Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:30 PM GMT

PDB ID	:	1XDY
Title	:	Structural and Biochemical Identification of a Novel Bacterial Oxidoreductase, W-containing cofactor
Authors	:	Loschi, L.; Brokx, S.J.; Hills, T.L.; Zhang, G.; Bertero, M.G.; Lovering, A.L.; Weiner, J.H.; Strynadka, N.C.
Deposited on	:	2004-09-08
Resolution	:	2.20 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 (i) symbol.

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

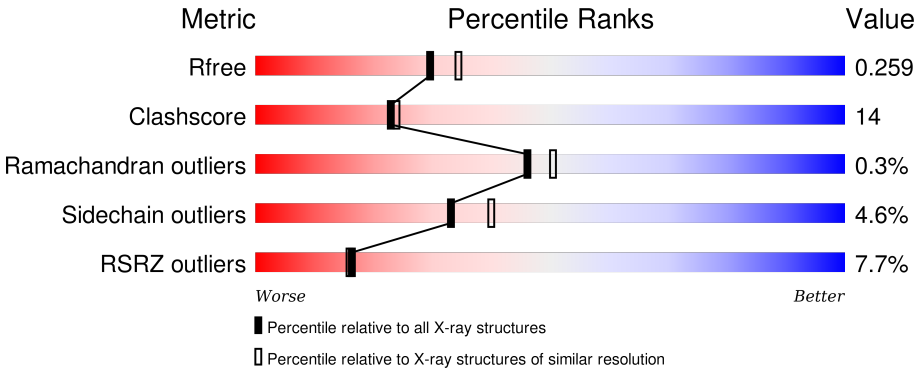
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	298	3% 67% 18% • 12%
1	B	298	11% 60% 27% • 12%
1	C	298	4% 67% 19% • 11%
1	D	298	2% 65% 22% • 12%
1	E	298	3% 69% 18% • 12%

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Mol	Chain	Length	Quality of chain
1	F	298	18% 60% 26% 12%
1	G	298	6% 63% 24% 12%
1	H	298	9% 61% 25% 11%
1	I	298	9% 61% 25% 12%
1	J	298	3% 63% 23% 12%

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
3	MTE	A	301	X	-	-	-
3	MTE	B	302	X	-	-	-
3	MTE	C	303	X	-	-	-
3	MTE	D	304	X	-	-	-
3	MTE	E	305	X	-	-	-
3	MTE	F	306	X	-	-	-
3	MTE	G	307	X	-	-	-
3	MTE	H	308	X	-	-	-
3	MTE	I	309	X	-	-	-
3	MTE	J	310	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21369 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 Bacterial Sulfite Oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2093	1358	354	375	6			
1	B	262	Total	C	N	O	S	0	0	0
			2088	1354	353	375	6			
1	C	264	Total	C	N	O	S	0	0	0
			2102	1363	356	377	6			
1	D	263	Total	C	N	O	S	0	0	0
			2094	1357	355	376	6			
1	E	262	Total	C	N	O	S	0	0	0
			2085	1351	353	375	6			
1	F	262	Total	C	N	O	S	1	0	0
			2084	1352	352	374	6			
1	G	261	Total	C	N	O	S	0	0	0
			2079	1349	351	373	6			
1	H	264	Total	C	N	O	S	11	0	0
			2102	1363	356	377	6			
1	I	262	Total	C	N	O	S	0	0	0
			2085	1351	353	375	6			
1	J	262	Total	C	N	O	S	0	0	0
			2085	1351	353	375	6			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	ASP	ALA	SEE REMARK 999	UNP P76342
A	291	LEU	-	EXPRESSION TAG	UNP P76342
A	292	GLU	-	EXPRESSION TAG	UNP P76342
A	293	HIS	-	EXPRESSION TAG	UNP P76342
A	294	HIS	-	EXPRESSION TAG	UNP P76342
A	295	HIS	-	EXPRESSION TAG	UNP P76342
A	296	HIS	-	EXPRESSION TAG	UNP P76342
A	297	HIS	-	EXPRESSION TAG	UNP P76342
A	298	HIS	-	EXPRESSION TAG	UNP P76342

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Chain	Residue	Modelled	Actual	Comment	Reference
B	275	ASP	ALA	SEE REMARK 999	UNP P76342
B	291	LEU	-	EXPRESSION TAG	UNP P76342
B	292	GLU	-	EXPRESSION TAG	UNP P76342
B	293	HIS	-	EXPRESSION TAG	UNP P76342
B	294	HIS	-	EXPRESSION TAG	UNP P76342
B	295	HIS	-	EXPRESSION TAG	UNP P76342
B	296	HIS	-	EXPRESSION TAG	UNP P76342
B	297	HIS	-	EXPRESSION TAG	UNP P76342
B	298	HIS	-	EXPRESSION TAG	UNP P76342
C	275	ASP	ALA	SEE REMARK 999	UNP P76342
C	291	LEU	-	EXPRESSION TAG	UNP P76342
C	292	GLU	-	EXPRESSION TAG	UNP P76342
C	293	HIS	-	EXPRESSION TAG	UNP P76342
C	294	HIS	-	EXPRESSION TAG	UNP P76342
C	295	HIS	-	EXPRESSION TAG	UNP P76342
C	296	HIS	-	EXPRESSION TAG	UNP P76342
C	297	HIS	-	EXPRESSION TAG	UNP P76342
C	298	HIS	-	EXPRESSION TAG	UNP P76342
D	275	ASP	ALA	SEE REMARK 999	UNP P76342
D	291	LEU	-	EXPRESSION TAG	UNP P76342
D	292	GLU	-	EXPRESSION TAG	UNP P76342
D	293	HIS	-	EXPRESSION TAG	UNP P76342
D	294	HIS	-	EXPRESSION TAG	UNP P76342
D	295	HIS	-	EXPRESSION TAG	UNP P76342
D	296	HIS	-	EXPRESSION TAG	UNP P76342
D	297	HIS	-	EXPRESSION TAG	UNP P76342
D	298	HIS	-	EXPRESSION TAG	UNP P76342
E	275	ASP	ALA	SEE REMARK 999	UNP P76342
E	291	LEU	-	EXPRESSION TAG	UNP P76342
E	292	GLU	-	EXPRESSION TAG	UNP P76342
E	293	HIS	-	EXPRESSION TAG	UNP P76342
E	294	HIS	-	EXPRESSION TAG	UNP P76342
E	295	HIS	-	EXPRESSION TAG	UNP P76342
E	296	HIS	-	EXPRESSION TAG	UNP P76342
E	297	HIS	-	EXPRESSION TAG	UNP P76342
E	298	HIS	-	EXPRESSION TAG	UNP P76342
F	275	ASP	ALA	SEE REMARK 999	UNP P76342
F	291	LEU	-	EXPRESSION TAG	UNP P76342
F	292	GLU	-	EXPRESSION TAG	UNP P76342
F	293	HIS	-	EXPRESSION TAG	UNP P76342
F	294	HIS	-	EXPRESSION TAG	UNP P76342
F	295	HIS	-	EXPRESSION TAG	UNP P76342

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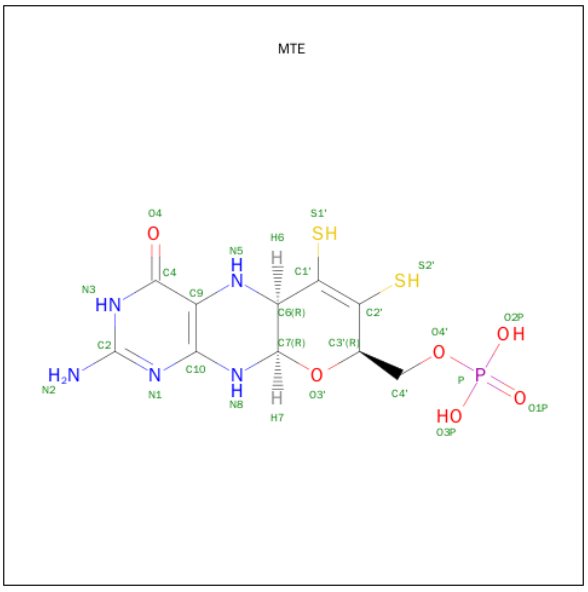
Chain	Residue	Modelled	Actual	Comment	Reference
F	296	HIS	-	EXPRESSION TAG	UNP P76342
F	297	HIS	-	EXPRESSION TAG	UNP P76342
F	298	HIS	-	EXPRESSION TAG	UNP P76342
G	275	ASP	ALA	SEE REMARK 999	UNP P76342
G	291	LEU	-	EXPRESSION TAG	UNP P76342
G	292	GLU	-	EXPRESSION TAG	UNP P76342
G	293	HIS	-	EXPRESSION TAG	UNP P76342
G	294	HIS	-	EXPRESSION TAG	UNP P76342
G	295	HIS	-	EXPRESSION TAG	UNP P76342
G	296	HIS	-	EXPRESSION TAG	UNP P76342
G	297	HIS	-	EXPRESSION TAG	UNP P76342
G	298	HIS	-	EXPRESSION TAG	UNP P76342
H	275	ASP	ALA	SEE REMARK 999	UNP P76342
H	291	LEU	-	EXPRESSION TAG	UNP P76342
H	292	GLU	-	EXPRESSION TAG	UNP P76342
H	293	HIS	-	EXPRESSION TAG	UNP P76342
H	294	HIS	-	EXPRESSION TAG	UNP P76342
H	295	HIS	-	EXPRESSION TAG	UNP P76342
H	296	HIS	-	EXPRESSION TAG	UNP P76342
H	297	HIS	-	EXPRESSION TAG	UNP P76342
H	298	HIS	-	EXPRESSION TAG	UNP P76342
I	275	ASP	ALA	SEE REMARK 999	UNP P76342
I	291	LEU	-	EXPRESSION TAG	UNP P76342
I	292	GLU	-	EXPRESSION TAG	UNP P76342
I	293	HIS	-	EXPRESSION TAG	UNP P76342
I	294	HIS	-	EXPRESSION TAG	UNP P76342
I	295	HIS	-	EXPRESSION TAG	UNP P76342
I	296	HIS	-	EXPRESSION TAG	UNP P76342
I	297	HIS	-	EXPRESSION TAG	UNP P76342
I	298	HIS	-	EXPRESSION TAG	UNP P76342
J	275	ASP	ALA	SEE REMARK 999	UNP P76342
J	291	LEU	-	EXPRESSION TAG	UNP P76342
J	292	GLU	-	EXPRESSION TAG	UNP P76342
J	293	HIS	-	EXPRESSION TAG	UNP P76342
J	294	HIS	-	EXPRESSION TAG	UNP P76342
J	295	HIS	-	EXPRESSION TAG	UNP P76342
J	296	HIS	-	EXPRESSION TAG	UNP P76342
J	297	HIS	-	EXPRESSION TAG	UNP P76342
J	298	HIS	-	EXPRESSION TAG	UNP P76342

- Molecule 2 is TUNGSTEN ION (three-letter code: W) (formula: W).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total W 1 1	0	0
2	J	1	Total W 1 1	0	0
2	D	1	Total W 1 1	0	0
2	E	1	Total W 1 1	0	0
2	H	1	Total W 1 1	0	0
2	B	1	Total W 1 1	0	0
2	I	1	Total W 1 1	0	0
2	C	1	Total W 1 1	0	0
2	A	1	Total W 1 1	0	0
2	F	1	Total W 1 1	0	0

- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	C	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	D	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	E	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	F	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	G	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	H	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	I	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	J	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 4 is water.

