Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:31 AM GMT

PDB ID	:	3IP3
Title	:	Structure of putative oxidoreductase (TM_0425) from Thermotoga maritima
Authors	:	Ramagopal, U.A.; Morano, C.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-08-16
Resolution	:	2.14 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

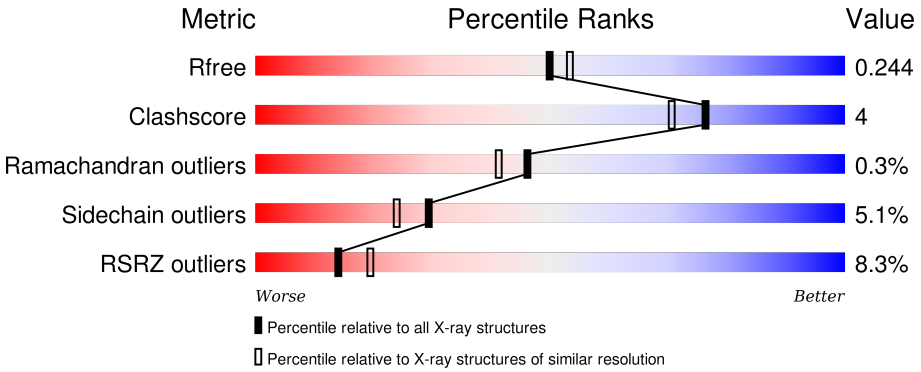
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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 >=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 <=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	337	86% 11%
1	B	337	91% 7%
1	C	337	6% 86% 10%
1	D	337	88% 9%
1	E	337	9% 84% 12%

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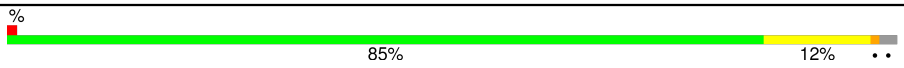
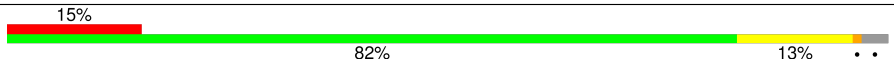
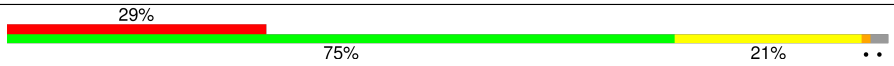
Mol	Chain	Length	Quality of chain
1	F	337	
1	G	337	
1	H	337	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	338	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21415 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 Oxidoreductase, putative.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	Se	0	0	0
			2632	1686	453	484	4	5			
1	B	331	Total	C	N	O	S	Se	0	0	0
			2657	1700	459	489	4	5			
1	C	330	Total	C	N	O	S	Se	0	0	0
			2647	1694	456	488	4	5			
1	D	328	Total	C	N	O	S	Se	0	1	0
			2640	1691	454	486	4	5			
1	E	328	Total	C	N	O	S	Se	0	0	0
			2634	1687	454	484	4	5			
1	F	330	Total	C	N	O	S	Se	0	0	0
			2647	1694	456	488	4	5			
1	G	327	Total	C	N	O	S	Se	0	0	0
			2628	1684	453	482	4	5			
1	H	329	Total	C	N	O	S	Se	0	0	0
			2641	1691	455	486	4	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MSE	-	EXPRESSION TAG	UNP Q9WYQ6
A	1	SER	-	EXPRESSION TAG	UNP Q9WYQ6
A	329	GLU	-	EXPRESSION TAG	UNP Q9WYQ6
A	330	GLY	-	EXPRESSION TAG	UNP Q9WYQ6
A	331	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
A	332	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
A	333	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
A	334	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
A	335	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
A	336	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
B	0	MSE	-	EXPRESSION TAG	UNP Q9WYQ6
B	1	SER	-	EXPRESSION TAG	UNP Q9WYQ6
B	329	GLU	-	EXPRESSION TAG	UNP Q9WYQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	330	GLY	-	EXPRESSION TAG	UNP Q9WYQ6
B	331	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
B	332	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
B	333	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
B	334	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
B	335	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
B	336	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
C	0	MSE	-	EXPRESSION TAG	UNP Q9WYQ6
C	1	SER	-	EXPRESSION TAG	UNP Q9WYQ6
C	329	GLU	-	EXPRESSION TAG	UNP Q9WYQ6
C	330	GLY	-	EXPRESSION TAG	UNP Q9WYQ6
C	331	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
C	332	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
C	333	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
C	334	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
C	335	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
C	336	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
D	0	MSE	-	EXPRESSION TAG	UNP Q9WYQ6
D	1	SER	-	EXPRESSION TAG	UNP Q9WYQ6
D	329	GLU	-	EXPRESSION TAG	UNP Q9WYQ6
D	330	GLY	-	EXPRESSION TAG	UNP Q9WYQ6
D	331	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
D	332	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
D	333	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
D	334	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
D	335	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
D	336	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
E	0	MSE	-	EXPRESSION TAG	UNP Q9WYQ6
E	1	SER	-	EXPRESSION TAG	UNP Q9WYQ6
E	329	GLU	-	EXPRESSION TAG	UNP Q9WYQ6
E	330	GLY	-	EXPRESSION TAG	UNP Q9WYQ6
E	331	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
E	332	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
E	333	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
E	334	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
E	335	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
E	336	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
F	0	MSE	-	EXPRESSION TAG	UNP Q9WYQ6
F	1	SER	-	EXPRESSION TAG	UNP Q9WYQ6
F	329	GLU	-	EXPRESSION TAG	UNP Q9WYQ6
F	330	GLY	-	EXPRESSION TAG	UNP Q9WYQ6
F	331	HIS	-	EXPRESSION TAG	UNP Q9WYQ6

