



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:09 PM UTC

PDB ID : 5GHA / pdb_00005gha
Title : Sulfur Transferase TtuA in complex with Sulfur Carrier TtuB
Authors : Chen, M.; Narai, S.; Tanaka, Y.; Yao, M.
Deposited on : 2016-06-19
Resolution : 2.50 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

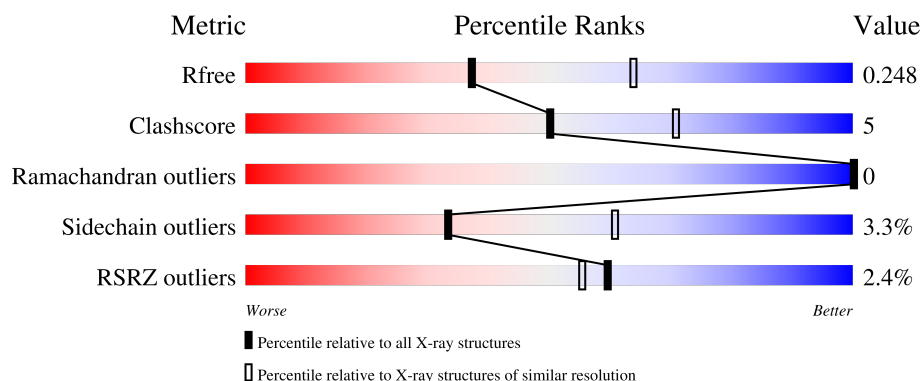
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	321	2% 84% 10% 5%
1	B	321	% 79% 16% • •
1	C	321	% 81% 12% 6%
1	D	321	% 83% 13% •
2	E	85	7% 55% 15% • 27%

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Mol	Chain	Length	Quality of chain
2	F	85	% 62%18%19%
2	G	85	9% 42%20%35%
2	H	85	4% 56%16%25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11849 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 Sulfur Transferase TtuA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2418	1539	447	418	14			
1	D	310	Total	C	N	O	S	0	0	0
			2457	1561	454	428	14			
1	B	309	Total	C	N	O	S	0	0	0
			2448	1556	454	424	14			
1	C	302	Total	C	N	O	S	0	0	0
			2402	1527	445	416	14			

- Molecule 2 is a protein called Sulfur Carrier TtuB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	62	Total	C	N	O		0	0	0
			495	307	87	101				
2	H	64	Total	C	N	O	S	0	0	0
			513	318	91	103	1			
2	F	69	Total	C	N	O	S	0	0	0
			550	342	99	108	1			
2	G	55	Total	C	N	O		0	0	0
			438	272	77	89				