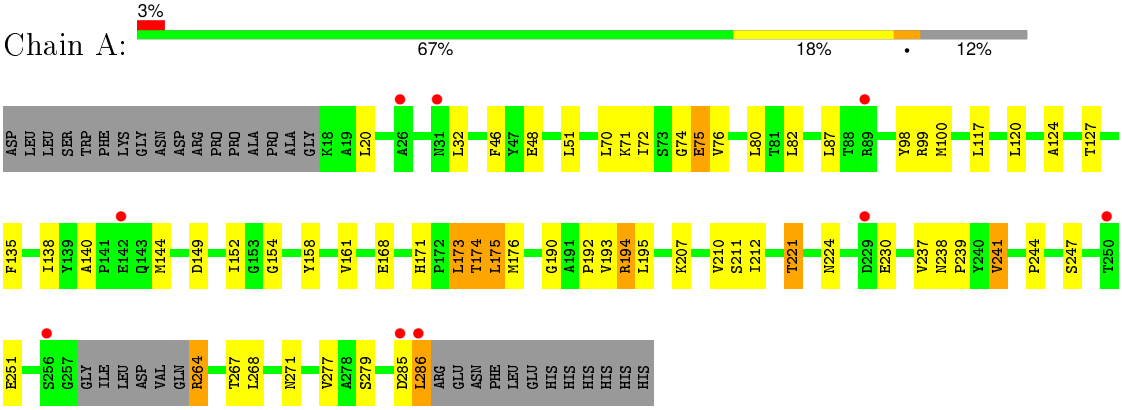
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	13	Total	O	0	0
			13	13		
4	C	32	Total	O	0	0
			32	32		
4	D	30	Total	O	0	0
			30	30		
4	E	29	Total	O	0	0
			29	29		
4	F	10	Total	O	0	0
			10	10		
4	G	22	Total	O	0	0
			22	22		
4	H	4	Total	O	0	0
			4	4		
4	I	12	Total	O	0	0
			12	12		
4	J	35	Total	O	0	0
			35	35		

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.

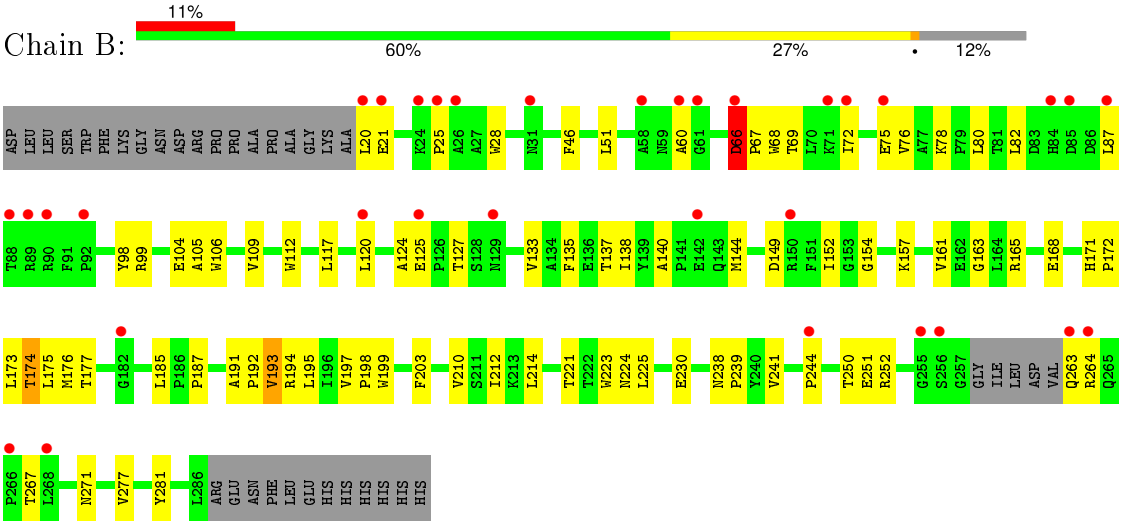
- Molecule 1: Bacterial Sulfite Oxidase

Chain A:



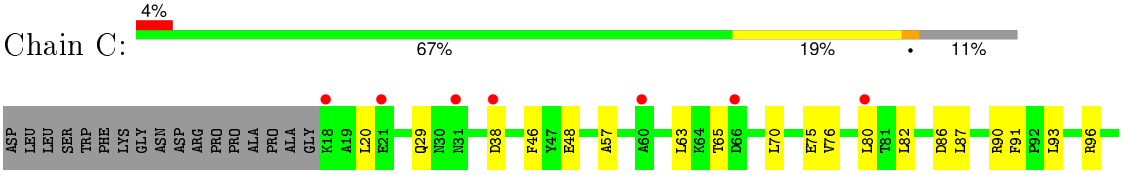
- Molecule 1: Bacterial Sulfite Oxidase

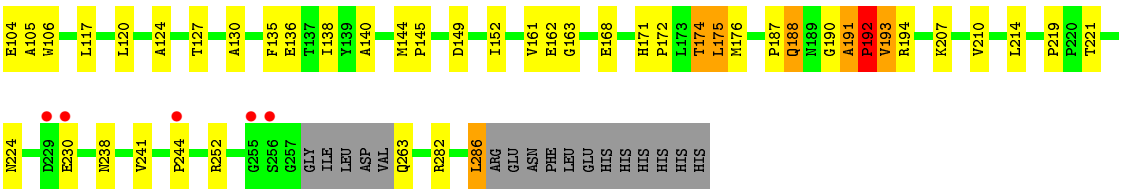
Chain B:



- Molecule 1: Bacterial Sulfite Oxidase

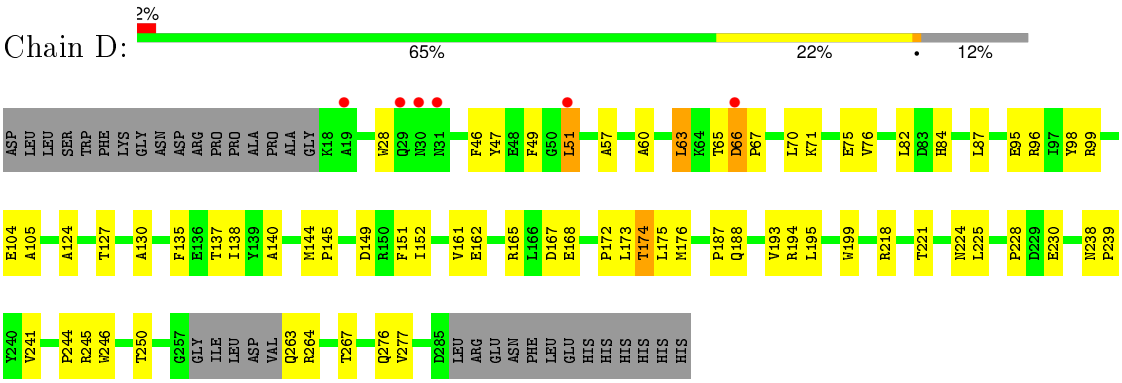
Chain C:





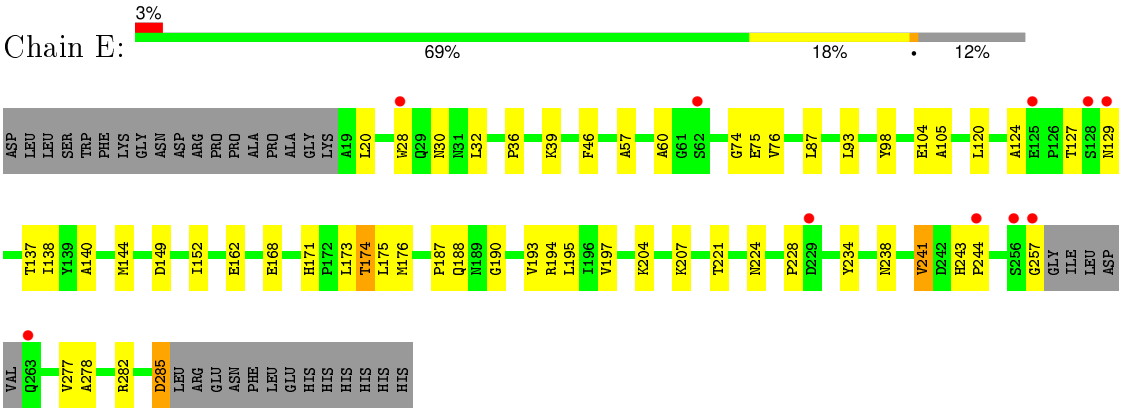
• Molecule 1: Bacterial Sulfite Oxidase

Chain D:



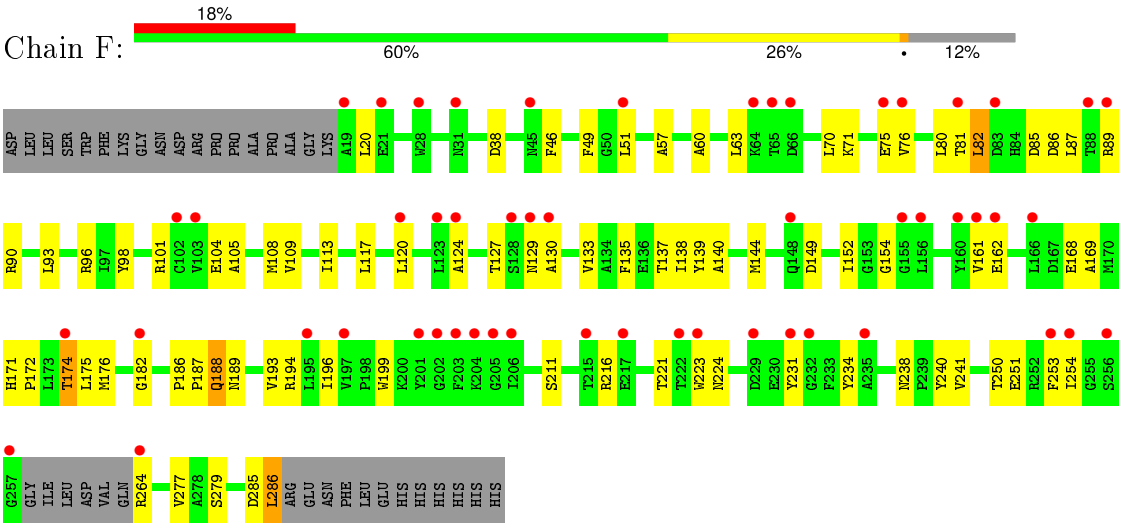
• Molecule 1: Bacterial Sulfite Oxidase

Chain E:



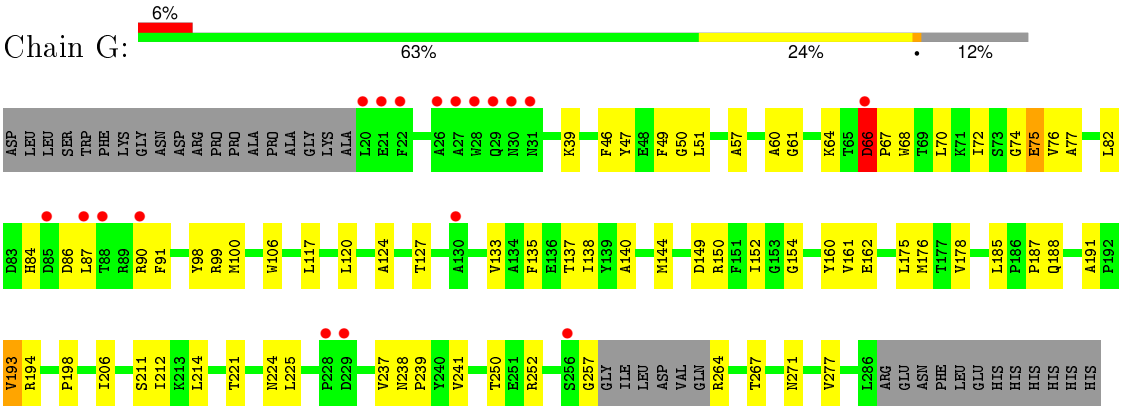
• Molecule 1: Bacterial Sulfite Oxidase

Chain F:



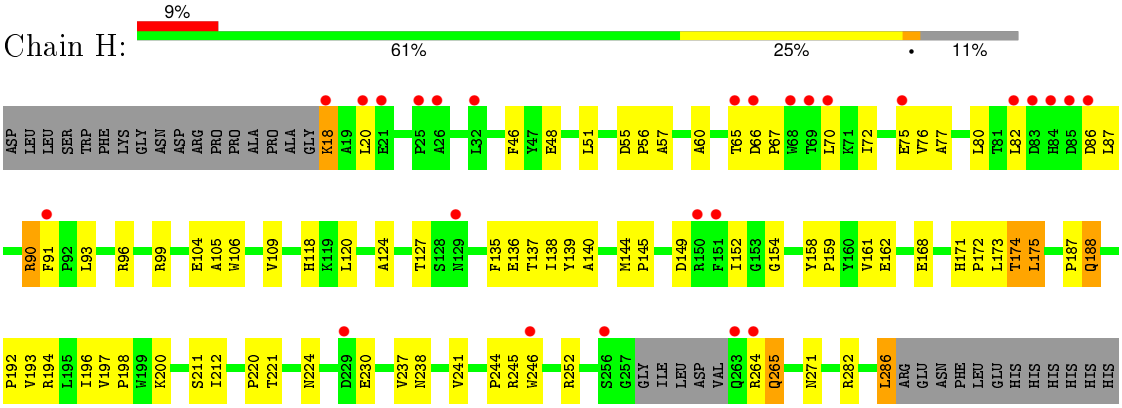
• Molecule 1: Bacterial Sulfite Oxidase

Chain G:



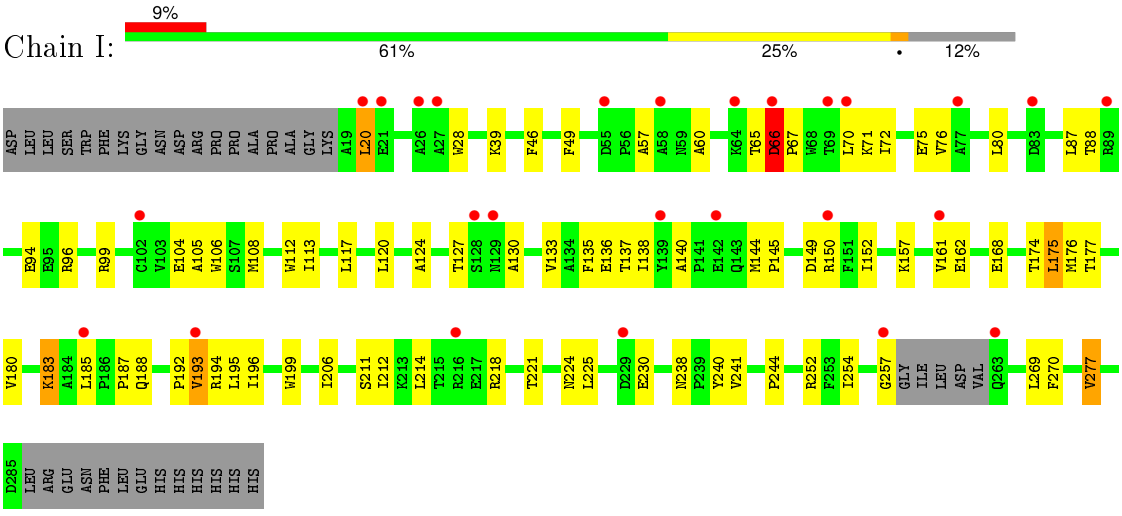
• Molecule 1: Bacterial Sulfite Oxidase

Chain H:



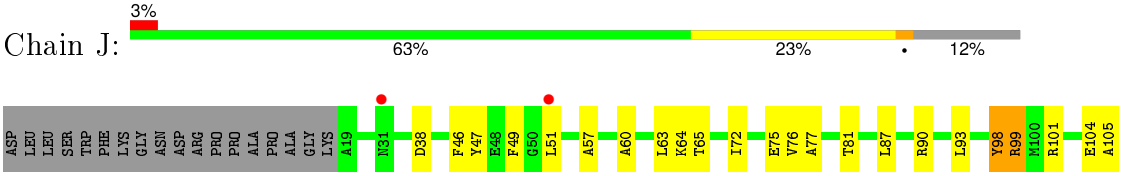
• Molecule 1: Bacterial Sulfite Oxidase

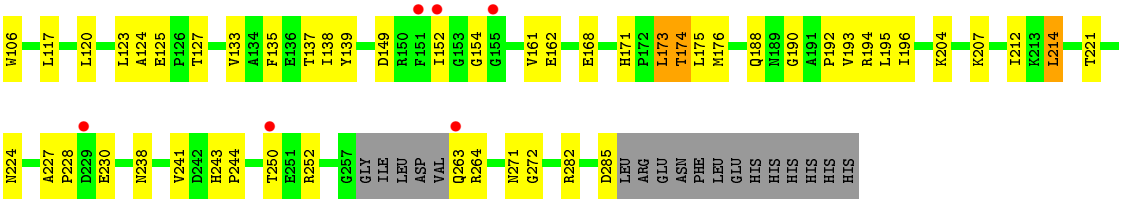
Chain I:



• Molecule 1: Bacterial Sulfite Oxidase

Chain J:




W106 L117 L120 L123 A124 E125 P126 T127 V133 A134 F135 E136 T137 I138 Y139 D149 R150 F151 I152 G153 G154 G155 V161 E162 E168 H171 P172 L173 T174 L175 M176 Q188 N189 G190 A191 P192 V193 R194 L195 I196 K204 K207 I212 K213 L214 T221
N224 A227 P228 D229 E230 N238 V241 D242 H243 P244 T250 E251 R252 G257 GLY ILE LEU ASP VAL Q263 R264 N271 G272 R282 D285 LEU ARG GLU ASN PHE LEU GLU 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	84.84Å 177.51Å 104.21Å 90.00° 109.73° 90.00°	Depositor
Resolution (Å)	38.96 – 2.20 38.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.96-2.20) 98.6 (38.96-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.258 0.224 , 0.259	Depositor DCC
R_{free} test set	4389 reflections (3.13%)	DCC
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 144703 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21369	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: W, MTE

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	0.57	1/2158 (0.0%)	0.76	2/2942 (0.1%)
1	B	0.43	0/2153	0.69	2/2936 (0.1%)
1	C	0.51	0/2167	0.85	3/2954 (0.1%)
1	D	0.53	0/2159	0.77	1/2943 (0.0%)
1	E	0.55	0/2150	0.75	1/2932 (0.0%)
1	F	0.42	0/2149	0.69	0/2931
1	G	0.53	0/2144	0.75	1/2924 (0.0%)
1	H	0.40	0/2167	0.67	1/2954 (0.0%)
1	I	0.45	0/2150	0.70	1/2932 (0.0%)
1	J	0.58	0/2150	0.77	0/2932
All	All	0.50	1/21547 (0.0%)	0.74	12/29380 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	J	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	ARG	CB-CG	-5.40	1.38	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	191	ALA	C-N-CD	-20.12	76.34	120.60
1	C	191	ALA	C-N-CA	13.52	178.78	122.00
1	A	175	LEU	CA-CB-CG	7.14	131.72	115.30
1	G	66	ASP	C-N-CD	7.09	143.29	128.40
1	B	66	ASP	C-N-CD	6.70	142.46	128.40
1	A	194	ARG	CG-CD-NE	-6.23	98.72	111.80
1	C	192	PRO	CA-N-CD	-5.92	103.21	111.50
1	I	66	ASP	C-N-CD	5.89	140.77	128.40
1	D	66	ASP	C-N-CD	5.83	140.65	128.40
1	E	197	VAL	N-CA-C	-5.82	95.29	111.00
1	B	109	VAL	N-CA-C	-5.30	96.69	111.00
1	H	109	VAL	N-CA-C	-5.23	96.88	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	TYR	Sidechain
1	E	234	TYR	Sidechain
1	J	98	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2093	0	2067	49	0
1	B	2088	0	2057	62	0
1	C	2102	0	2075	53	0
1	D	2094	0	2064	63	0
1	E	2085	0	2051	46	0
1	F	2084	0	2054	63	0
1	G	2079	0	2049	54	0
1	H	2102	0	2075	58	0
1	I	2085	0	2051	67	0
1	J	2085	0	2051	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	24	0	9	0	0
3	B	24	0	9	0	0
3	C	24	0	9	0	0
3	D	24	0	9	0	0
3	E	24	0	9	0	0
3	F	24	0	9	0	0
3	G	24	0	9	0	0
3	H	24	0	9	0	0
3	I	24	0	9	0	0
3	J	24	0	9	0	0
4	A	35	0	0	1	0
4	B	13	0	0	1	0
4	C	32	0	0	2	0
4	D	30	0	0	0	0
4	E	29	0	0	1	0
4	F	10	0	0	0	0
4	G	22	0	0	1	0
4	H	4	0	0	0	0
4	I	12	0	0	0	0
4	J	35	0	0	2	0
All	All	21369	0	20684	565	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 14.