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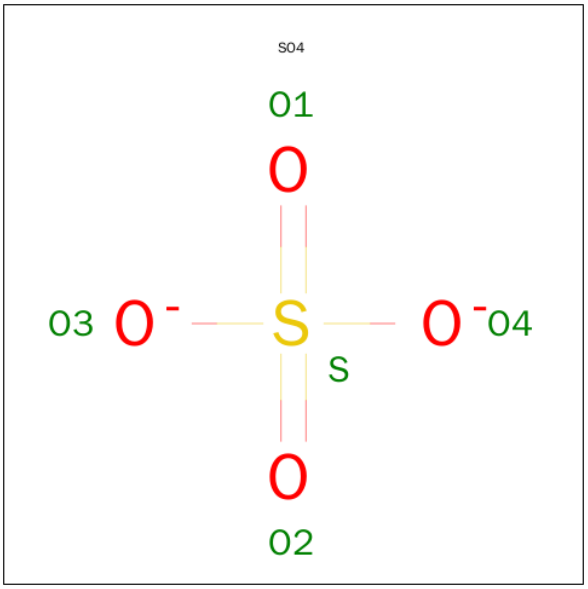
Chain	Residue	Modelled	Actual	Comment	Reference
F	332	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
F	333	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
F	334	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
F	335	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
F	336	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
G	0	MSE	-	EXPRESSION TAG	UNP Q9WYQ6
G	1	SER	-	EXPRESSION TAG	UNP Q9WYQ6
G	329	GLU	-	EXPRESSION TAG	UNP Q9WYQ6
G	330	GLY	-	EXPRESSION TAG	UNP Q9WYQ6
G	331	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
G	332	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
G	333	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
G	334	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
G	335	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
G	336	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
H	0	MSE	-	EXPRESSION TAG	UNP Q9WYQ6
H	1	SER	-	EXPRESSION TAG	UNP Q9WYQ6
H	329	GLU	-	EXPRESSION TAG	UNP Q9WYQ6
H	330	GLY	-	EXPRESSION TAG	UNP Q9WYQ6
H	331	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
H	332	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
H	333	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
H	334	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
H	335	HIS	-	EXPRESSION TAG	UNP Q9WYQ6
H	336	HIS	-	EXPRESSION TAG	UNP Q9WYQ6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

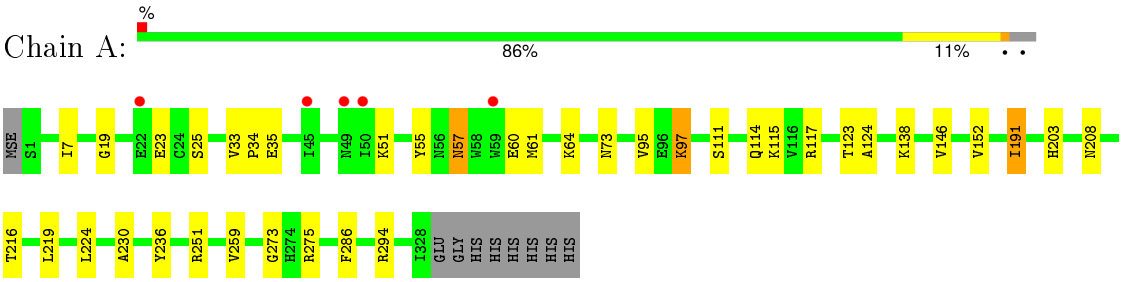
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	59	Total O 59 59	0	0
3	B	67	Total O 67 67	0	0
3	C	18	Total O 18 18	0	0
3	D	30	Total O 30 30	0	0
3	E	19	Total O 19 19	0	0
3	F	59	Total O 59 59	0	0
3	G	8	Total O 8 8	0	0
3	H	4	Total O 4 4	0	0

3 Residue-property plots (i)

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.

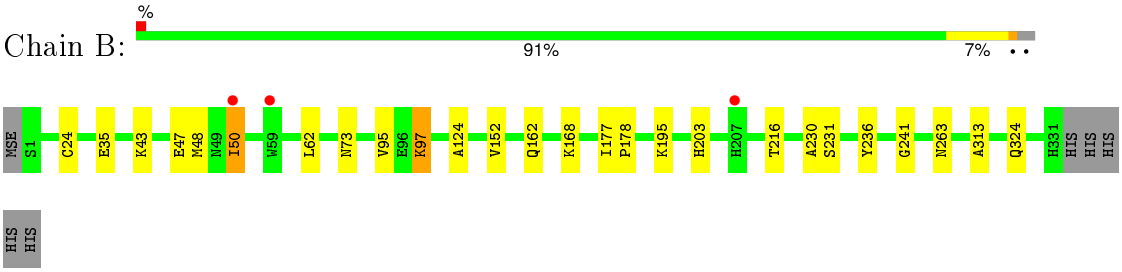
- Molecule 1: Oxidoreductase, putative

Chain A:



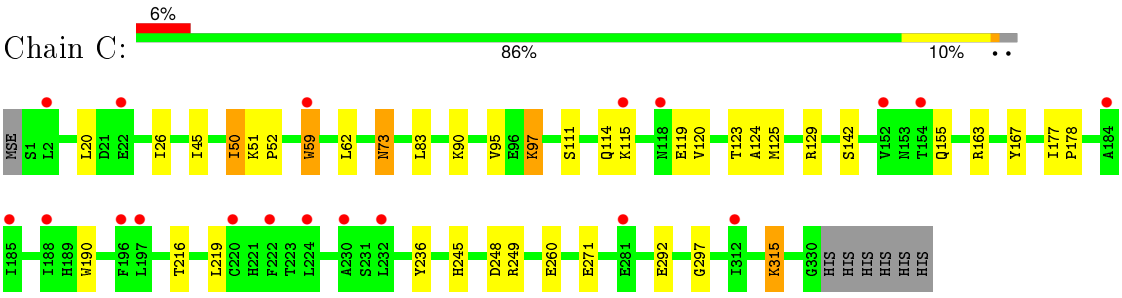
- Molecule 1: Oxidoreductase, putative

Chain B:



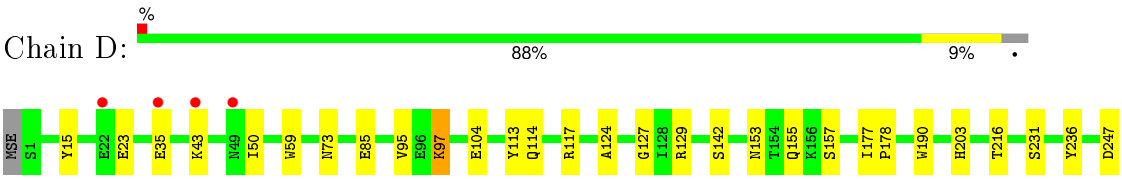
- Molecule 1: Oxidoreductase, putative

Chain C:



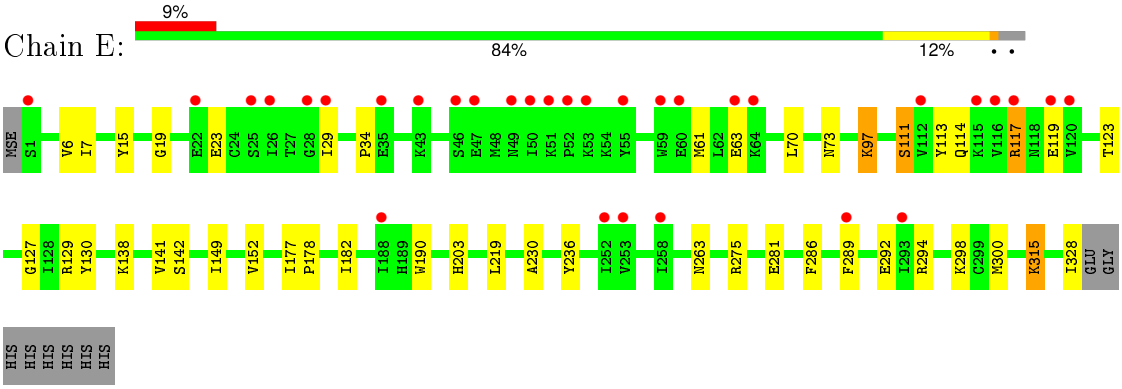
- Molecule 1: Oxidoreductase, putative

Chain D:



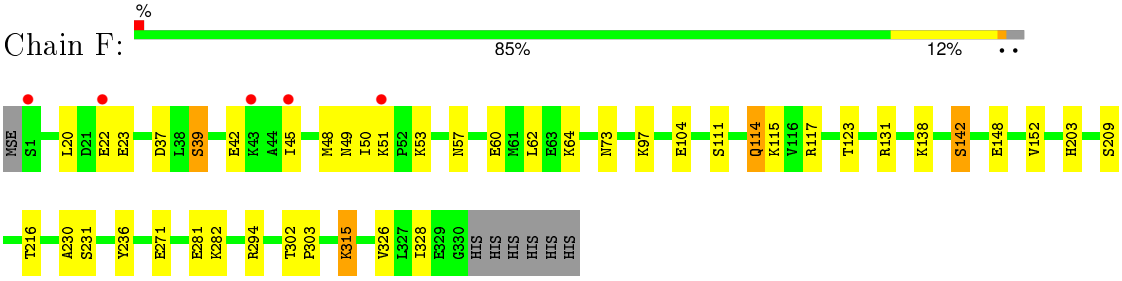
• Molecule 1: Oxidoreductase, putative

Chain E:



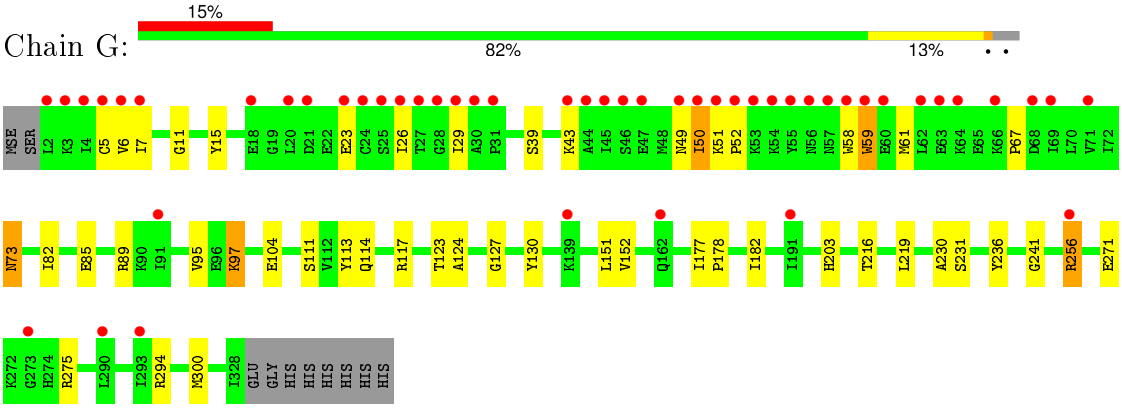
• Molecule 1: Oxidoreductase, putative

Chain F:



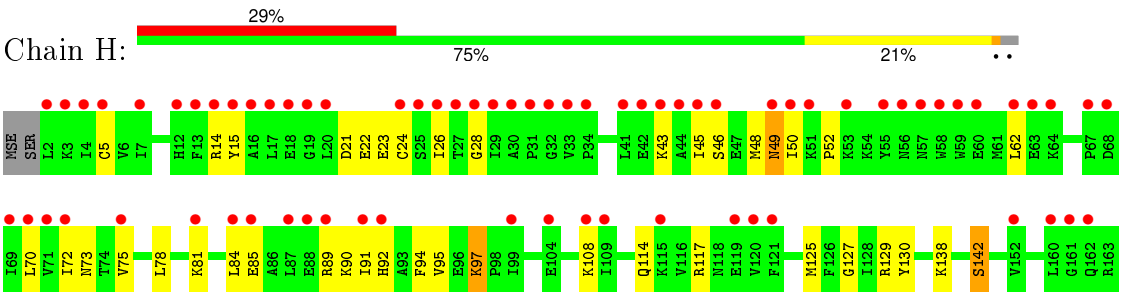
• Molecule 1: Oxidoreductase, putative

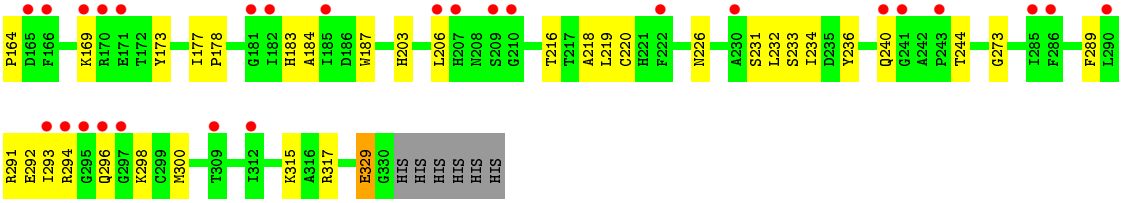
Chain G:



• Molecule 1: Oxidoreductase, putative

Chain H:




P164 D165 F166 K169 R170 E171 T172 Y173 I177 P178 G181 I182 H183 A184 I185 D186 W187 H203 L206 H207 N208 S209 G210 T216 T217 A218 I219 C220 H221 F222 N226 A230 S231 L232 S233 I234 D235 Y236 Q240 G241 A242 P243 T244 G273 I285 F286 F289 L290
R291 E292 I293 R294 G295 Q296 G297 K298 C299 M300 T309 I312 K315 A316 R317 E329 G330 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	118.01Å 94.18Å 142.85Å 90.00° 91.91° 90.00°	Depositor
Resolution (Å)	50.00 – 2.14 44.65 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.14) 99.4 (44.65-2.14)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.204 , 0.242 0.208 , 0.244	Depositor DCC
R_{free} test set	8541 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.5	EDS
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 170307 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21415	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.66	0/2683	0.69	2/3615 (0.1%)
1	B	0.76	1/2709 (0.0%)	0.69	0/3649
1	C	0.58	0/2698	0.65	2/3634 (0.1%)
1	D	0.60	0/2694	0.65	0/3629
1	E	0.53	0/2685	0.63	0/3617
1	F	0.65	0/2698	0.67	0/3634
1	G	0.48	0/2679	0.57	0/3609
1	H	0.47	0/2692	0.59	0/3626
All	All	0.60	1/21538 (0.0%)	0.64	4/29013 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	24	CYS	CB-SG	-6.75	1.70	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	251	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	C	59	TRP	CA-CB-CG	5.61	124.35	113.70
1	A	251	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	248	ASP	CB-CG-OD1	5.11	122.90	118.30

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	2632	0	2659	18	0
1	B	2657	0	2682	11	0
1	C	2647	0	2675	19	0
1	D	2640	0	2672	16	0
1	E	2634	0	2666	22	0
1	F	2647	0	2675	18	0
1	G	2628	0	2658	26	0
1	H	2641	0	2667	40	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	F	10	0	0	0	0
3	A	59	0	0	0	0
3	B	67	0	0	1	0
3	C	18	0	0	0	0
3	D	30	0	0	0	0
3	E	19	0	0	0	0
3	F	59	0	0	1	0
3	G	8	0	0	1	0
3	H	4	0	0	0	0
All	All	21415	0	21354	161	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 4.