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	expression tag	UNP Q72LF4
E	-18	GLY	-	expression tag	UNP Q72LF4
E	-17	SER	-	expression tag	UNP Q72LF4
E	-16	SER	-	expression tag	UNP Q72LF4
E	-15	HIS	-	expression tag	UNP Q72LF4
E	-14	HIS	-	expression tag	UNP Q72LF4
E	-13	HIS	-	expression tag	UNP Q72LF4
E	-12	HIS	-	expression tag	UNP Q72LF4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	HIS	-	expression tag	UNP Q72LF4
E	-10	HIS	-	expression tag	UNP Q72LF4
E	-9	SER	-	expression tag	UNP Q72LF4
E	-8	SER	-	expression tag	UNP Q72LF4
E	-7	GLY	-	expression tag	UNP Q72LF4
E	-6	LEU	-	expression tag	UNP Q72LF4
E	-5	VAL	-	expression tag	UNP Q72LF4
E	-4	PRO	-	expression tag	UNP Q72LF4
E	-3	ARG	-	expression tag	UNP Q72LF4
E	-2	GLY	-	expression tag	UNP Q72LF4
E	-1	SER	-	expression tag	UNP Q72LF4
E	0	HIS	-	expression tag	UNP Q72LF4
E	65	CYS	-	expression tag	UNP Q72LF4
H	-19	MET	-	expression tag	UNP Q72LF4
H	-18	GLY	-	expression tag	UNP Q72LF4
H	-17	SER	-	expression tag	UNP Q72LF4
H	-16	SER	-	expression tag	UNP Q72LF4
H	-15	HIS	-	expression tag	UNP Q72LF4
H	-14	HIS	-	expression tag	UNP Q72LF4
H	-13	HIS	-	expression tag	UNP Q72LF4
H	-12	HIS	-	expression tag	UNP Q72LF4
H	-11	HIS	-	expression tag	UNP Q72LF4
H	-10	HIS	-	expression tag	UNP Q72LF4
H	-9	SER	-	expression tag	UNP Q72LF4
H	-8	SER	-	expression tag	UNP Q72LF4
H	-7	GLY	-	expression tag	UNP Q72LF4
H	-6	LEU	-	expression tag	UNP Q72LF4
H	-5	VAL	-	expression tag	UNP Q72LF4
H	-4	PRO	-	expression tag	UNP Q72LF4
H	-3	ARG	-	expression tag	UNP Q72LF4
H	-2	GLY	-	expression tag	UNP Q72LF4
H	-1	SER	-	expression tag	UNP Q72LF4
H	0	HIS	-	expression tag	UNP Q72LF4
H	65	CYS	-	expression tag	UNP Q72LF4
F	-19	MET	-	expression tag	UNP Q72LF4
F	-18	GLY	-	expression tag	UNP Q72LF4
F	-17	SER	-	expression tag	UNP Q72LF4
F	-16	SER	-	expression tag	UNP Q72LF4
F	-15	HIS	-	expression tag	UNP Q72LF4
F	-14	HIS	-	expression tag	UNP Q72LF4
F	-13	HIS	-	expression tag	UNP Q72LF4
F	-12	HIS	-	expression tag	UNP Q72LF4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	HIS	-	expression tag	UNP Q72LF4
F	-10	HIS	-	expression tag	UNP Q72LF4
F	-9	SER	-	expression tag	UNP Q72LF4
F	-8	SER	-	expression tag	UNP Q72LF4
F	-7	GLY	-	expression tag	UNP Q72LF4
F	-6	LEU	-	expression tag	UNP Q72LF4
F	-5	VAL	-	expression tag	UNP Q72LF4
F	-4	PRO	-	expression tag	UNP Q72LF4
F	-3	ARG	-	expression tag	UNP Q72LF4
F	-2	GLY	-	expression tag	UNP Q72LF4
F	-1	SER	-	expression tag	UNP Q72LF4
F	0	HIS	-	expression tag	UNP Q72LF4
F	65	CYS	-	expression tag	UNP Q72LF4
G	-19	MET	-	expression tag	UNP Q72LF4
G	-18	GLY	-	expression tag	UNP Q72LF4
G	-17	SER	-	expression tag	UNP Q72LF4
G	-16	SER	-	expression tag	UNP Q72LF4
G	-15	HIS	-	expression tag	UNP Q72LF4
G	-14	HIS	-	expression tag	UNP Q72LF4
G	-13	HIS	-	expression tag	UNP Q72LF4
G	-12	HIS	-	expression tag	UNP Q72LF4
G	-11	HIS	-	expression tag	UNP Q72LF4
G	-10	HIS	-	expression tag	UNP Q72LF4
G	-9	SER	-	expression tag	UNP Q72LF4
G	-8	SER	-	expression tag	UNP Q72LF4
G	-7	GLY	-	expression tag	UNP Q72LF4
G	-6	LEU	-	expression tag	UNP Q72LF4
G	-5	VAL	-	expression tag	UNP Q72LF4
G	-4	PRO	-	expression tag	UNP Q72LF4
G	-3	ARG	-	expression tag	UNP Q72LF4
G	-2	GLY	-	expression tag	UNP Q72LF4
G	-1	SER	-	expression tag	UNP Q72LF4
G	0	HIS	-	expression tag	UNP Q72LF4
G	65	CYS	-	expression tag	UNP Q72LF4

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	0
			16	16		
6	D	25	Total	O	0	0
			25	25		
6	B	16	Total	O	0	0
			16	16		
6	C	19	Total	O	0	0
			19	19		
6	E	2	Total	O	0	0
			2	2		
6	H	2	Total	O	0	0
			2	2		