All (565) 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:250:THR:HG23	1:D:264:ARG:HH21	1.33	0.92
1:H:57:ALA:HA	1:H:188:GLN:HG2	1.51	0.92
1:B:20:LEU:HG	1:B:21:GLU:H	1.35	0.90
1:A:140:ALA:HB3	1:A:144:MET:HE3	1.52	0.88
1:E:140:ALA:HB3	1:E:144:MET:HE3	1.56	0.86
1:I:57:ALA:HA	1:I:188:GLN:HG2	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:ALA:HA	1:E:188:GLN:HG2	1.60	0.84
1:J:221:THR:HG21	4:J:440:HOH:O	1.76	0.84
1:E:87:LEU:HD13	1:E:193:VAL:HG22	1.59	0.83
1:J:250:THR:HG23	1:J:264:ARG:HE	1.44	0.82
1:G:250:THR:HG23	1:G:264:ARG:HH21	1.44	0.81
1:H:66:ASP:HB3	1:H:67:PRO:HD3	1.63	0.81
1:E:30:ASN:HD22	1:E:32:LEU:H	1.29	0.81
1:C:57:ALA:HA	1:C:188:GLN:HG2	1.60	0.81
1:D:230:GLU:HG2	1:D:244:PRO:HG2	1.61	0.80
1:G:76:VAL:HG13	1:G:124:ALA:O	1.82	0.79
1:E:57:ALA:HA	1:E:188:GLN:CG	2.12	0.79
1:J:57:ALA:HA	1:J:188:GLN:CG	2.13	0.79
1:A:87:LEU:HD13	1:A:193:VAL:HG22	1.62	0.79
1:F:211:SER:OG	1:H:282:ARG:HD3	1.84	0.78
1:A:76:VAL:HG13	1:A:124:ALA:O	1.83	0.78
1:D:75:GLU:HG3	1:D:127:THR:OG1	1.84	0.78
1:H:286:LEU:HD22	1:H:286:LEU:H	1.47	0.78
1:H:76:VAL:HG13	1:H:124:ALA:O	1.84	0.78
1:I:75:GLU:HG3	1:I:127:THR:OG1	1.84	0.78
1:I:230:GLU:HG2	1:I:244:PRO:HG2	1.66	0.78
1:I:28:TRP:CG	1:I:96:ARG:HG2	2.19	0.77
1:G:140:ALA:HB3	1:G:144:MET:HE3	1.65	0.77
1:H:168:GLU:O	1:H:174:THR:HG21	1.83	0.77
1:B:176:MET:HE1	1:B:195:LEU:HD13	1.65	0.77
1:C:57:ALA:HA	1:C:188:GLN:CG	2.15	0.77
1:J:230:GLU:HG2	1:J:244:PRO:HG2	1.64	0.77
1:G:87:LEU:HD13	1:G:193:VAL:HG22	1.66	0.77
1:J:149:ASP:HB3	1:J:152:ILE:HB	1.68	0.76
1:I:72:ILE:HD13	1:I:212:ILE:HB	1.67	0.76
1:C:65:THR:HB	1:C:192:PRO:CD	2.16	0.76
1:D:57:ALA:HA	1:D:188:GLN:CG	2.16	0.76
1:D:87:LEU:HD13	1:D:193:VAL:HG22	1.67	0.75
1:H:57:ALA:HA	1:H:188:GLN:CG	2.16	0.74
1:J:87:LEU:HD13	1:J:193:VAL:CG2	2.17	0.74
1:B:99:ARG:HG3	1:B:271:ASN:ND2	2.03	0.74
1:C:221:THR:HG21	4:C:426:HOH:O	1.85	0.74
1:I:57:ALA:HA	1:I:188:GLN:CG	2.18	0.73
1:J:221:THR:HG22	1:J:224:ASN:H	1.53	0.73
1:H:230:GLU:HG2	1:H:244:PRO:HG2	1.68	0.73
1:H:87:LEU:HD13	1:H:193:VAL:HG22	1.69	0.72
1:C:238:ASN:HB3	1:C:241:VAL:HG12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:ASN:HB3	1:J:241:VAL:HG12	1.72	0.72
1:A:221:THR:HG22	1:A:224:ASN:H	1.55	0.71
1:A:168:GLU:O	1:A:174:THR:HG21	1.91	0.71
1:I:87:LEU:HD13	1:I:193:VAL:HG22	1.73	0.71
1:C:140:ALA:HB3	1:C:144:MET:HE3	1.71	0.71
1:H:238:ASN:HB3	1:H:241:VAL:HG12	1.72	0.71
1:F:57:ALA:HA	1:F:188:GLN:CG	2.21	0.70
1:I:137:THR:HG22	1:I:138:ILE:N	2.06	0.70
1:I:39:LYS:NZ	1:I:257:GLY:H	1.89	0.70
1:G:57:ALA:HA	1:G:188:GLN:HG3	1.73	0.70
1:C:168:GLU:O	1:C:174:THR:HG21	1.92	0.70
1:D:162:GLU:OE2	1:D:221:THR:HG23	1.91	0.70
1:E:238:ASN:HB3	1:E:241:VAL:CG1	2.22	0.70
1:H:60:ALA:HB1	1:H:187:PRO:HB2	1.75	0.69
1:A:99:ARG:HD2	1:A:271:ASN:O	1.91	0.69
1:F:60:ALA:HB1	1:F:187:PRO:HB2	1.72	0.69
1:C:187:PRO:HA	1:C:191:ALA:HB2	1.75	0.69
1:C:65:THR:HB	1:C:192:PRO:HD3	1.74	0.68
1:A:176:MET:HE1	1:A:195:LEU:HD13	1.76	0.68
1:B:87:LEU:HD13	1:B:193:VAL:HG22	1.75	0.68
1:H:96:ARG:HD2	1:H:175:LEU:HD13	1.75	0.68
1:I:162:GLU:OE2	1:I:221:THR:HG23	1.94	0.68
1:I:133:VAL:HG22	1:I:214:LEU:HD13	1.75	0.68
1:J:75:GLU:HG3	1:J:127:THR:OG1	1.93	0.68
1:H:162:GLU:OE2	1:H:221:THR:HG23	1.94	0.68
1:J:168:GLU:O	1:J:174:THR:HG21	1.93	0.68
1:E:87:LEU:HD13	1:E:193:VAL:CG2	2.24	0.68
1:B:230:GLU:HG2	1:B:244:PRO:HG2	1.74	0.68
1:G:51:LEU:HD21	1:G:154:GLY:CA	2.23	0.68
1:F:120:LEU:O	1:F:120:LEU:HD23	1.93	0.68
1:H:149:ASP:HB3	1:H:152:ILE:HB	1.75	0.67
1:I:66:ASP:HB3	1:I:67:PRO:HD3	1.75	0.67
1:A:32:LEU:HD11	1:A:99:ARG:HH11	1.59	0.67
1:D:238:ASN:HB3	1:D:241:VAL:HG12	1.77	0.67
1:G:51:LEU:HD21	1:G:154:GLY:N	2.09	0.67
1:J:87:LEU:HD22	1:J:193:VAL:HG21	1.77	0.66
1:A:51:LEU:HD21	1:A:154:GLY:CA	2.25	0.66
1:E:221:THR:HG22	1:E:224:ASN:H	1.60	0.66
1:D:250:THR:HG23	1:D:264:ARG:NH2	2.07	0.66
1:B:241:VAL:HG13	4:B:413:HOH:O	1.96	0.66
1:J:250:THR:CG2	1:J:264:ARG:HE	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:LEU:HD13	1:F:193:VAL:CG2	2.25	0.66
1:J:57:ALA:HA	1:J:188:GLN:HG3	1.77	0.66
1:B:238:ASN:HB3	1:B:241:VAL:CG1	2.26	0.66
1:F:238:ASN:HB3	1:F:241:VAL:HG12	1.78	0.66
1:A:99:ARG:HG3	1:A:271:ASN:ND2	2.11	0.65
1:G:221:THR:HG22	1:G:224:ASN:H	1.61	0.65
1:E:241:VAL:HG13	4:E:427:HOH:O	1.95	0.65
1:D:57:ALA:HA	1:D:188:GLN:HG2	1.80	0.64
1:I:76:VAL:HG13	1:I:124:ALA:O	1.97	0.64
1:C:238:ASN:HB3	1:C:241:VAL:CG1	2.27	0.64
1:F:51:LEU:HD21	1:F:154:GLY:CA	2.27	0.64
1:J:63:LEU:HD12	1:J:65:THR:HG23	1.80	0.64
1:D:149:ASP:OD2	1:D:152:ILE:HG12	1.97	0.64
1:I:180:VAL:HG12	1:I:185:LEU:HD23	1.78	0.64
1:D:135:PHE:O	1:D:161:VAL:HG23	1.98	0.64
1:H:57:ALA:CA	1:H:188:GLN:HG2	2.25	0.63
1:B:117:LEU:HD13	1:B:176:MET:HE3	1.79	0.63
1:F:51:LEU:HD21	1:F:154:GLY:HA3	1.81	0.63
1:F:162:GLU:OE2	1:F:221:THR:HG23	1.97	0.63
1:E:57:ALA:CA	1:E:188:GLN:HG2	2.26	0.63
1:B:168:GLU:O	1:B:174:THR:HG21	1.99	0.63
1:I:57:ALA:CA	1:I:188:GLN:HG2	2.29	0.62
1:H:286:LEU:N	1:H:286:LEU:HD22	2.14	0.62
1:F:75:GLU:HG3	1:F:127:THR:OG1	1.98	0.62
1:B:76:VAL:HG11	1:B:124:ALA:HB1	1.82	0.62
1:I:140:ALA:H	1:I:144:MET:HE3	1.64	0.62
1:E:162:GLU:OE2	1:E:221:THR:HG23	1.99	0.62
1:B:238:ASN:HB3	1:B:241:VAL:HG12	1.80	0.62
1:D:28:TRP:CG	1:D:96:ARG:HG2	2.34	0.62
1:J:176:MET:HE1	1:J:195:LEU:HD13	1.81	0.62
1:B:75:GLU:HG3	1:B:127:THR:OG1	2.00	0.62
1:D:76:VAL:HG13	1:D:124:ALA:O	2.00	0.61
1:C:57:ALA:CA	1:C:188:GLN:HG2	2.30	0.61
1:H:221:THR:HG22	1:H:224:ASN:H	1.65	0.61
1:A:149:ASP:HB3	1:A:152:ILE:HB	1.82	0.61
1:H:197:VAL:HG11	1:H:200:LYS:HD2	1.82	0.61
1:J:57:ALA:HA	1:J:188:GLN:HG2	1.82	0.61
1:C:187:PRO:HA	1:C:191:ALA:CB	2.30	0.61
1:I:221:THR:HG22	1:I:224:ASN:H	1.67	0.60
1:G:72:ILE:HD13	1:G:212:ILE:HB	1.81	0.60
1:J:99:ARG:HD3	1:J:271:ASN:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:149:ASP:OD2	1:J:152:ILE:HG12	2.01	0.60
1:E:60:ALA:HB1	1:E:187:PRO:HB2	1.84	0.60
1:B:99:ARG:HD2	1:B:271:ASN:O	2.02	0.60
1:G:135:PHE:O	1:G:161:VAL:HG23	2.01	0.60
1:A:75:GLU:HG3	1:A:127:THR:OG1	2.02	0.60
1:G:72:ILE:HG13	1:G:120:LEU:HD21	1.84	0.60
1:I:20:LEU:HD23	1:I:88:THR:HG21	1.84	0.59
1:J:117:LEU:HD13	1:J:176:MET:HE3	1.83	0.59
1:B:250:THR:HG23	1:B:264:ARG:NH2	2.16	0.59
1:H:82:LEU:HD12	1:H:82:LEU:N	2.17	0.59
1:C:241:VAL:HG13	4:C:435:HOH:O	2.01	0.59
1:D:51:LEU:HD23	1:D:152:ILE:O	2.03	0.59
1:D:250:THR:CG2	1:D:264:ARG:HH21	2.12	0.59
1:F:221:THR:HG22	1:F:224:ASN:H	1.67	0.59
1:F:76:VAL:HG11	1:F:124:ALA:HB1	1.84	0.58
1:C:87:LEU:HD13	1:C:193:VAL:HG22	1.85	0.58
1:F:82:LEU:HD12	1:F:82:LEU:N	2.18	0.58
1:I:199:TRP:CD2	1:I:277:VAL:HG21	2.37	0.58
1:H:18:LYS:HA	1:H:18:LYS:NZ	2.18	0.58
1:A:176:MET:CE	1:A:195:LEU:HD13	2.32	0.58
1:D:176:MET:HE1	1:D:195:LEU:HD13	1.85	0.58
1:D:168:GLU:O	1:D:174:THR:HG21	2.04	0.58
1:I:39:LYS:HZ1	1:I:257:GLY:H	1.52	0.58
1:H:75:GLU:HG3	1:H:127:THR:OG1	2.04	0.58
1:D:57:ALA:HA	1:D:188:GLN:HG3	1.85	0.57
1:I:137:THR:CG2	1:I:138:ILE:N	2.67	0.57
1:B:98:TYR:HE1	1:B:175:LEU:HD22	1.68	0.57
1:D:66:ASP:HB3	1:D:67:PRO:HD3	1.86	0.57
1:G:250:THR:CG2	1:G:264:ARG:HH21	2.16	0.57
1:G:66:ASP:O	1:G:84:HIS:HB2	2.04	0.57
1:G:99:ARG:HG3	1:G:271:ASN:ND2	2.18	0.57
1:E:140:ALA:HB3	1:E:144:MET:CE	2.32	0.57
1:A:99:ARG:NH2	1:A:268:LEU:HD12	2.20	0.57
1:F:129:ASN:HB3	1:F:216:ARG:NH1	2.20	0.57
1:A:285:ASP:O	1:A:286:LEU:HB3	2.05	0.57
1:H:238:ASN:HB3	1:H:241:VAL:CG1	2.33	0.57
1:F:135:PHE:O	1:F:161:VAL:HG23	2.05	0.57
1:I:168:GLU:O	1:I:174:THR:HG21	2.05	0.57
1:E:120:LEU:HD23	1:E:120:LEU:O	2.05	0.57
1:F:250:THR:HG23	1:F:264:ARG:HH21	1.70	0.57
1:E:149:ASP:HB3	1:E:152:ILE:HB	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASN:HB3	1:A:241:VAL:CG1	2.35	0.56
1:I:28:TRP:CB	1:I:96:ARG:HG2	2.35	0.56
1:I:238:ASN:HB3	1:I:241:VAL:HG12	1.86	0.56
1:A:80:LEU:HD23	1:A:80:LEU:H	1.71	0.56
1:F:57:ALA:HA	1:F:188:GLN:HG3	1.86	0.56
1:G:133:VAL:HG22	1:G:214:LEU:HD13	1.88	0.56
1:C:65:THR:HB	1:C:192:PRO:CG	2.36	0.56
1:B:60:ALA:HB1	1:B:187:PRO:HB2	1.87	0.56
1:B:120:LEU:HD23	1:B:120:LEU:O	2.06	0.56
1:A:239:PRO:HB3	1:A:267:THR:HB	1.88	0.56
1:H:120:LEU:O	1:H:120:LEU:HD23	2.05	0.56
1:G:57:ALA:HA	1:G:188:GLN:CG	2.36	0.55
1:E:285:ASP:N	1:E:285:ASP:OD2	2.39	0.55
1:B:69:THR:O	1:B:210:VAL:HG23	2.06	0.55
1:B:20:LEU:HG	1:B:21:GLU:N	2.14	0.55
1:A:285:ASP:OD1	1:A:286:LEU:N	2.38	0.55
1:F:211:SER:HB2	1:H:282:ARG:NH2	2.21	0.55
1:I:49:PHE:CZ	1:I:144:MET:HG2	2.41	0.55
1:E:39:LYS:NZ	1:E:257:GLY:H	2.05	0.55
1:F:234:TYR:CD2	1:F:286:LEU:HB3	2.41	0.55
1:C:149:ASP:OD2	1:C:152:ILE:HG12	2.06	0.55
