	B	434	ASN
1	B	530	ASN
1	C	126	ASN
1	C	382	GLN
1	C	502	ASN
1	D	342	ASN
1	D	360	GLN
1	D	437	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	605	2	4,4,4	0.62	0	6,6,6	0.52	0
3	SO4	C	604	-	4,4,4	0.42	0	6,6,6	0.41	0
4	EDO	C	608	-	3,3,3	0.50	0	2,2,2	0.24	0
3	SO4	C	606[B]	-	4,4,4	0.38	0	6,6,6	0.26	0
3	SO4	D	605	-	4,4,4	0.49	0	6,6,6	0.31	0
4	EDO	C	609	-	3,3,3	0.64	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	607	-	3,3,3	0.67	0	2,2,2	0.49	0
3	SO4	A	604	-	4,4,4	0.58	0	6,6,6	1.45	1 (16%)
4	EDO	D	606	-	3,3,3	0.60	0	2,2,2	0.20	0
3	SO4	C	606[A]	-	4,4,4	0.74	0	6,6,6	0.43	0
3	SO4	D	604	2	4,4,4	0.90	0	6,6,6	0.40	0
3	SO4	C	605	-	4,4,4	0.33	0	6,6,6	0.83	0
3	SO4	C	607	-	4,4,4	0.51	0	6,6,6	0.54	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	D	606	-	-	0/1/1/1	-
4	EDO	D	607	-	-	0/1/1/1	-
4	EDO	C	608	-	-	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	2.54	122.86	109.56

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	467/467 (100%)	-1.37	0 100 100	10, 18, 28, 44	13 (2%)
1	B	467/467 (100%)	-1.37	0 100 100	11, 18, 27, 49	10 (2%)
1	C	467/467 (100%)	-1.39	0 100 100	9, 17, 26, 42	9 (1%)
1	D	467/467 (100%)	-1.39	0 100 100	10, 17, 26, 43	17 (3%)
All	All	1868/1868 (100%)	-1.38	0 100 100	9, 18, 27, 49	49 (2%)

There are no RSRZ outliers to report.

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CU	A	602	1/1	0.99	0.07	27,27,27,27	1
2	CU	B	601	1/1	0.99	0.05	21,21,21,21	1
2	CU	B	602	1/1	0.99	0.05	15,15,15,15	1
2	CU	B	603	1/1	0.99	0.14	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	B	604	1/1	0.99	0.03	25,25,25,25	1
2	CU	D	602	1/1	0.99	0.03	15,15,15,15	1
2	CU	D	603	1/1	0.99	0.08	30,30,30,30	1
3	SO4	A	604	5/5	0.99	0.06	26,27,32,32	0
3	SO4	B	605	5/5	0.99	0.06	25,26,27,29	0
3	SO4	C	606[A]	5/5	0.99	0.04	19,19,20,23	5
3	SO4	C	606[B]	5/5	0.99	0.04	19,20,20,21	5
3	SO4	C	607	5/5	0.99	0.04	31,31,35,37	0
3	SO4	D	604	5/5	0.99	0.05	27,27,30,33	0
3	SO4	D	605	5/5	0.99	0.06	29,30,31,36	0
2	CU	C	602	1/1	1.00	0.05	29,29,29,29	1
3	SO4	C	604	5/5	1.00	0.04	23,24,27,28	0
3	SO4	C	605	5/5	1.00	0.02	23,23,26,28	0
2	CU	C	603	1/1	1.00	0.03	25,25,25,25	1
2	CU	D	601	1/1	1.00	0.01	22,22,22,22	1
2	CU	A	601	1/1	1.00	0.01	20,20,20,20	1
2	CU	A	603	1/1	1.00	0.03	33,33,33,33	1
2	CU	C	601	1/1	1.00	0.03	19,19,19,19	1
4	EDO	C	608	4/4	1.00	0.02	20,21,21,21	0
4	EDO	C	609	4/4	1.00	0.02	18,19,19,20	0
4	EDO	D	606	4/4	1.00	0.02	17,19,20,20	0
4	EDO	D	607	4/4	1.00	0.02	17,17,18,19	0

6.5 Other polymers

There are no such residues in this entry.