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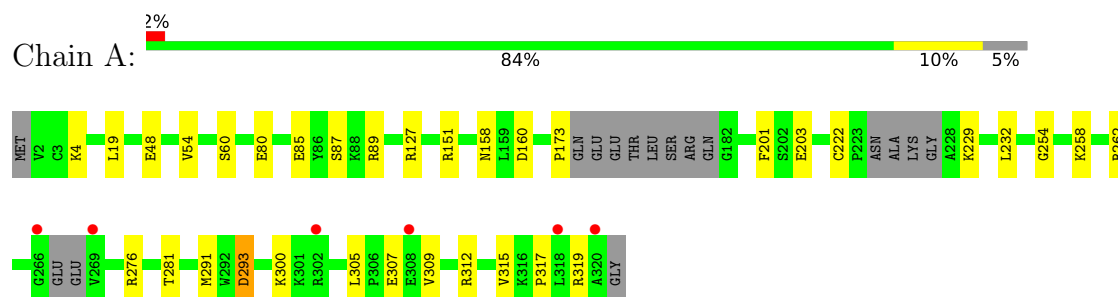
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	O	0	0
			1	1		

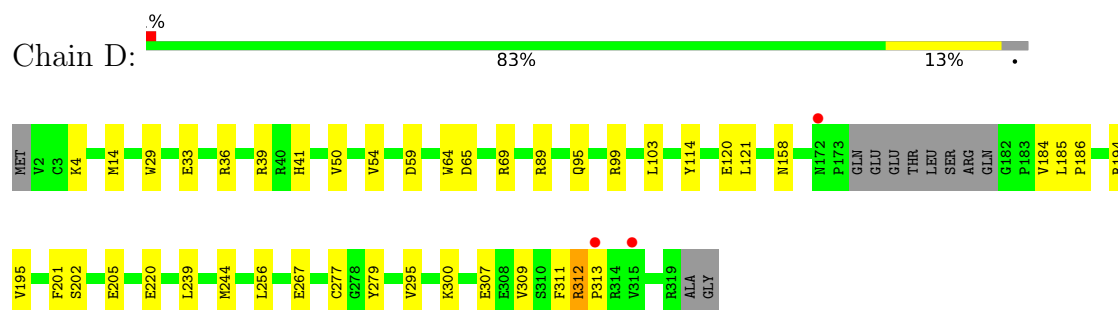
3 Residue-property plots [i](#)

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.