1:G:117:LEU:HD13	1:G:176:MET:HE3	1.88	0.55
1:C:93:LEU:HD12	1:C:93:LEU:N	2.21	0.55
1:C:65:THR:HB	1:C:192:PRO:HG3	1.88	0.54
1:J:133:VAL:HG22	1:J:214:LEU:HD13	1.89	0.54
1:D:225:LEU:O	1:D:228:PRO:HD3	2.07	0.54
1:D:96:ARG:NH1	1:D:172:PRO:O	2.40	0.54
1:J:138:ILE:HG12	1:J:139:TYR:N	2.22	0.54
1:F:171:HIS:ND1	1:F:172:PRO:HD2	2.22	0.54
1:D:75:GLU:HG3	1:D:127:THR:HG1	1.70	0.54
1:F:82:LEU:CD1	1:F:82:LEU:N	2.71	0.54
1:G:60:ALA:HB1	1:G:187:PRO:HB2	1.90	0.54
1:H:87:LEU:HD13	1:H:193:VAL:CG2	2.36	0.54
1:D:263:GLN:HE21	1:D:264:ARG:H	1.54	0.54
1:J:117:LEU:HD13	1:J:176:MET:CE	2.38	0.54
1:G:238:ASN:HB3	1:G:241:VAL:HG12	1.90	0.54
1:E:30:ASN:ND2	1:E:32:LEU:H	2.03	0.54
1:D:238:ASN:HB3	1:D:241:VAL:CG1	2.37	0.54
1:D:28:TRP:CB	1:D:96:ARG:HG2	2.38	0.54
1:J:51:LEU:HD21	1:J:154:GLY:CA	2.38	0.53
1:H:66:ASP:HB3	1:H:67:PRO:CD	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:HD13	1:A:193:VAL:CG2	2.37	0.53
1:J:238:ASN:HB3	1:J:241:VAL:CG1	2.37	0.53
1:F:87:LEU:HD22	1:F:193:VAL:HG21	1.89	0.53
1:C:76:VAL:HG13	1:C:124:ALA:O	2.08	0.53
1:F:57:ALA:HA	1:F:188:GLN:HG2	1.90	0.53
1:I:140:ALA:H	1:I:144:MET:CE	2.21	0.53
1:F:20:LEU:HD11	1:F:113:ILE:HG21	1.91	0.53
1:I:20:LEU:H	1:I:20:LEU:HD12	1.73	0.53
1:C:75:GLU:HG3	1:C:127:THR:OG1	2.09	0.53
1:E:76:VAL:HG13	1:E:124:ALA:O	2.08	0.53
1:B:192:PRO:HG2	1:B:193:VAL:HG23	1.90	0.53
1:B:117:LEU:HD13	1:B:176:MET:CE	2.38	0.53
1:C:190:GLY:HA3	1:C:207:LYS:HB3	1.91	0.53
1:E:238:ASN:HB3	1:E:241:VAL:HG13	1.92	0.52
1:J:90:ARG:NH1	1:J:123:LEU:HD11	2.24	0.52
1:H:220:PRO:HB3	1:J:285:ASP:OD1	2.10	0.52
1:C:230:GLU:HG2	1:C:244:PRO:HG2	1.91	0.52
1:A:138:ILE:HG23	1:A:144:MET:CE	2.40	0.52
1:I:20:LEU:HD23	1:I:88:THR:CG2	2.39	0.52
1:C:120:LEU:C	1:C:120:LEU:HD23	2.30	0.52
1:F:98:TYR:HE1	1:F:175:LEU:HD22	1.74	0.52
1:D:221:THR:HG22	1:D:224:ASN:H	1.74	0.52
1:G:162:GLU:OE2	1:G:221:THR:HG23	2.10	0.52
1:D:104:GLU:O	1:D:105:ALA:HB3	2.10	0.52
1:H:120:LEU:HD23	1:H:120:LEU:C	2.30	0.52
1:B:149:ASP:HB3	1:B:152:ILE:HB	1.92	0.52
1:E:98:TYR:HE1	1:E:175:LEU:HD22	1.75	0.51
1:B:99:ARG:HG3	1:B:271:ASN:HD21	1.75	0.51
1:I:149:ASP:HB3	1:I:152:ILE:HB	1.92	0.51
1:J:57:ALA:CA	1:J:188:GLN:HG2	2.40	0.51
1:D:241:VAL:HG13	1:D:241:VAL:O	2.11	0.51
1:F:238:ASN:HB3	1:F:241:VAL:CG1	2.40	0.51
1:G:106:TRP:HA	1:G:252:ARG:O	2.10	0.51
1:I:106:TRP:HA	1:I:252:ARG:O	2.11	0.51
1:G:82:LEU:HD12	1:G:82:LEU:N	2.25	0.51
1:J:76:VAL:HG13	1:J:124:ALA:O	2.10	0.51
1:C:138:ILE:HG23	1:C:144:MET:CE	2.41	0.51
1:A:117:LEU:HD13	1:A:176:MET:HE3	1.93	0.51
1:B:51:LEU:HD21	1:B:154:GLY:CA	2.40	0.51
1:B:104:GLU:O	1:B:105:ALA:HB3	2.10	0.51
1:A:99:ARG:HH21	1:A:268:LEU:HD12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:VAL:CG1	1:B:281:TYR:HE2	2.24	0.51
1:G:150:ARG:NH1	1:I:240:TYR:HA	2.26	0.51
1:H:136:GLU:HB3	1:H:211:SER:HB3	1.92	0.51
1:B:137:THR:HG22	1:B:138:ILE:N	2.25	0.51
1:C:190:GLY:CA	1:C:207:LYS:HB3	2.40	0.51
1:B:171:HIS:CE1	1:B:172:PRO:HG2	2.46	0.51
1:J:241:VAL:O	1:J:241:VAL:HG13	2.10	0.50
1:F:76:VAL:CG1	1:F:124:ALA:HB1	2.40	0.50
1:C:75:GLU:HB3	1:C:130:ALA:HB2	1.92	0.50
1:F:137:THR:HG22	1:F:138:ILE:N	2.26	0.50
1:F:138:ILE:HG12	1:F:139:TYR:N	2.26	0.50
1:G:239:PRO:HG3	1:G:267:THR:O	2.12	0.50
1:A:48:GLU:HG3	1:A:158:TYR:CE2	2.46	0.50
1:J:63:LEU:HD13	1:J:63:LEU:C	2.32	0.50
1:D:149:ASP:HB3	1:D:152:ILE:HB	1.93	0.50
1:A:192:PRO:HG2	1:A:193:VAL:HG23	1.93	0.50
1:J:65:THR:HB	1:J:192:PRO:HD3	1.93	0.50
1:F:96:ARG:HD2	1:F:175:LEU:HD13	1.92	0.50
1:A:190:GLY:HA3	1:A:207:LYS:HG2	1.92	0.50
1:H:241:VAL:HG13	1:H:241:VAL:O	2.12	0.50
1:D:49:PHE:CE2	1:D:60:ALA:HA	2.47	0.50
1:J:98:TYR:HE1	1:J:175:LEU:HD22	1.77	0.50
1:F:104:GLU:O	1:F:105:ALA:HB3	2.12	0.50
1:F:140:ALA:H	1:F:144:MET:CE	2.24	0.50
1:A:72:ILE:HD13	1:A:212:ILE:HB	1.94	0.50
1:D:221:THR:HB	1:D:224:ASN:HB3	1.93	0.50
1:F:86:ASP:O	1:F:90:ARG:HB2	2.11	0.50
1:D:98:TYR:HE1	1:D:175:LEU:HD22	1.76	0.49
1:B:251:GLU:O	1:B:264:ARG:HA	2.12	0.49
1:F:223:TRP:HE3	1:F:231:TYR:CE2	2.31	0.49
1:C:93:LEU:CD1	1:C:93:LEU:N	2.74	0.49
1:G:239:PRO:HB3	1:G:267:THR:HB	1.93	0.49
1:G:39:LYS:NZ	1:G:257:GLY:O	2.34	0.49
1:D:173:LEU:HD11	1:D:276:GLN:NE2	2.28	0.49
1:F:117:LEU:HD13	1:F:176:MET:CE	2.41	0.49
1:E:137:THR:HG22	1:E:138:ILE:N	2.26	0.49
1:J:63:LEU:HD12	1:J:65:THR:CG2	2.41	0.49
1:D:28:TRP:HB3	1:D:96:ARG:HG2	1.93	0.49
1:F:171:HIS:CG	1:F:172:PRO:HD2	2.47	0.49
1:J:224:ASN:O	1:J:228:PRO:HG3	2.13	0.49
1:D:75:GLU:HB3	1:D:130:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:GLU:OE1	1:E:204:LYS:NZ	2.45	0.49
1:H:139:TYR:HB2	1:H:159:PRO:HB3	1.95	0.49
1:D:82:LEU:N	1:D:82:LEU:HD12	2.28	0.49
1:I:96:ARG:HD3	1:I:175:LEU:HD13	1.95	0.48
1:H:245:ARG:O	1:H:246:TRP:HB3	2.13	0.48
1:E:104:GLU:O	1:E:105:ALA:HB3	2.13	0.48
1:J:77:ALA:HB3	1:J:125:GLU:HB2	1.95	0.48
1:F:250:THR:HG23	1:F:264:ARG:NH2	2.28	0.48
1:F:140:ALA:H	1:F:144:MET:HE3	1.78	0.48
1:E:168:GLU:O	1:E:174:THR:HG21	2.13	0.48
1:G:185:LEU:O	1:G:191:ALA:HB2	2.12	0.48
1:H:90:ARG:HB3	1:H:91:PHE:CD1	2.48	0.48
1:G:117:LEU:HD13	1:G:176:MET:CE	2.43	0.48
1:A:251:GLU:HA	1:A:264:ARG:HH22	1.78	0.48
1:D:176:MET:CE	1:D:195:LEU:HD13	2.43	0.48
1:B:210:VAL:O	1:B:210:VAL:HG22	2.12	0.48
1:C:286:LEU:HD13	1:C:286:LEU:N	2.28	0.48
1:C:80:LEU:N	1:C:80:LEU:HD23	2.28	0.48
1:A:80:LEU:HD23	1:A:80:LEU:N	2.29	0.48
1:A:211:SER:OG	1:C:282:ARG:HD3	2.12	0.48
1:B:106:TRP:HA	1:B:252:ARG:O	2.13	0.48
1:H:48:GLU:HG3	1:H:158:TYR:CE2	2.48	0.48
1:D:263:GLN:HA	1:D:263:GLN:NE2	2.27	0.48
1:H:135:PHE:O	1:H:161:VAL:HG23	2.14	0.48
1:G:120:LEU:HD23	1:G:120:LEU:O	2.14	0.47
1:H:171:HIS:O	1:H:174:THR:HG23	2.14	0.47
1:J:87:LEU:HD13	1:J:193:VAL:HG22	1.93	0.47
1:C:136:GLU:OE1	1:E:282:ARG:HD3	2.14	0.47
1:G:74:GLY:O	1:G:76:VAL:N	2.43	0.47
1:G:99:ARG:HD2	1:G:271:ASN:O	2.14	0.47
1:J:175:LEU:HD23	1:J:175:LEU:H	1.79	0.47
1:J:272:GLY:HA2	4:J:434:HOH:O	2.14	0.47
1:J:171:HIS:ND1	1:J:173:LEU:HB2	2.28	0.47
1:H:80:LEU:H	1:H:80:LEU:HD23	1.78	0.47
1:B:87:LEU:CD1	1:B:193:VAL:HG22	2.43	0.47
1:C:29:GLN:HG2	1:G:61:GLY:HA3	1.95	0.47
1:A:140:ALA:HB3	1:A:144:MET:CE	2.35	0.47
1:D:245:ARG:O	1:D:246:TRP:HB3	2.14	0.47
1:B:51:LEU:HD21	1:B:154:GLY:HA3	1.97	0.47
1:B:199:TRP:CD1	1:B:277:VAL:HG11	2.49	0.47
1:G:75:GLU:HG3	1:G:127:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:PHE:CE2	1:J:60:ALA:HA	2.49	0.47
1:B:176:MET:CE	1:B:195:LEU:HD13	2.41	0.47
1:D:51:LEU:HD21	1:D:151:PHE:O	2.14	0.47
1:G:66:ASP:O	1:G:68:TRP:N	2.47	0.47
1:B:149:ASP:OD2	1:B:152:ILE:HG12	2.14	0.47
1:B:66:ASP:O	1:B:67:PRO:C	2.51	0.47
1:F:168:GLU:O	1:F:174:THR:HG21	2.15	0.47
1:F:240:TYR:HA	1:I:150:ARG:NH1	2.30	0.47
1:H:140:ALA:HB3	1:H:144:MET:HE3	1.97	0.47
1:I:60:ALA:HB1	1:I:187:PRO:HB2	1.95	0.47
1:I:138:ILE:O	1:I:144:MET:HE1	2.15	0.47
1:F:140:ALA:HB3	1:F:144:MET:HE3	1.97	0.47
1:I:112:TRP:CE3	1:I:177:THR:HG21	2.50	0.47
1:C:96:ARG:HD2	1:C:175:LEU:HD13	1.97	0.47
1:D:57:ALA:CA	1:D:188:GLN:HG2	2.42	0.46
1:A:135:PHE:O	1:A:161:VAL:HG23	2.14	0.46
1:G:237:VAL:HG21	1:G:271:ASN:HB2	1.97	0.46
1:E:75:GLU:HG3	1:E:127:THR:OG1	2.15	0.46
1:D:60:ALA:HB1	1:D:187:PRO:HB2	1.97	0.46
1:F:223:TRP:CE3	1:F:231:TYR:CE2	3.03	0.46
1:A:171:HIS:ND1	1:A:173:LEU:HB2	2.31	0.46
1:B:185:LEU:O	1:B:191:ALA:HB2	2.16	0.46
1:I:175:LEU:HD23	1:I:196:ILE:HB	1.98	0.46
1:E:39:LYS:HZ1	1:E:257:GLY:H	1.64	0.46
1:I:136:GLU:HB3	1:I:211:SER:HB3	1.96	0.46
1:C:162:GLU:OE2	1:C:221:THR:HG23	2.16	0.46
1:F:120:LEU:C	1:F:120:LEU:HD23	2.36	0.46
1:J:104:GLU:O	1:J:105:ALA:HB3	2.16	0.46
1:D:63:LEU:HD13	1:D:65:THR:CG2	2.45	0.46
1:B:133:VAL:HG22	1:B:214:LEU:HD13	1.97	0.46
1:I:133:VAL:HG22	1:I:214:LEU:CD1	2.44	0.46
1:H:211:SER:OG	1:J:282:ARG:HD3	2.16	0.46
1:H:264:ARG:O	1:H:265:GLN:HB3	2.15	0.46
1:F:109:VAL:HG23	1:F:253:PHE:HE1	1.80	0.46
1:B:221:THR:HG22	1:B:224:ASN:H	1.81	0.46
1:I:221:THR:HB	1:I:224:ASN:HB3	1.98	0.46
1:D:95:GLU:O	1:D:96:ARG:HG3	2.16	0.45
1:B:76:VAL:CG1	1:B:124:ALA:HB1	2.45	0.45
1:A:286:LEU:C	1:A:286:LEU:HD22	2.36	0.45
1:A:82:LEU:N	1:A:82:LEU:HD12	2.31	0.45
1:I:66:ASP:HB3	1:I:67:PRO:CD	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:VAL:HG11	1:A:124:ALA:HB1	1.97	0.45
1:B:25:PRO:HB2	1:B:28:TRP:CD1	2.51	0.45
1:A:277:VAL:HG12	1:A:277:VAL:O	2.15	0.45
1:I:238:ASN:HB3	1:I:241:VAL:CG1	2.47	0.45
1:B:171:HIS:CG	1:B:172:PRO:HD2	2.51	0.45
1:F:80:LEU:N	1:F:80:LEU:HD23	2.32	0.45
1:C:144:MET:HA	1:C:145:PRO:HD2	1.85	0.45
1:F:76:VAL:HG13	1:F:124:ALA:O	2.16	0.45
1:F:171:HIS:ND1	1:F:172:PRO:CD	2.80	0.45
1:C:135:PHE:O	1:C:161:VAL:HG23	2.17	0.45
1:F:108:MET:HG2	1:F:254:ILE:HB	1.99	0.45