All (161) 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:G:256:ARG:HG3	1:G:256:ARG:HH11	1.28	0.98
1:H:129:ARG:HD2	1:H:300:MSE:HE3	1.68	0.73
1:F:131:ARG:HD3	3:F:365:HOH:O	1.89	0.72
1:G:256:ARG:HG3	1:G:256:ARG:NH1	2.03	0.71
1:H:291:ARG:HG2	1:H:296:GLN:HB2	1.74	0.70
1:C:111:SER:O	1:C:114:GLN:HG2	1.94	0.68
1:C:45:ILE:HB	1:C:50:ILE:CD1	2.24	0.67
1:E:130:TYR:CZ	1:E:300:MSE:HE2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:GLU:HB2	1:E:294:ARG:NH2	2.11	0.66
1:A:57:ASN:ND2	1:A:60:GLU:H	1.95	0.65
1:E:113:TYR:O	1:E:117:ARG:HB3	1.97	0.64
1:F:138:LYS:O	1:F:142:SER:HB2	1.98	0.64
1:D:59:TRP:CH2	1:D:85[A]:GLU:HG2	2.34	0.63
1:H:177:ILE:HB	1:H:178:PRO:HD3	1.80	0.63
1:C:45:ILE:HB	1:C:50:ILE:HD13	1.82	0.62
1:H:220:CYS:HB2	1:H:232:LEU:HB3	1.81	0.61
1:G:113:TYR:O	1:G:117:ARG:HB3	2.01	0.61
1:E:130:TYR:CE2	1:E:300:MSE:HE2	2.37	0.60
1:E:7:ILE:HG12	1:E:61:MSE:HE1	1.84	0.59
1:G:241:GLY:O	1:H:273:GLY:HA2	2.04	0.58
1:B:195:LYS:HE2	3:G:338:HOH:O	2.03	0.58
1:A:55:TYR:HE2	1:A:64:LYS:HD2	1.66	0.58
1:H:294:ARG:HB3	1:H:296:GLN:HE22	1.70	0.57
1:E:292:GLU:OE2	1:E:298:LYS:HA	2.05	0.57
1:H:97:LYS:HE3	1:H:97:LYS:O	2.05	0.56
1:E:97:LYS:HD2	1:E:182:ILE:CG2	2.35	0.56
1:H:15:TYR:CE1	1:H:127:GLY:HA3	2.41	0.56
1:C:260:GLU:OE2	1:D:249:ARG:NH1	2.29	0.56
1:D:23:GLU:HB2	1:D:294:ARG:NH2	2.22	0.55
1:E:315:LYS:HG2	1:E:328:ILE:HG12	1.88	0.55
1:F:315:LYS:HG3	1:F:326:VAL:HG11	1.90	0.54
1:G:23:GLU:HB2	1:G:294:ARG:NH2	2.23	0.54
1:G:5:CYS:HB2	1:G:67:PRO:HG3	1.90	0.53
1:D:15:TYR:CZ	1:D:127:GLY:HA3	2.44	0.53
1:H:89:ARG:O	1:H:91:ILE:HG13	2.08	0.53
1:H:240:GLN:HA	1:H:240:GLN:HE21	1.74	0.52
1:H:72:ILE:HB	1:H:95:VAL:HG23	1.92	0.52
1:E:6:VAL:HB	1:E:29:ILE:HG22	1.92	0.52
1:E:129:ARG:HD2	1:E:300:MSE:HE3	1.92	0.52
1:H:92:HIS:CD2	1:H:293:ILE:HD12	2.45	0.52
1:H:43:LYS:HD2	1:H:43:LYS:N	2.25	0.51
1:D:104:GLU:H	1:D:104:GLU:CD	2.12	0.51
1:H:22:GLU:C	1:H:24:CYS:H	2.14	0.51
1:G:39:SER:O	1:G:43:LYS:HD3	2.10	0.51
1:G:15:TYR:CE1	1:G:127:GLY:HA3	2.46	0.51
1:D:153:ASN:HD21	1:D:251:ARG:HH11	1.58	0.50
1:H:84:LEU:HD13	1:H:108:LYS:HB3	1.94	0.50
1:F:114:GLN:NE2	1:F:115:LYS:HE3	2.26	0.50
1:G:130:TYR:CZ	1:G:300:MSE:HE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LEU:HD11	1:D:231:SER:HB3	1.94	0.50
1:A:152:VAL:O	1:A:230:ALA:HA	2.12	0.49
1:H:97:LYS:HD3	1:H:183:HIS:CE1	2.47	0.49
1:F:302:THR:HB	1:F:303:PRO:HD2	1.94	0.49
1:B:35:GLU:CD	1:B:35:GLU:H	2.16	0.49
1:E:7:ILE:HG13	1:E:70:LEU:HD11	1.93	0.49
1:F:114:GLN:HE21	1:F:115:LYS:HG3	1.77	0.49
1:F:152:VAL:O	1:F:230:ALA:HA	2.13	0.49
1:B:152:VAL:O	1:B:230:ALA:HA	2.12	0.49
1:A:57:ASN:HD22	1:A:57:ASN:C	2.17	0.49
1:D:155:GLN:HB3	1:D:249:ARG:HB2	1.95	0.49
1:G:6:VAL:HB	1:G:29:ILE:HG22	1.95	0.49
1:H:26:ILE:HG22	1:H:28:GLY:H	1.78	0.48
1:H:85:GLU:OE1	1:H:89:ARG:HD2	2.12	0.48
1:H:169:LYS:O	1:H:173:TYR:HB3	2.13	0.48
1:G:152:VAL:O	1:G:230:ALA:HA	2.13	0.48
1:G:7:ILE:HG12	1:G:61:MSE:HE1	1.95	0.48
1:A:57:ASN:HD21	1:A:60:GLU:H	1.62	0.48
1:F:37:ASP:OD1	1:F:39:SER:OG	2.32	0.48
1:C:155:GLN:HB3	1:C:249:ARG:HB2	1.96	0.48
1:E:19:GLY:HA3	1:E:286:PHE:HB3	1.95	0.48
1:F:23:GLU:HB2	1:F:294:ARG:NH2	2.29	0.47
1:A:138:LYS:HA	1:A:191:ILE:CD1	2.45	0.47
1:F:315:LYS:HG2	1:F:328:ILE:HG12	1.96	0.47
1:E:292:GLU:OE1	1:E:298:LYS:NZ	2.46	0.47
1:G:50:ILE:HG23	1:G:52:PRO:HD3	1.97	0.47
1:A:111:SER:O	1:A:114:GLN:HG2	2.15	0.47
1:G:97:LYS:HD2	1:G:182:ILE:CG2	2.45	0.46
1:A:19:GLY:HA3	1:A:286:PHE:HB3	1.97	0.46
1:B:48:MSE:HB2	1:B:50:ILE:HD13	1.96	0.46
1:D:113:TYR:O	1:D:117:ARG:HB3	2.16	0.46
1:G:58:TRP:HH2	1:G:85:GLU:HG3	1.81	0.46
1:G:151:LEU:HD21	1:H:233:SER:OG	2.14	0.46
1:C:95:VAL:O	1:C:124:ALA:HA	2.16	0.45
1:B:168:LYS:HE3	3:B:370:HOH:O	2.16	0.45
1:G:59:TRP:CZ3	1:G:89:ARG:NH2	2.84	0.45
1:G:256:ARG:CG	1:G:256:ARG:NH1	2.75	0.45
1:E:138:LYS:HG2	1:E:190:TRP:CZ2	2.51	0.45
1:D:97:LYS:HG3	1:D:97:LYS:H	1.56	0.45
1:G:95:VAL:O	1:G:124:ALA:HA	2.16	0.45
1:D:177:ILE:HB	1:D:178:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:HG3	1:A:97:LYS:H	1.57	0.45
1:D:95:VAL:O	1:D:124:ALA:HA	2.16	0.45
1:E:15:TYR:CZ	1:E:127:GLY:HA3	2.51	0.45