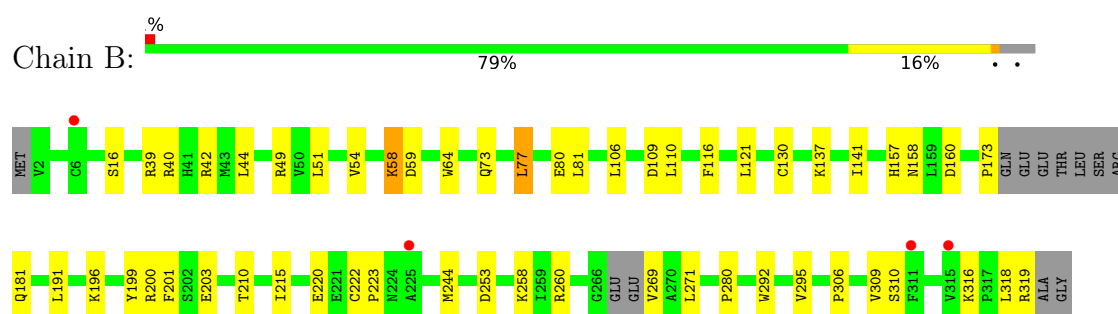
• Molecule 1: Sulfur Transferase TtuA



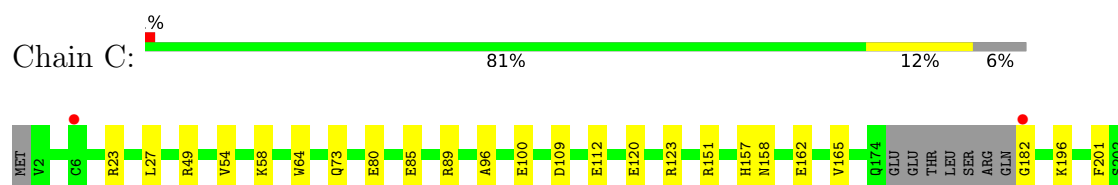
• Molecule 1: Sulfur Transferase TtuA

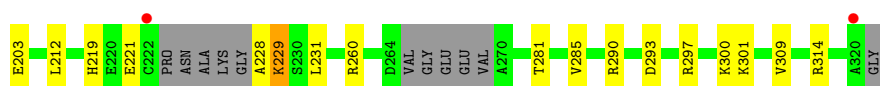


• Molecule 1: Sulfur Transferase TtuA

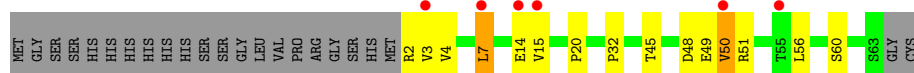


• Molecule 1: Sulfur Transferase TtuA

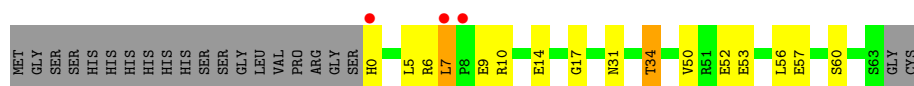




• Molecule 2: Sulfur Carrier TtuB



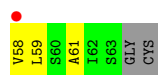
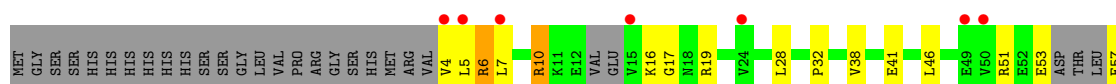
• Molecule 2: Sulfur Carrier TtuB



• Molecule 2: Sulfur Carrier TtuB



• Molecule 2: Sulfur Carrier TtuB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.14Å 93.87Å 97.53Å 109.21° 104.57° 106.86°	Depositor
Resolution (Å)	47.84 – 2.50 47.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.84-2.50) 97.4 (47.84-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.196 , 0.246 0.201 , 0.248	Depositor DCC
R_{free} test set	2752 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.099 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11849	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: ZN, SO4, 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	0.29	0/2461	0.70	0/3310
1	B	0.29	0/2492	0.72	0/3352
1	C	0.29	0/2444	0.71	0/3285
1	D	0.29	0/2502	0.71	0/3367
2	E	0.26	0/497	0.72	0/672
2	F	0.28	0/554	0.72	0/749
2	G	0.28	0/438	0.76	0/588
2	H	0.27	0/516	0.73	0/697
All	All	0.29	0/11904	0.71	0/16020

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2418	0	2489	21	0
1	B	2448	0	2520	31	0
1	C	2402	0	2469	24	0
1	D	2457	0	2525	22	0
2	E	495	0	513	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	550	0	575	9	0
2	G	438	0	452	12	0
2	H	513	0	532	7	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	10	0	0	1	0
4	C	5	0	0	1	0
5	B	8	0	12	1	0
5	C	4	0	6	0	0
5	D	8	0	12	1	0
5	E	4	0	6	1	0
6	A	16	0	0	0	0
6	B	16	0	0	0	0
6	C	19	0	0	0	1
6	D	25	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	H	2	0	0	0	0
All	All	11849	0	12111	127	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 5.