1:I:221:THR:O	1:I:225:LEU:HB2	2.17	0.45
1:I:72:ILE:CD1	1:I:212:ILE:HB	2.41	0.45
1:E:39:LYS:NZ	1:E:257:GLY:N	2.65	0.45
1:F:113:ILE:HD11	1:F:182:GLY:HA2	1.99	0.45
1:J:72:ILE:HD13	1:J:212:ILE:HB	1.99	0.45
1:F:285:ASP:OD1	1:F:286:LEU:N	2.50	0.45
1:J:106:TRP:HA	1:J:252:ARG:O	2.18	0.45
1:G:50:GLY:HA2	1:G:152:ILE:O	2.17	0.45
1:C:221:THR:HG22	1:C:224:ASN:H	1.82	0.44
1:G:238:ASN:HB3	1:G:241:VAL:CG1	2.46	0.44
1:B:112:TRP:CE3	1:B:177:THR:HG21	2.53	0.44
1:I:135:PHE:O	1:I:161:VAL:HG23	2.16	0.44
1:E:39:LYS:HZ1	1:E:257:GLY:N	2.16	0.44
1:D:140:ALA:H	1:D:144:MET:HE3	1.82	0.44
1:F:57:ALA:CA	1:F:188:GLN:HG2	2.47	0.44
1:D:82:LEU:N	1:D:82:LEU:CD1	2.81	0.44
1:G:90:ARG:HB3	1:G:91:PHE:CD1	2.52	0.44
1:B:76:VAL:HG12	1:B:78:LYS:N	2.33	0.44
1:C:82:LEU:HD12	1:C:82:LEU:N	2.32	0.44
1:C:63:LEU:CD1	1:C:65:THR:HG22	2.48	0.44
1:C:171:HIS:CG	1:C:172:PRO:HD2	2.53	0.44
1:J:190:GLY:CA	1:J:207:LYS:HB3	2.48	0.44
1:C:117:LEU:HD13	1:C:176:MET:CE	2.48	0.44
1:B:82:LEU:N	1:B:82:LEU:HD12	2.32	0.44
1:I:120:LEU:HD23	1:I:120:LEU:O	2.18	0.44
1:I:80:LEU:HD23	1:I:80:LEU:N	2.33	0.44
1:I:183:LYS:HG2	1:I:183:LYS:H	1.65	0.44
1:D:199:TRP:CD1	1:D:277:VAL:HG11	2.53	0.44
1:F:101:ARG:NE	1:F:251:GLU:OE2	2.51	0.44
1:J:243:HIS:O	1:J:244:PRO:C	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:VAL:HG11	1:D:124:ALA:HB1	1.99	0.44
1:H:138:ILE:HG23	1:H:144:MET:CE	2.48	0.44
1:B:133:VAL:O	1:B:163:GLY:HA2	2.18	0.44
1:J:135:PHE:O	1:J:161:VAL:HG23	2.17	0.44
1:G:76:VAL:HG11	1:G:124:ALA:HB1	1.99	0.44
1:H:82:LEU:CD1	1:H:82:LEU:N	2.81	0.44
1:C:106:TRP:HA	1:C:252:ARG:O	2.18	0.44
1:E:57:ALA:HA	1:E:188:GLN:HG3	1.96	0.43
1:C:57:ALA:HA	1:C:188:GLN:HG3	1.96	0.43
1:I:75:GLU:HB3	1:I:130:ALA:HB2	1.98	0.43
1:D:87:LEU:CD1	1:D:193:VAL:HG22	2.41	0.43
1:I:87:LEU:CD1	1:I:193:VAL:HG22	2.46	0.43
1:J:51:LEU:HD21	1:J:154:GLY:HA3	1.98	0.43
1:D:137:THR:HG22	1:D:138:ILE:N	2.32	0.43
1:D:165:ARG:NH2	1:D:167:ASP:OD2	2.47	0.43
1:H:137:THR:HG22	1:H:138:ILE:N	2.33	0.43
1:H:196:ILE:HG22	1:H:198:PRO:HD3	2.00	0.43
1:E:190:GLY:HA2	1:E:207:LYS:HB3	2.00	0.43
1:D:76:VAL:CG1	1:D:124:ALA:HB1	2.49	0.43
1:B:72:ILE:HD13	1:B:212:ILE:HB	2.00	0.43
1:A:230:GLU:HG2	1:A:244:PRO:HG2	1.99	0.43
1:E:75:GLU:CG	1:E:129:ASN:HB2	2.49	0.43
1:G:149:ASP:HB3	1:G:152:ILE:HB	2.01	0.43
1:G:98:TYR:CE1	1:G:198:PRO:HG3	2.53	0.43
1:E:224:ASN:O	1:E:228:PRO:HG3	2.19	0.43
1:B:66:ASP:O	1:B:68:TRP:N	2.52	0.43
1:D:140:ALA:HB3	1:D:144:MET:HE3	2.00	0.43
1:H:104:GLU:O	1:H:105:ALA:HB3	2.19	0.43
1:C:86:ASP:O	1:C:90:ARG:HB2	2.18	0.43
1:C:138:ILE:HG23	1:C:144:MET:HE1	2.01	0.43
1:A:51:LEU:HD21	1:A:154:GLY:N	2.34	0.43
1:H:80:LEU:N	1:H:80:LEU:HD23	2.34	0.43
1:F:186:PRO:HG2	1:F:189:ASN:OD1	2.19	0.43
1:D:140:ALA:HB3	1:D:144:MET:CE	2.49	0.43
1:C:163:GLY:HA3	1:C:219:PRO:HG2	2.00	0.43
1:B:80:LEU:HD23	1:B:80:LEU:N	2.34	0.43
1:I:104:GLU:O	1:I:105:ALA:HB3	2.18	0.43
1:A:138:ILE:HG23	1:A:144:MET:HE1	2.00	0.42
1:B:238:ASN:CB	1:B:241:VAL:HG12	2.47	0.42
1:J:63:LEU:HD13	1:J:64:LYS:N	2.34	0.42
1:J:214:LEU:CD2	1:J:214:LEU:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:LEU:HB3	1:G:86:ASP:HB2	2.00	0.42
1:D:63:LEU:HD13	1:D:65:THR:HG22	2.00	0.42
1:G:90:ARG:HB3	1:G:91:PHE:CE1	2.53	0.42
1:I:117:LEU:HD13	1:I:176:MET:CE	2.49	0.42
1:E:138:ILE:HG23	1:E:144:MET:CE	2.49	0.42
1:J:263:GLN:HG3	1:J:264:ARG:H	1.83	0.42
1:F:49:PHE:CE2	1:F:60:ALA:HA	2.53	0.42
1:E:204:LYS:HE3	1:E:204:LYS:HB3	1.89	0.42
1:I:20:LEU:HD12	1:I:20:LEU:N	2.33	0.42
1:G:66:ASP:O	1:G:67:PRO:C	2.52	0.42
1:C:149:ASP:HB3	1:C:152:ILE:HB	2.00	0.42
1:H:144:MET:HA	1:H:145:PRO:HD2	1.83	0.42
1:G:160:TYR:CD1	1:G:206:ILE:HG13	2.53	0.42
1:H:55:ASP:HB2	1:H:56:PRO:HD3	2.01	0.42
1:A:71:LYS:HB2	1:A:71:LYS:HE3	1.84	0.42
1:F:133:VAL:HG21	1:F:169:ALA:CB	2.49	0.42
1:J:227:ALA:N	1:J:228:PRO:HD3	2.34	0.42
1:H:86:ASP:O	1:H:90:ARG:HB2	2.19	0.42
1:B:140:ALA:H	1:B:144:MET:HE3	1.84	0.42
1:F:199:TRP:CD1	1:F:277:VAL:HG11	2.54	0.42
1:I:28:TRP:CD1	1:I:96:ARG:HG2	2.52	0.42
1:C:171:HIS:O	1:C:174:THR:HG23	2.19	0.42
1:F:238:ASN:ND2	1:I:157:LYS:HE3	2.34	0.42
1:J:175:LEU:CD2	1:J:196:ILE:HB	2.50	0.42
1:D:140:ALA:H	1:D:144:MET:CE	2.33	0.42
1:E:138:ILE:HG23	1:E:144:MET:HE1	2.02	0.42
1:C:286:LEU:CD1	1:C:286:LEU:N	2.82	0.42
1:H:286:LEU:CD2	1:H:286:LEU:H	2.26	0.42
1:G:49:PHE:CE2	1:G:60:ALA:HA	2.54	0.42
1:B:171:HIS:HE1	1:B:173:LEU:HD13	1.84	0.42
1:C:90:ARG:HB3	1:C:91:PHE:CD1	2.54	0.42
1:D:239:PRO:HB3	1:D:267:THR:HB	2.01	0.42
1:H:72:ILE:HD13	1:H:212:ILE:HB	2.00	0.42
1:C:104:GLU:O	1:C:105:ALA:HB3	2.19	0.42
1:G:138:ILE:HG23	1:G:144:MET:CE	2.50	0.42
1:I:135:PHE:CB	1:I:206:ILE:HG21	2.49	0.42
1:G:47:TYR:CE2	1:G:51:LEU:HD22	2.55	0.42
1:G:178:VAL:C	1:G:185:LEU:HG	2.40	0.42
1:F:101:ARG:HD3	1:F:251:GLU:OE2	2.20	0.42
1:I:94:GLU:O	1:I:113:ILE:HA	2.20	0.42
1:E:243:HIS:O	1:E:244:PRO:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:VAL:O	1:E:278:ALA:C	2.58	0.42
1:D:71:LYS:HE3	1:D:71:LYS:HB2	1.76	0.42
1:A:237:VAL:HG21	1:A:271:ASN:HB2	2.01	0.42
1:A:99:ARG:NH2	1:A:268:LEU:CD1	2.83	0.42
1:B:157:LYS:HE3	1:D:238:ASN:ND2	2.35	0.42
1:E:98:TYR:CE1	1:E:175:LEU:HD22	2.55	0.42
1:B:221:THR:O	1:B:225:LEU:HD13	2.19	0.42
1:I:65:THR:HB	1:I:192:PRO:HG3	2.01	0.42
1:G:137:THR:HG22	1:G:138:ILE:N	2.35	0.41
1:H:51:LEU:HD21	1:H:154:GLY:CA	2.49	0.41
1:I:108:MET:HG2	1:I:254:ILE:HB	2.02	0.41
1:A:100:MET:HG2	4:A:428:HOH:O	2.20	0.41
1:B:263:GLN:OE1	1:B:263:GLN:HA	2.20	0.41
1:G:76:VAL:CG1	1:G:77:ALA:N	2.83	0.41
1:D:66:ASP:O	1:D:84:HIS:HB2	2.20	0.41
1:I:176:MET:HE1	1:I:195:LEU:HD13	2.02	0.41
1:C:48:GLU:OE2	1:C:48:GLU:N	2.46	0.41
1:G:277:VAL:O	1:G:277:VAL:CG1	2.68	0.41
1:F:175:LEU:HD23	1:F:196:ILE:HB	2.03	0.41
1:B:197:VAL:HA	1:B:198:PRO:HD2	1.86	0.41
1:F:149:ASP:HB3	1:F:152:ILE:HB	2.03	0.41
1:E:171:HIS:ND1	1:E:173:LEU:HB2	2.36	0.41
1:B:135:PHE:O	1:B:161:VAL:HG23	2.20	0.41
1:B:20:LEU:CG	1:B:21:GLU:H	2.12	0.41
1:H:106:TRP:HA	1:H:252:ARG:O	2.20	0.41
1:I:71:LYS:HB2	1:I:71:LYS:HE3	1.84	0.41
1:F:71:LYS:HB2	1:F:71:LYS:HE3	1.81	0.41
1:A:74:GLY:O	1:A:76:VAL:N	2.47	0.41
1:I:137:THR:CG2	1:I:138:ILE:H	2.32	0.41
1:J:101:ARG:NH1	1:J:105:ALA:HA	2.35	0.41
1:A:277:VAL:O	1:A:277:VAL:CG1	2.68	0.41
1:J:137:THR:HG22	1:J:138:ILE:N	2.35	0.41
1:D:47:TYR:CD1	1:D:47:TYR:N	2.89	0.41
1:E:176:MET:CE	1:E:195:LEU:HD13	2.51	0.41
1:D:224:ASN:O	1:D:228:PRO:HG3	2.20	0.41
1:G:161:VAL:HG22	1:G:162:GLU:N	2.36	0.41
1:J:214:LEU:N	1:J:214:LEU:HD22	2.35	0.41
1:H:65:THR:HB	1:H:192:PRO:HD3	2.03	0.41
1:H:93:LEU:N	1:H:93:LEU:HD12	2.36	0.41
1:A:138:ILE:HG23	1:A:144:MET:HE2	2.03	0.41
1:H:76:VAL:CG1	1:H:77:ALA:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASP:OD1	1:A:286:LEU:HD13	2.20	0.41
1:B:239:PRO:HB3	1:B:267:THR:HB	2.03	0.41
1:I:70:LEU:HD12	1:I:193:VAL:HG21	2.03	0.41
1:I:144:MET:HA	1:I:145:PRO:HD2	1.87	0.41
1:I:66:ASP:O	1:I:67:PRO:C	2.56	0.41
1:J:162:GLU:OE1	1:J:204:LYS:HD2	2.21	0.41
1:I:269:LEU:O	1:I:270:PHE:HB2	2.20	0.41
1:F:85:ASP:O	1:F:89:ARG:HB2	2.21	0.41
1:E:36:PRO:HG2	1:E:39:LYS:HD2	2.04	0.40
1:B:66:ASP:HB3	1:B:67:PRO:CD	2.51	0.40
1:B:203:PHE:HB2	1:B:223:TRP:CD1	2.55	0.40
1:J:99:ARG:HG3	1:J:271:ASN:ND2	2.36	0.40
1:E:28:TRP:CH2	1:E:173:LEU:CD1	3.04	0.40
1:H:237:VAL:HG21	1:H:271:ASN:HB2	2.04	0.40
1:H:171:HIS:CG	1:H:172:PRO:HD2	2.57	0.40
1:E:74:GLY:O	1:E:76:VAL:N	2.52	0.40
1:J:47:TYR:C	1:J:49:PHE:N	2.73	0.40
1:J:190:GLY:HA2	1:J:207:LYS:HB3	2.03	0.40
1:E:173:LEU:HD12	1:E:173:LEU:HA	1.78	0.40
1:G:100:MET:HG2	4:G:421:HOH:O	2.21	0.40
1:C:138:ILE:HG23	1:C:144:MET:HE2	2.02	0.40
1:A:51:LEU:HD21	1:A:154:GLY:HA3	2.00	0.40
1:F:75:GLU:HB3	1:F:130:ALA:HB2	2.02	0.40
1:J:87:LEU:HD13	1:J:193:VAL:HG23	2.00	0.40
1:I:161:VAL:HG22	1:I:162:GLU:N	2.36	0.40
1:D:144:MET:HA	1:D:145:PRO:HD2	1.88	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	259/298 (87%)	249 (96%)	9 (4%)	1 (0%)	39	42
1	B	258/298 (87%)	242 (94%)	15 (6%)	1 (0%)	39	42
1	C	260/298 (87%)	246 (95%)	13 (5%)	1 (0%)	39	42
1	D	259/298 (87%)	248 (96%)	11 (4%)	0	100	100
1	E	258/298 (87%)	241 (93%)	17 (7%)	0	100	100
1	F	258/298 (87%)	243 (94%)	15 (6%)	0	100	100
1	G	257/298 (86%)	242 (94%)	13 (5%)	2 (1%)	24	22
1	H	260/298 (87%)	236 (91%)	23 (9%)	1 (0%)	39	42
1	I	258/298 (87%)	239 (93%)	18 (7%)	1 (0%)	39	42
1	J	258/298 (87%)	244 (95%)	14 (5%)	0	100	100
All	All	2585/2980 (87%)	2430 (94%)	148 (6%)	7 (0%)	46	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	192	PRO
1	G	75	GLU
1	A	75	GLU
1	B	66	ASP
1	G	66	ASP
1	H	265	GLN
1	I	66	ASP