1:H:45:ILE:HG13	1:H:46:SER:N	2.31	0.45
1:D:153:ASN:ND2	1:D:251:ARG:HH11	2.14	0.44
1:A:273:GLY:HA2	1:B:241:GLY:O	2.17	0.44
1:H:138:LYS:O	1:H:142:SER:HB3	2.17	0.44
1:A:138:LYS:HA	1:A:191:ILE:HD11	1.99	0.44
1:C:163:ARG:HD2	1:C:167:TYR:CE2	2.53	0.44
1:H:240:GLN:NE2	1:H:240:GLN:HA	2.32	0.44
1:F:114:GLN:HA	1:F:117:ARG:NH1	2.33	0.44
1:F:114:GLN:HE21	1:F:115:LYS:HE3	1.83	0.44
1:F:281:GLU:HG3	1:F:282:LYS:N	2.31	0.44
1:E:97:LYS:H	1:E:97:LYS:HG3	1.67	0.43
1:F:315:LYS:HG3	1:F:326:VAL:CG1	2.47	0.43
1:G:219:LEU:HD11	1:H:231:SER:HB3	2.00	0.43
1:C:177:ILE:HB	1:C:178:PRO:HD3	2.00	0.43
1:B:97:LYS:H	1:B:97:LYS:HG3	1.59	0.43
1:A:35:GLU:N	1:A:35:GLU:OE2	2.35	0.43
1:E:289:PHE:O	1:E:292:GLU:HB3	2.18	0.43
1:H:218:ALA:HB3	1:H:234:ILE:HB	2.00	0.43
1:B:178:PRO:HA	1:B:313:ALA:HB1	2.00	0.43
1:C:83:LEU:HD22	1:C:95:VAL:HG11	2.01	0.43
1:H:130:TYR:CZ	1:H:300:MSE:HE2	2.53	0.43
1:E:177:ILE:HB	1:E:178:PRO:HD3	2.01	0.43
1:H:94:PHE:CE2	1:H:125:MSE:HG2	2.54	0.43
1:F:42:GLU:HA	1:F:45:ILE:HG12	2.00	0.43
1:A:7:ILE:HG12	1:A:61:MSE:HE1	2.01	0.43
1:A:219:LEU:HD11	1:B:231:SER:HB3	2.01	0.43
1:B:95:VAL:O	1:B:124:ALA:HA	2.18	0.43
1:H:21:ASP:H	1:H:24:CYS:HB2	1.84	0.43
1:A:208:ASN:HA	1:A:216:THR:HG21	2.00	0.43
1:C:111:SER:O	1:C:114:GLN:CG	2.64	0.43
1:C:97:LYS:H	1:C:97:LYS:HG3	1.48	0.43
1:H:48:MSE:O	1:H:49:ASN:HB2	2.19	0.42
1:H:78:LEU:HA	1:H:81:LYS:HD3	2.00	0.42
1:G:7:ILE:HD12	1:G:82:ILE:HG21	2.01	0.42
1:C:315:LYS:HA	1:C:315:LYS:HD2	1.81	0.42
1:E:141:VAL:HG11	1:E:149:ILE:HD11	2.02	0.42
1:H:5:CYS:O	1:H:70:LEU:HD12	2.19	0.42
1:A:23:GLU:HB2	1:A:294:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:LEU:HD11	1:F:231:SER:HB3	2.01	0.42
1:G:26:ILE:O	1:G:52:PRO:HB3	2.20	0.42
1:G:11:GLY:HA3	1:G:73:ASN:HB2	2.02	0.42
1:E:111:SER:O	1:E:114:GLN:HG2	2.20	0.42
1:C:114:GLN:HE21	1:C:115:LYS:NZ	2.17	0.42
1:H:329:GLU:HA	1:H:329:GLU:OE2	2.20	0.41
1:H:23:GLU:HB2	1:H:294:ARG:NH2	2.35	0.41
1:C:292:GLU:HA	1:C:297:GLY:O	2.20	0.41
1:C:129:ARG:HD3	1:C:190:TRP:CD2	2.55	0.41
1:C:45:ILE:HD12	1:C:52:PRO:HG2	2.03	0.41
1:F:57:ASN:HD22	1:F:60:GLU:CD	2.23	0.41
1:H:84:LEU:HD22	1:H:108:LYS:HD3	2.02	0.41
1:H:184:ALA:HA	1:H:187:TRP:CD2	2.55	0.41
1:G:231:SER:HB3	1:H:219:LEU:HD21	2.02	0.41
1:H:289:PHE:O	1:H:293:ILE:HG12	2.20	0.41
1:D:157:SER:HB3	1:D:247:ASP:HB3	2.03	0.41
1:D:35:GLU:HG2	1:D:35:GLU:O	2.20	0.41
1:D:129:ARG:HD3	1:D:190:TRP:CD2	2.55	0.41
1:C:20:LEU:HD11	1:C:26:ILE:HD11	2.02	0.41
1:E:152:VAL:O	1:E:230:ALA:HA	2.21	0.41
1:H:178:PRO:HG2	1:H:317:ARG:HD3	2.03	0.40
1:H:184:ALA:HA	1:H:187:TRP:CE3	2.56	0.40
1:C:73:ASN:HB3	1:C:125:MSE:HE1	2.04	0.40
1:F:20:LEU:HD12	1:F:48:MSE:HE1	2.03	0.40
1:H:292:GLU:OE2	1:H:298:LYS:HA	2.22	0.40
1:A:95:VAL:O	1:A:124:ALA:HA	2.22	0.40
1:A:146:VAL:CG1	1:A:259:VAL:HG23	2.52	0.40
1:G:50:ILE:HD13	1:G:51:LYS:N	2.36	0.40
1:B:177:ILE:HB	1:B:178:PRO:HD3	2.02	0.40
1:G:177:ILE:HB	1:G:178:PRO:HD3	2.02	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	326/337 (97%)	313 (96%)	12 (4%)	1 (0%)	46 41
1	B	329/337 (98%)	318 (97%)	11 (3%)	0	100 100
1	C	328/337 (97%)	315 (96%)	13 (4%)	0	100 100
1	D	327/337 (97%)	316 (97%)	11 (3%)	0	100 100
1	E	326/337 (97%)	309 (95%)	16 (5%)	1 (0%)	46 41
1	F	328/337 (97%)	319 (97%)	9 (3%)	0	100 100
1	G	325/337 (96%)	304 (94%)	20 (6%)	1 (0%)	46 41
1	H	327/337 (97%)	297 (91%)	25 (8%)	5 (2%)	13 5
All	All	2616/2696 (97%)	2491 (95%)	117 (4%)	8 (0%)	46 41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	49	ASN
1	E	34	PRO
1	G	49	ASN
1	H	90	LYS
1	H	164	PRO
1	H	52	PRO
1	A	34	PRO
1	H	75	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	286/289 (99%)	272 (95%)	14 (5%)	31 25
1	B	289/289 (100%)	277 (96%)	12 (4%)	36 32
1	C	288/289 (100%)	272 (94%)	16 (6%)	26 20
1	D	288/289 (100%)	278 (96%)	10 (4%)	43 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	287/289 (99%)	273 (95%)	14 (5%)	31	25
1	F	288/289 (100%)	266 (92%)	22 (8%)	16	10
1	G	286/289 (99%)	272 (95%)	14 (5%)	31	25
1	H	287/289 (99%)	271 (94%)	16 (6%)	26	20
All	All	2299/2312 (99%)	2181 (95%)	118 (5%)	29	24