All (127) 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:33:GLU:OE1	1:D:36:ARG:NH1	1.96	0.97
1:A:127:ARG:NH1	1:A:291:MET:SD	2.39	0.96
1:C:285:VAL:O	1:C:290:ARG:NH1	2.08	0.87
1:B:181:GLN:O	1:B:260:ARG:NH1	2.14	0.80
1:A:300:LYS:NZ	1:A:309:VAL:O	2.18	0.76
1:A:312:ARG:HH12	1:A:315:VAL:HG23	1.55	0.70
2:H:50:VAL:HG11	2:H:56:LEU:HD11	1.73	0.70
1:C:219:HIS:CD2	2:G:6:ARG:HH12	2.10	0.70
1:C:219:HIS:HD2	2:G:6:ARG:HH12	1.40	0.68
2:H:52:GLU:HG2	2:H:53:GLU:HG2	1.76	0.67
1:B:121:LEU:HD12	1:B:295:VAL:HG21	1.79	0.65
1:B:39:ARG:NH1	1:B:44:LEU:O	2.31	0.63
2:H:0:HIS:N	2:H:14:GLU:OE1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:ARG:N	2:F:49:GLU:OE2	2.33	0.61
1:A:85:GLU:HB3	1:A:89:ARG:NH1	2.16	0.61
1:C:120:GLU:OE2	1:C:123:ARG:NH1	2.35	0.59
1:B:42:ARG:HD2	1:C:151:ARG:HG3	1.86	0.57
1:D:59:ASP:HB2	5:D:403:EDO:H12	1.87	0.56
1:D:121:LEU:HD12	1:D:295:VAL:HG21	1.87	0.56
2:E:45:THR:OG1	2:E:48:ASP:OD2	2.23	0.56
2:F:-6:LEU:HD23	2:F:-4:PRO:HD2	1.88	0.55
1:A:232:LEU:HD23	1:B:244:MET:HE3	1.89	0.55
1:B:199:TYR:CZ	1:B:200:ARG:HD3	2.41	0.55
2:E:7:LEU:HA	2:E:60:SER:HB2	1.87	0.55
1:D:14:MET:HE1	1:D:29:TRP:CZ3	2.41	0.55
1:B:16:SER:HB2	5:B:403:EDO:H21	1.87	0.55
1:B:318:LEU:HD12	1:B:319:ARG:HG2	1.90	0.54
2:H:31:ASN:HB3	2:H:34:THR:HB	1.90	0.54
1:C:300:LYS:NZ	1:C:309:VAL:O	2.26	0.54
2:E:50:VAL:HG21	2:E:56:LEU:HD11	1.90	0.54
2:H:7:LEU:HB3	2:H:60:SER:HB2	1.90	0.54
2:G:17:GLY:HA3	2:G:19:ARG:HH21	1.72	0.53
1:C:281:THR:OG1	4:C:403:SO4:O4	2.27	0.53
1:B:200:ARG:NH2	1:B:253:ASP:OD1	2.42	0.53
1:B:49:ARG:HA	1:B:73:GLN:HB2	1.91	0.53
1:C:49:ARG:HA	1:C:73:GLN:HB2	1.91	0.52
2:E:2:ARG:NH2	2:E:15:VAL:O	2.42	0.52
2:G:6:ARG:HH21	2:G:10:ARG:NH1	2.07	0.52
2:G:16:LYS:O	2:G:19:ARG:NH2	2.42	0.52
1:B:80:GLU:HG2	1:B:109:ASP:OD2	2.08	0.52
1:A:4:LYS:HD3	1:A:19:LEU:HD12	1.92	0.51
1:A:48:GLU:OE2	1:A:151:ARG:HD3	2.09	0.51
1:D:89:ARG:HD2	1:D:220:GLU:OE2	2.11	0.51
1:A:158:ASN:HB2	1:A:201:PHE:O	2.11	0.51
2:G:6:ARG:HA	2:G:10:ARG:H	1.75	0.51
1:C:157:HIS:HB2	1:C:196:LYS:HD3	1.91	0.50
1:C:85:GLU:HB3	1:C:89:ARG:NH1	2.26	0.50
1:B:40:ARG:HH12	1:B:200:ARG:NH1	2.09	0.50
2:E:3:VAL:HG22	2:E:56:LEU:HB2	1.94	0.50
1:D:267:GLU:OE1	1:D:267:GLU:N	2.38	0.50
1:A:281:THR:OG1	4:A:403:SO4:O1	2.29	0.49
1:A:173:PRO:HB2	1:B:258:LYS:HD3	1.94	0.49
1:C:158:ASN:HB2	1:C:201:PHE:O	2.13	0.49
1:C:162:GLU:HA	1:C:165:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:HD12	1:B:141:ILE:HG12	1.96	0.47
2:G:32:PRO:HB3	2:G:46:LEU:HD21	1.97	0.47
2:G:5:LEU:HD12	2:G:58:VAL:HB	1.97	0.46
2:E:32:PRO:O	5:E:101:EDO:O2	2.32	0.46
1:A:229:LYS:HD2	1:B:244:MET:HE2	1.96	0.46
1:D:4:LYS:HA	1:D:4:LYS:HD2	1.70	0.46
2:F:0:HIS:HA	2:F:52:GLU:OE2	2.14	0.46
2:F:1:MET:HE1	2:F:50:VAL:HB	1.97	0.46
2:F:-6:LEU:HD22	2:F:-3:ARG:HD2	1.96	0.46
1:A:160:ASP:HB2	1:A:203:GLU:HG3	1.98	0.45