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	219/249 (88%)	204 (93%)	15 (7%)	20	21
1	B	219/249 (88%)	213 (97%)	6 (3%)	52	64
1	C	220/249 (88%)	207 (94%)	13 (6%)	24	27
1	D	219/249 (88%)	211 (96%)	8 (4%)	41	50
1	E	218/249 (88%)	211 (97%)	7 (3%)	46	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	218/249 (88%)	206 (94%)	12 (6%)	27 30
1	G	218/249 (88%)	210 (96%)	8 (4%)	41 50
1	H	220/249 (88%)	207 (94%)	13 (6%)	24 27
1	I	218/249 (88%)	209 (96%)	9 (4%)	37 45
1	J	218/249 (88%)	208 (95%)	10 (5%)	33 40
All	All	2187/2490 (88%)	2086 (95%)	101 (5%)	33 40

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	46	PHE
1	A	70	LEU
1	A	120	LEU
1	A	173	LEU
1	A	174	THR
1	A	175	LEU
1	A	194	ARG
1	A	210	VAL
1	A	221	THR
1	A	241	VAL
1	A	247	SER
1	A	264	ARG
1	A	279	SER
1	A	286	LEU
1	B	46	PHE
1	B	125	GLU
1	B	165	ARG
1	B	174	THR
1	B	193	VAL
1	B	194	ARG
1	C	20	LEU
1	C	38	ASP
1	C	46	PHE
1	C	70	LEU
1	C	174	THR
1	C	175	LEU
1	C	188	GLN
1	C	193	VAL
1	C	194	ARG