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	33	VAL
1	A	51	LYS
1	A	57	ASN
1	A	73	ASN
1	A	97	LYS
1	A	115	LYS
1	A	117	ARG
1	A	123	THR
1	A	191	ILE
1	A	203	HIS
1	A	224	LEU
1	A	236	TYR
1	A	275	ARG
1	B	43	LYS
1	B	47	GLU
1	B	50	ILE
1	B	62	LEU
1	B	73	ASN
1	B	97	LYS
1	B	162	GLN
1	B	203	HIS
1	B	216	THR
1	B	236	TYR
1	B	263	ASN
1	B	324	GLN
1	C	50	ILE
1	C	51	LYS
1	C	59	TRP
1	C	62	LEU
1	C	73	ASN
1	C	90	LYS

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Mol	Chain	Res	Type
1	C	97	LYS
1	C	119	GLU
1	C	120	VAL
1	C	123	THR
1	C	142	SER
1	C	216	THR
1	C	236	TYR
1	C	245	HIS
1	C	271	GLU
1	C	315	LYS
1	D	43	LYS
1	D	50	ILE
1	D	73	ASN
1	D	97	LYS
1	D	114	GLN
1	D	142	SER
1	D	203	HIS
1	D	216	THR
1	D	236	TYR
1	D	271	GLU
1	E	63	GLU
1	E	73	ASN
1	E	97	LYS
1	E	111	SER
1	E	117	ARG
1	E	119	GLU
1	E	123	THR
1	E	142	SER
1	E	203	HIS
1	E	236	TYR
1	E	263	ASN
1	E	275	ARG
1	E	281	GLU
1	E	315	LYS
1	F	22	GLU
1	F	39	SER
1	F	49	ASN
1	F	50	ILE
1	F	51	LYS
1	F	53	LYS
1	F	62	LEU
1	F	64	LYS

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Mol	Chain	Res	Type
1	F	73	ASN
1	F	97	LYS
1	F	104	GLU
1	F	111	SER
1	F	114	GLN
1	F	123	THR
1	F	142	SER
1	F	148	GLU
1	F	203	HIS
1	F	209	SER
1	F	216	THR
1	F	236	TYR
1	F	271	GLU
1	F	315	LYS
1	G	50	ILE
1	G	59	TRP
1	G	73	ASN
1	G	97	LYS
1	G	104	GLU
1	G	111	SER
1	G	114	GLN
1	G	123	THR
1	G	203	HIS
1	G	216	THR
1	G	236	TYR
1	G	256	ARG
1	G	271	GLU
1	G	275	ARG
1	H	14	ARG
1	H	50	ILE
1	H	62	LEU
1	H	73	ASN
1	H	97	LYS
1	H	114	GLN
1	H	117	ARG
1	H	142	SER
1	H	203	HIS
1	H	206	LEU
1	H	216	THR
1	H	226	ASN
1	H	236	TYR
1	H	244	THR

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Mol	Chain	Res	Type
1	H	315	LYS
1	H	329	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	114	GLN
1	A	118	ASN
1	A	240	GLN
1	A	245	HIS
1	B	114	GLN
1	B	118	ASN
1	C	114	GLN
1	C	203	HIS
1	D	153	ASN
1	D	207	HIS
1	F	57	ASN
1	F	114	GLN
1	F	240	GLN
1	F	274	HIS
1	G	240	GLN
1	H	114	GLN
1	H	226	ASN
1	H	240	GLN
1	H	296	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

5 ligands 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	$\#\|Z\| > 2$
2	SO4	A	337	-	4,4,4	0.18	0	6,6,6	0.16	0
2	SO4	B	337	-	4,4,4	0.18	0	6,6,6	0.16	0
2	SO4	B	338	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	F	337	-	4,4,4	0.19	0	6,6,6	0.07	0
2	SO4	F	338	-	4,4,4	0.18	0	6,6,6	0.11	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	337	-	-	0/0/0/0	0/0/0/0
2	SO4	B	337	-	-	0/0/0/0	0/0/0/0
2	SO4	B	338	-	-	0/0/0/0	0/0/0/0
2	SO4	F	337	-	-	0/0/0/0	0/0/0/0
2	SO4	F	338	-	-	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 (i)