1:A:80:GLU:OE1	1:A:87:SER:HB3	2.16	0.45
1:D:300:LYS:HD3	1:D:307:GLU:HA	1.97	0.45
2:F:6:ARG:NH1	2:F:10:ARG:HE	2.14	0.45
1:A:317:PRO:C	1:A:319:ARG:H	2.24	0.45
1:C:27:LEU:HD21	1:C:212:LEU:HB3	1.97	0.45
2:E:7:LEU:HD22	2:E:60:SER:HB2	1.99	0.45
2:G:51:ARG:HB3	2:G:53:GLU:HG2	1.99	0.45
1:B:306:PRO:HB2	1:B:309:VAL:HG13	1.99	0.45
1:C:109:ASP:HB3	1:C:112:GLU:HB2	1.98	0.45
2:F:-6:LEU:O	2:F:-2:GLY:N	2.46	0.45
1:B:271:LEU:HD13	1:B:280:PRO:HB2	1.98	0.44
1:A:300:LYS:HZ2	1:A:309:VAL:HG22	1.82	0.44
1:D:185:LEU:HA	1:D:186:PRO:HD3	1.84	0.44
1:B:191:LEU:HB2	1:B:280:PRO:HG3	2.00	0.44
2:H:0:HIS:CD2	2:H:17:GLY:H	2.36	0.44
1:D:41:HIS:HB3	1:D:184:VAL:HG21	1.98	0.44
1:B:81:LEU:HD11	1:B:137:LYS:HE3	2.00	0.44
1:A:85:GLU:HB3	1:A:89:ARG:HH12	1.83	0.44
1:A:254:GLY:HA3	1:B:173:PRO:HG3	1.99	0.44
1:B:157:HIS:HB2	1:B:196:LYS:HD3	2.00	0.44
2:G:6:ARG:HH21	2:G:10:ARG:HH11	1.66	0.44
1:D:158:ASN:HB2	1:D:201:PHE:O	2.18	0.43
1:B:51:LEU:HD11	1:B:77:LEU:HB2	1.99	0.43
2:F:1:MET:HG2	2:F:15:VAL:O	2.18	0.43
1:C:80:GLU:HB3	1:C:109:ASP:HA	1.99	0.43
1:A:276:ARG:NH2	1:A:293:ASP:OD1	2.46	0.43
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.80	0.43
2:G:4:VAL:HB	2:G:57:GLU:HB3	2.00	0.43
1:A:258:LYS:O	1:A:262:ARG:HD3	2.19	0.42
2:E:2:ARG:HB3	2:E:14:GLU:HA	2.00	0.42
1:D:185:LEU:HB2	1:D:194:ARG:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ALA:O	1:C:100:GLU:HB2	2.18	0.42
1:C:182:GLY:N	1:C:260:ARG:HH12	2.16	0.42
1:C:297:ARG:O	1:C:301:LYS:HG2	2.19	0.42
1:B:222:CYS:HA	1:B:223:PRO:HD3	1.90	0.42
1:C:54:VAL:HG11	1:C:64:TRP:CE3	2.54	0.42
1:D:95:GLN:O	1:D:99:ARG:HG2	2.20	0.42
1:A:54:VAL:HA	1:A:60:SER:HB2	2.01	0.42
1:D:54:VAL:HG11	1:D:64:TRP:CE3	2.55	0.41
1:B:158:ASN:HB2	1:B:201:PHE:O	2.19	0.41
1:B:160:ASP:HB2	1:B:203:GLU:HG3	2.02	0.41
1:B:77:LEU:HD23	1:B:106:LEU:HB2	2.01	0.41
2:E:49:GLU:OE2	2:E:51:ARG:NH2	2.53	0.41
1:C:203:GLU:HB3	2:G:61:ALA:O	2.20	0.41
1:B:54:VAL:HG11	1:B:64:TRP:CE3	2.55	0.41
1:C:228:ALA:HB3	1:C:231:LEU:HD12	2.02	0.41
1:D:114:TYR:HD1	1:D:311:PHE:HE1	1.68	0.41
1:D:277:CYS:SG	1:D:279:TYR:HB2	2.61	0.41
1:C:293:ASP:O	1:C:297:ARG:HG3	2.21	0.41
1:A:300:LYS:HZ2	1:A:309:VAL:CG2	2.34	0.41
1:B:58:LYS:NZ	1:B:59:ASP:OD2	2.28	0.41
1:B:116:PHE:HD2	1:B:292:TRP:HZ3	1.69	0.41
2:F:53:GLU:OE1	2:F:53:GLU:N	2.53	0.41
1:D:65:ASP:CG	1:D:69:ARG:HE	2.29	0.41
1:D:312:ARG:HA	1:D:313:PRO:HD3	1.79	0.41
1:D:202:SER:OG	1:D:205:GLU:HG3	2.22	0.40
2:E:20:PRO:HA	2:E:49:GLU:HA	2.03	0.40
1:D:64:TRP:CE2	1:D:103:LEU:HD13	2.56	0.40
1:D:114:TYR:CD1	1:D:311:PHE:HE1	2.38	0.40
1:D:244:MET:HE3	1:C:229:LYS:HG3	2.04	0.40
1:B:210:THR:HG23	1:B:215:ILE:HB	2.03	0.40
2:H:5:LEU:O	2:H:10:ARG:HA	2.20	0.40
1:C:23:ARG:HG3	1:C:212:LEU:HG	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)
6:C:506:HOH:O	6:C:518:HOH:O[1_455]	2.16	0.04