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^{th} 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	323/337 (95%)	0.05	5 (1%) 76 82	27, 41, 68, 80	0
1	B	326/337 (96%)	-0.03	3 (0%) 85 89	26, 35, 54, 70	0
1	C	325/337 (96%)	0.42	19 (5%) 26 35	35, 50, 65, 74	0
1	D	323/337 (95%)	-0.07	4 (1%) 81 85	30, 45, 59, 70	0
1	E	323/337 (95%)	0.67	32 (9%) 9 14	32, 53, 89, 96	0
1	F	325/337 (96%)	-0.07	5 (1%) 76 82	28, 38, 53, 65	0
1	G	322/337 (95%)	0.97	50 (15%) 3 4	33, 65, 104, 109	0
1	H	324/337 (96%)	1.59	98 (30%) 1 1	36, 77, 120, 122	0
All	All	2591/2696 (96%)	0.44	216 (8%) 14 19	26, 47, 94, 122	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	34	PRO	11.3
1	G	6	VAL	8.0
1	G	50	ILE	7.7
1	H	5	CYS	7.7
1	H	33	VAL	7.7
1	H	50	ILE	7.5
1	H	59	TRP	7.4
1	G	26	ILE	7.3
1	H	26	ILE	7.3
1	G	59	TRP	6.9
1	H	45	ILE	6.7
1	G	5	CYS	6.5
1	H	13	PHE	6.5
1	H	20	LEU	6.5
1	G	49	ASN	6.3
1	G	45	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
1	G	62	LEU	6.0
1	H	69	ILE	6.0
1	H	68	ASP	5.9
1	H	62	LEU	5.9
1	E	26	ILE	5.9
1	G	55	TYR	5.5
1	G	64	LYS	5.4
1	G	24	CYS	5.4
1	H	166	PHE	5.4
1	H	290	LEU	5.3
1	G	60	GLU	5.2
1	H	84	LEU	5.2
1	H	28	GLY	5.2
1	G	4	ILE	5.0
1	H	293	ILE	5.0
1	E	59	TRP	4.9
1	H	162	GLN	4.8
1	G	46	SER	4.8
1	H	49	ASN	4.7
1	H	297	GLY	4.7
1	G	28	GLY	4.6
1	H	2	LEU	4.5
1	H	53	LYS	4.4
1	H	286	PHE	4.4
1	H	27	THR	4.4
1	H	24	CYS	4.3
1	E	51	LYS	4.2
1	G	20	LEU	4.2
1	H	19	GLY	4.1
1	H	31	PRO	4.1
1	G	68	ASP	4.1
1	H	7	ILE	4.1
1	C	59	TRP	4.1
1	H	55	TYR	4.0
1	G	63	GLU	4.0
1	G	23	GLU	4.0
1	E	46	SER	3.9
1	E	293	ILE	3.9
1	G	2	LEU	3.9
1	H	295	GLY	3.9
1	G	56	ASN	3.9
1	H	58	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	52	PRO	3.8
1	H	67	PRO	3.8
1	H	115	LYS	3.8
1	G	3	LYS	3.8
1	H	120	VAL	3.8
1	G	29	ILE	3.8
1	G	30	ALA	3.7
1	H	75	VAL	3.7
1	E	50	ILE	3.7
1	G	293	ILE	3.7
1	E	22	GLU	3.7
1	G	54	LYS	3.7
1	H	60	GLU	3.6
1	H	63	GLU	3.6
1	E	43	LYS	3.6
1	E	49	ASN	3.6
1	H	70	LEU	3.5
1	H	87	LEU	3.5
1	G	53	LYS	3.5
1	E	60	GLU	3.4
1	E	117	ARG	3.4
1	G	44	ALA	3.3
1	G	25	SER	3.3
1	E	119	GLU	3.2
1	H	43	LYS	3.2
1	G	69	ILE	3.2
1	H	160	LEU	3.2
1	H	56	ASN	3.1
1	G	7	ILE	3.1
1	G	71	VAL	3.1
1	H	64	LYS	3.1
1	A	49	ASN	3.1
1	G	256	ARG	3.1
1	H	30	ALA	3.1
1	H	207	HIS	3.1
1	E	120	VAL	3.0
1	G	66	LYS	3.0
1	H	17	LEU	3.0
1	C	118	ASN	3.0
1	H	240	GLN	3.0
1	H	119	GLU	3.0
1	G	31	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	27	THR	3.0
1	G	51	LYS	3.0
1	C	220	CYS	2.9
1	H	169	LYS	2.9
1	B	207	HIS	2.9
1	H	230	ALA	2.9
1	E	115	LYS	2.9
1	C	185	ILE	2.9
1	H	41	LEU	2.9
1	G	43	LYS	2.9
1	A	45	ILE	2.8
1	B	59	TRP	2.8
1	E	258	ILE	2.8
1	H	3	LYS	2.8
1	C	152	VAL	2.8
1	F	1	SER	2.8
1	H	161	GLY	2.8
1	H	285	ILE	2.8
1	H	12	HIS	2.7
1	H	121	PHE	2.7
1	E	55	TYR	2.7
1	H	32	GLY	2.7
1	E	53	LYS	2.7
1	H	25	SER	2.7
1	H	312	ILE	2.7
1	E	116	VAL	2.7
1	E	47	GLU	2.7
1	E	25	SER	2.7
1	D	22	GLU	2.6
1	E	1	SER	2.6
1	H	165	ASP	2.6
1	H	171	GLU	2.6
1	H	182	ILE	2.6
1	C	224	LEU	2.6
1	G	273	GLY	2.6
1	H	72	ILE	2.6
1	G	58	TRP	2.5
1	C	312	ILE	2.5
1	H	152	VAL	2.5
1	H	185	ILE	2.5
1	C	22	GLU	2.5
1	E	63	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	209	SER	2.5
1	H	92	HIS	2.5
1	G	52	PRO	2.5
1	G	21	ASP	2.4
1	G	47	GLU	2.4
1	B	50	ILE	2.4
1	C	232	LEU	2.4
1	G	162	GLN	2.4
1	H	44	ALA	2.4
1	D	49	ASN	2.4
1	A	59	TRP	2.4
1	H	42	GLU	2.3
1	H	210	GLY	2.3
1	G	290	LEU	2.3
1	H	71	VAL	2.3
1	F	45	ILE	2.3
1	E	28	GLY	2.3
1	H	46	SER	2.3
1	H	14	ARG	2.3
1	E	35	GLU	2.3
1	G	18	GLU	2.3
1	H	81	LYS	2.3
1	E	289	PHE	2.3
1	H	104	GLU	2.3
1	C	154	THR	2.3
1	H	16	ALA	2.3
1	H	88	GLU	2.3
1	D	43	LYS	2.3
1	H	29	ILE	2.3
1	H	91	ILE	2.3
1	A	22	GLU	2.3
1	H	294	ARG	2.3
1	D	35	GLU	2.2
1	H	15	TYR	2.2
1	H	243	PRO	2.2
1	H	57	ASN	2.2
1	G	191	ILE	2.2
1	H	99	ILE	2.2
1	E	112	VAL	2.2
1	H	206	LEU	2.2
1	C	222	PHE	2.2
1	A	50	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	281	GLU	2.2
1	C	2	LEU	2.2
1	F	22	GLU	2.2
1	G	57	ASN	2.2
1	E	29	ILE	2.2
1	C	184	ALA	2.1
1	E	252	ILE	2.1
1	F	43	LYS	2.1
1	G	139	LYS	2.1
1	H	181	GLY	2.1
1	C	196	PHE	2.1
1	H	89	ARG	2.1
1	H	222	PHE	2.1
1	G	91	ILE	2.1
1	H	4	ILE	2.1
1	E	64	LYS	2.1
1	H	108	LYS	2.1
1	C	188	ILE	2.1
1	C	230	ALA	2.1
1	E	188	ILE	2.0
1	H	109	ILE	2.0
1	H	170	ARG	2.0
1	H	241	GLY	2.0
1	H	18	GLU	2.0
1	F	51	LYS	2.0
1	C	197	LEU	2.0
1	C	115	LYS	2.0
1	H	296	GLN	2.0
1	H	309	THR	2.0
1	E	253	VAL	2.0
1	H	85	GLU	2.0
1	H	51	LYS	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 carbohydrates in this entry.

6.4 Ligands

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^{th} 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^2)	Q<0.9
2	SO4	B	338	5/5	0.80	0.20	5.29	108,108,108,109	0
2	SO4	F	337	5/5	0.91	0.14	0.15	102,102,102,102	0
2	SO4	F	338	5/5	0.93	0.09	-1.09	96,96,96,96	0
2	SO4	B	337	5/5	0.94	0.11	-1.76	88,88,89,89	0
2	SO4	A	337	5/5	0.95	0.11	-2.44	105,105,106,106	0

6.5 Other polymers

There are no such residues in this entry.