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	297/321 (92%)	294 (99%)	3 (1%)	0	100	100
1	B	303/321 (94%)	296 (98%)	7 (2%)	0	100	100
1	C	294/321 (92%)	290 (99%)	4 (1%)	0	100	100
1	D	306/321 (95%)	301 (98%)	5 (2%)	0	100	100
2	E	60/85 (71%)	56 (93%)	4 (7%)	0	100	100
2	F	67/85 (79%)	64 (96%)	3 (4%)	0	100	100
2	G	49/85 (58%)	48 (98%)	1 (2%)	0	100	100
2	H	62/85 (73%)	61 (98%)	1 (2%)	0	100	100
All	All	1438/1624 (88%)	1410 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	253/266 (95%)	249 (98%)	4 (2%)	55	79
1	B	256/266 (96%)	249 (97%)	7 (3%)	39	67
1	C	251/266 (94%)	247 (98%)	4 (2%)	55	79
1	D	257/266 (97%)	249 (97%)	8 (3%)	35	62
2	E	57/76 (75%)	54 (95%)	3 (5%)	20	42
2	F	63/76 (83%)	60 (95%)	3 (5%)	23	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	50/76 (66%)	43 (86%)	7 (14%)	3	7
2	H	59/76 (78%)	54 (92%)	5 (8%)	10	22
All	All	1246/1368 (91%)	1205 (97%)	41 (3%)	33	61

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	CYS
1	A	293	ASP
1	A	305	LEU
1	A	307	GLU
1	D	39	ARG
1	D	50	VAL
1	D	120	GLU
1	D	195	VAL
1	D	239	LEU
1	D	256	LEU
1	D	309	VAL
1	D	312	ARG
1	B	58	LYS
1	B	77	LEU
1	B	130	CYS
1	B	220	GLU
1	B	269	VAL
1	B	310	SER
1	B	316	LYS
1	C	58	LYS
1	C	221	GLU
1	C	229	LYS
1	C	314	ARG
2	E	4	VAL
2	E	7	LEU
2	E	50	VAL
2	H	6	ARG
2	H	7	LEU
2	H	9	GLU
2	H	34	THR
2	H	57	GLU
2	F	-6	LEU
2	F	24	VAL
2	F	58	VAL

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Mol	Chain	Res	Type
2	G	6	ARG
2	G	7	LEU
2	G	10	ARG
2	G	28	LEU
2	G	38	VAL
2	G	41	GLU
2	G	59	LEU

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

Mol	Chain	Res	Type
1	B	219	HIS
1	B	224	ASN
1	C	95	GLN
1	C	172	ASN
2	F	18	ASN

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 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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
5	EDO	C	404	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	E	101	-	3,3,3	0.42	0	2,2,2	0.39	0
5	EDO	D	403	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	D	404	-	3,3,3	0.51	0	2,2,2	0.19	0
5	EDO	B	403	-	3,3,3	0.48	0	2,2,2	0.23	0
4	SO4	A	403	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	C	403	-	4,4,4	0.23	0	6,6,6	0.06	0
4	SO4	A	404	-	4,4,4	0.24	0	6,6,6	0.08	0
5	EDO	B	404	-	3,3,3	0.44	0	2,2,2	0.32	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
5	EDO	C	404	-	-	0/1/1/1	-
5	EDO	E	101	-	-	0/1/1/1	-
5	EDO	D	403	-	-	0/1/1/1	-
5	EDO	D	404	-	-	0/1/1/1	-
5	EDO	B	403	-	-	0/1/1/1	-
5	EDO	B	404	-	-	0/1/1/1	-

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.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	101	EDO	1	0
5	D	403	EDO	1	0
5	B	403	EDO	1	0
4	A	403	SO4	1	0
4	C	403	SO4	1	0

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, 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	305/321 (95%)	-0.14	6 (1%) 65 61	22, 38, 68, 80	0
1	B	309/321 (96%)	0.04	4 (1%) 75 71	25, 42, 72, 95	0
1	C	302/321 (94%)	-0.13	4 (1%) 75 71	24, 40, 62, 78	0
1	D	310/321 (96%)	-0.23	3 (0%) 79 76	25, 37, 64, 87	0
2	E	62/85 (72%)	0.86	6 (9%) 13 11	41, 74, 94, 110	0
2	F	69/85 (81%)	0.13	1 (1%) 73 70	35, 53, 68, 74	0
2	G	55/85 (64%)	1.21	8 (14%) 6 5	52, 75, 96, 101	0
2	H	64/85 (75%)	0.16	3 (4%) 36 32	31, 52, 76, 83	0
All	All	1476/1624 (90%)	0.00	35 (2%) 59 55	22, 42, 76, 110	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	ALA	3.5
1	D	315	VAL	3.3
2	G	15	VAL	3.2
1	D	313	PRO	3.1
2	E	55	THR	3.1
2	G	4	VAL	3.0
1	C	182	GLY	2.9
2	G	50	VAL	2.9
1	A	269	VAL	2.8
1	A	302	ARG	2.8
1	D	172	ASN	2.7
1	A	266	GLY	2.6
1	B	311	PHE	2.6
2	G	7	LEU	2.6
2	E	15	VAL	2.5
2	H	0	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	50	VAL	2.4
1	C	6	CYS	2.4
2	E	14	GLU	2.4
2	H	8	PRO	2.4
1	C	222	CYS	2.3
1	B	315	VAL	2.3
1	A	320	ALA	2.3
2	E	7	LEU	2.2
2	G	58	VAL	2.2
2	G	24	VAL	2.2
2	E	3	VAL	2.2
1	A	318	LEU	2.2
1	B	6	CYS	2.1
2	G	49	GLU	2.1
2	F	-5	VAL	2.0
1	C	320	ALA	2.0
2	H	7	LEU	2.0
1	A	308	GLU	2.0
2	G	5	LEU	2.0

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($\text{\AA}^2$)	Q<0.9
5	EDO	B	403	4/4	0.72	0.18	31,33,34,36	0
5	EDO	B	404	4/4	0.78	0.15	40,50,54,55	0
5	EDO	D	404	4/4	0.83	0.14	27,30,31,34	0
5	EDO	D	403	4/4	0.85	0.15	37,41,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	C	404	4/4	0.85	0.14	43,45,49,62	0
4	SO4	A	403	5/5	0.88	0.10	59,61,69,77	0
4	SO4	C	403	5/5	0.90	0.11	63,67,68,77	0
4	SO4	A	404	5/5	0.91	0.07	62,70,75,80	0
5	EDO	E	101	4/4	0.91	0.09	45,48,49,53	0
3	ZN	C	401	1/1	0.96	0.05	75,75,75,75	0
3	ZN	B	401	1/1	0.97	0.06	65,65,65,65	0
3	ZN	A	401	1/1	0.98	0.05	59,59,59,59	0
3	ZN	C	402	1/1	0.99	0.05	54,54,54,54	0
3	ZN	D	402	1/1	0.99	0.03	53,53,53,53	0
3	ZN	A	402	1/1	0.99	0.03	56,56,56,56	0
3	ZN	B	402	1/1	0.99	0.03	65,65,65,65	0
3	ZN	D	401	1/1	0.99	0.04	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.