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Mol	Chain	Res	Type
1	C	210	VAL
1	C	214	LEU
1	C	263	GLN
1	C	286	LEU
1	D	46	PHE
1	D	51	LEU
1	D	63	LEU
1	D	70	LEU
1	D	99	ARG
1	D	174	THR
1	D	194	ARG
1	D	218	ARG
1	E	20	LEU
1	E	46	PHE
1	E	93	LEU
1	E	174	THR
1	E	194	ARG
1	E	241	VAL
1	E	285	ASP
1	F	38	ASP
1	F	46	PHE
1	F	63	LEU
1	F	70	LEU
1	F	81	THR
1	F	82	LEU
1	F	93	LEU
1	F	174	THR
1	F	188	GLN
1	F	194	ARG
1	F	279	SER
1	F	286	LEU
1	G	46	PHE
1	G	64	LYS
1	G	70	LEU
1	G	175	LEU
1	G	193	VAL
1	G	194	ARG
1	G	211	SER
1	G	225	LEU
1	H	18	LYS
1	H	20	LEU
1	H	46	PHE

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Mol	Chain	Res	Type
1	H	70	LEU
1	H	90	ARG
1	H	99	ARG
1	H	118	HIS
1	H	173	LEU
1	H	174	THR
1	H	175	LEU
1	H	188	GLN
1	H	194	ARG
1	H	286	LEU
1	I	20	LEU
1	I	46	PHE
1	I	99	ARG
1	I	175	LEU
1	I	183	LYS
1	I	193	VAL
1	I	194	ARG
1	I	218	ARG
1	I	277	VAL
1	J	38	ASP
1	J	46	PHE
1	J	81	THR
1	J	93	LEU
1	J	99	ARG
1	J	120	LEU
1	J	173	LEU
1	J	174	THR
1	J	194	ARG
1	J	214	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	276	GLN
1	D	263	GLN
1	D	276	GLN
1	E	30	ASN
1	G	59	ASN
1	J	31	ASN
1	J	263	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

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	MTE	A	301	2	19,26,26	2.87	10 (52%)	19,40,40	6.31	13 (68%)
3	MTE	B	302	2	19,26,26	2.69	11 (57%)	19,40,40	6.10	15 (78%)
3	MTE	C	303	2	19,26,26	2.58	9 (47%)	19,40,40	6.60	13 (68%)
3	MTE	D	304	2	19,26,26	2.64	7 (36%)	19,40,40	6.14	12 (63%)
3	MTE	E	305	2	19,26,26	2.37	7 (36%)	19,40,40	6.67	13 (68%)
3	MTE	F	306	2	19,26,26	2.78	8 (42%)	19,40,40	6.34	15 (78%)
3	MTE	G	307	2	19,26,26	2.52	9 (47%)	19,40,40	6.47	12 (63%)
3	MTE	H	308	2	19,26,26	2.82	9 (47%)	19,40,40	6.02	15 (78%)
3	MTE	I	309	2	19,26,26	2.83	9 (47%)	19,40,40	6.17	14 (73%)
3	MTE	J	310	2	19,26,26	2.83	9 (47%)	19,40,40	6.60	13 (68%)

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
3	MTE	A	301	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	B	302	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	C	303	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	D	304	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	E	305	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	F	306	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	G	307	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	H	308	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	I	309	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	J	310	2	1/1/6/8	0/6/34/34	0/3/3/3

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	309	MTE	P-O4'	-5.46	1.42	1.60
3	H	308	MTE	P-O4'	-5.19	1.42	1.60
3	J	310	MTE	P-O4'	-5.00	1.43	1.60
3	A	301	MTE	P-O1P	-4.97	1.34	1.51
3	C	303	MTE	P-O4'	-4.88	1.43	1.60
3	F	306	MTE	P-O4'	-4.74	1.44	1.60
3	B	302	MTE	P-O4'	-4.46	1.45	1.60
3	D	304	MTE	P-O4'	-4.30	1.45	1.60
3	A	301	MTE	P-O4'	-4.28	1.45	1.60
3	E	305	MTE	P-O4'	-4.14	1.46	1.60
3	A	301	MTE	C2-N3	-4.02	1.28	1.35
3	H	308	MTE	P-O1P	-3.68	1.39	1.51
3	B	302	MTE	P-O1P	-3.60	1.39	1.51
3	G	307	MTE	P-O4'	-3.58	1.48	1.60
3	G	307	MTE	C2-N3	-3.28	1.29	1.35
3	F	306	MTE	P-O1P	-3.17	1.40	1.51
3	J	310	MTE	C2-N3	-2.87	1.30	1.35
3	I	309	MTE	C2-N3	-2.87	1.30	1.35
3	D	304	MTE	P-O1P	-2.79	1.42	1.51
3	E	305	MTE	P-O1P	-2.78	1.42	1.51
3	I	309	MTE	P-O1P	-2.78	1.42	1.51
3	D	304	MTE	C2-N3	-2.76	1.30	1.35
3	J	310	MTE	P-O1P	-2.65	1.42	1.51
3	C	303	MTE	P-O1P	-2.55	1.42	1.51
3	B	302	MTE	C2-N3	-2.49	1.31	1.35
3	J	310	MTE	C2-N2	-2.44	1.29	1.34
3	E	305	MTE	C2-N2	-2.41	1.29	1.34
3	A	301	MTE	C2-N2	-2.38	1.29	1.34
3	C	303	MTE	C2-N3	-2.37	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	307	MTE	P-O1P	-2.35	1.43	1.51
3	E	305	MTE	C2-N3	-2.07	1.31	1.35
3	B	302	MTE	P-O2P	-2.06	1.47	1.54
3	H	308	MTE	C2-N3	-2.04	1.31	1.35
3	B	302	MTE	C2-N1	2.01	1.39	1.35
3	I	309	MTE	O3'-C3'	2.05	1.46	1.43
3	B	302	MTE	O4'-C4'	2.10	1.53	1.44
3	G	307	MTE	C4-N3	2.11	1.37	1.33
3	I	309	MTE	C4-N3	2.25	1.37	1.33
3	B	302	MTE	C4-N3	2.33	1.37	1.33
3	G	307	MTE	C10-N8	2.40	1.39	1.35
3	A	301	MTE	O3'-C7	2.42	1.47	1.43
3	I	309	MTE	O3'-C7	2.43	1.47	1.43
3	H	308	MTE	O3'-C3'	2.55	1.47	1.43
3	F	306	MTE	O3'-C7	2.57	1.47	1.43
3	J	310	MTE	C4-N3	2.63	1.38	1.33
3	G	307	MTE	O3'-C3'	2.66	1.47	1.43
3	B	302	MTE	O3'-C7	2.67	1.47	1.43
3	C	303	MTE	O3'-C3'	2.70	1.47	1.43
3	C	303	MTE	O3'-C7	2.72	1.47	1.43
3	H	308	MTE	C9-N5	2.73	1.44	1.38
3	H	308	MTE	C4-N3	2.99	1.38	1.33
3	A	301	MTE	C9-N5	3.02	1.45	1.38
3	C	303	MTE	C9-N5	3.07	1.45	1.38
3	B	302	MTE	C9-N5	3.12	1.45	1.38
3	I	309	MTE	C9-N5	3.15	1.45	1.38
3	C	303	MTE	C6-N5	3.16	1.50	1.45
3	J	310	MTE	C9-N5	3.17	1.45	1.38
3	C	303	MTE	C4-N3	3.20	1.39	1.33
3	F	306	MTE	C9-N5	3.21	1.45	1.38
3	F	306	MTE	O3'-C3'	3.22	1.48	1.43
3	F	306	MTE	C4-N3	3.26	1.39	1.33
3	A	301	MTE	C4-N3	3.30	1.39	1.33
3	D	304	MTE	C6-N5	3.34	1.50	1.45
3	E	305	MTE	C6-N5	3.42	1.50	1.45
3	G	307	MTE	C9-N5	3.44	1.46	1.38
3	H	308	MTE	O3'-C7	3.46	1.48	1.43
3	A	301	MTE	O3'-C3'	3.56	1.48	1.43
3	H	308	MTE	C6-N5	3.70	1.50	1.45
3	E	305	MTE	C7-C6	3.83	1.56	1.53
3	G	307	MTE	C6-N5	3.93	1.51	1.45
3	D	304	MTE	O3'-C7	4.03	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	304	MTE	O3'-C3'	4.21	1.49	1.43
3	A	301	MTE	C6-N5	4.35	1.51	1.45
3	B	302	MTE	C6-N5	4.41	1.51	1.45
3	J	310	MTE	O3'-C7	4.64	1.50	1.43
3	F	306	MTE	C6-N5	4.75	1.52	1.45
3	A	301	MTE	C9-C10	4.85	1.51	1.41
3	J	310	MTE	C6-N5	5.02	1.52	1.45
3	D	304	MTE	C9-C10	5.64	1.53	1.41
3	I	309	MTE	C6-N5	5.72	1.53	1.45
3	B	302	MTE	C9-C10	5.73	1.53	1.41
3	E	305	MTE	C9-C10	5.76	1.53	1.41
3	I	309	MTE	C9-C10	5.82	1.53	1.41
3	C	303	MTE	C9-C10	5.85	1.53	1.41
3	J	310	MTE	C9-C10	6.11	1.54	1.41
3	G	307	MTE	C9-C10	6.13	1.54	1.41
3	F	306	MTE	C9-C10	6.34	1.54	1.41
3	H	308	MTE	C9-C10	6.74	1.55	1.41

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	305	MTE	O3'-C7-C6	-23.92	92.61	108.96
3	J	310	MTE	O3'-C7-C6	-23.89	92.63	108.96
3	C	303	MTE	O3'-C7-C6	-23.76	92.72	108.96
3	G	307	MTE	O3'-C7-C6	-22.50	93.59	108.96
3	A	301	MTE	O3'-C7-C6	-22.29	93.73	108.96
3	F	306	MTE	O3'-C7-C6	-22.13	93.84	108.96
3	D	304	MTE	O3'-C7-C6	-21.32	94.39	108.96
3	I	309	MTE	O3'-C7-C6	-21.05	94.58	108.96
3	B	302	MTE	O3'-C7-C6	-20.72	94.80	108.96
3	H	308	MTE	O3'-C7-C6	-20.43	95.00	108.96
3	I	309	MTE	N3-C2-N1	-4.97	117.39	125.53
3	G	307	MTE	N3-C2-N1	-4.88	117.54	125.53
3	F	306	MTE	N3-C2-N1	-4.68	117.86	125.53
3	D	304	MTE	N3-C2-N1	-4.58	118.02	125.53
3	H	308	MTE	N3-C2-N1	-4.57	118.05	125.53
3	J	310	MTE	N3-C2-N1	-4.56	118.06	125.53
3	A	301	MTE	N3-C2-N1	-4.52	118.13	125.53
3	C	303	MTE	N3-C2-N1	-4.49	118.17	125.53
3	B	302	MTE	N3-C2-N1	-4.45	118.23	125.53
3	E	305	MTE	N3-C2-N1	-4.33	118.43	125.53
3	E	305	MTE	C9-C10-N1	-3.65	111.20	118.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	MTE	C9-C10-N1	-3.64	111.23	118.76
3	G	307	MTE	C9-C10-N1	-3.63	111.23	118.76
3	D	304	MTE	C9-C10-N1	-3.58	111.34	118.76
3	C	303	MTE	C9-C10-N1	-3.52	111.46	118.76
3	I	309	MTE	C9-C10-N1	-3.49	111.53	118.76
3	B	302	MTE	C9-C10-N1	-3.42	111.68	118.76
3	H	308	MTE	C9-C10-N1	-3.32	111.89	118.76
3	J	310	MTE	C9-C10-N1	-3.30	111.92	118.76
3	F	306	MTE	C9-C10-N1	-3.16	112.21	118.76
3	G	307	MTE	C9-C10-N8	-2.88	115.32	118.34
3	F	306	MTE	C9-C10-N8	-2.87	115.34	118.34
3	B	302	MTE	C9-C10-N8	-2.67	115.55	118.34
3	J	310	MTE	C9-C10-N8	-2.65	115.56	118.34
3	H	308	MTE	O2P-P-O1P	-2.64	102.07	110.58
3	F	306	MTE	O2P-P-O1P	-2.52	102.46	110.58
3	E	305	MTE	C10-C9-N5	-2.48	115.72	118.85
3	A	301	MTE	C10-C9-N5	-2.45	115.76	118.85
3	H	308	MTE	C9-C10-N8	-2.39	115.84	118.34
3	I	309	MTE	C9-C10-N8	-2.35	115.88	118.34
3	G	307	MTE	C10-C9-N5	-2.32	115.92	118.85
3	C	303	MTE	C9-C10-N8	-2.32	115.91	118.34
3	H	308	MTE	O3P-P-O4'	-2.27	100.04	106.56
3	F	306	MTE	O3P-P-O4'	-2.22	100.19	106.56
3	B	302	MTE	O2P-P-O1P	-2.19	103.52	110.58
3	I	309	MTE	C10-C9-N5	-2.17	116.11	118.85
3	E	305	MTE	O2P-P-O1P	-2.16	103.61	110.58
3	D	304	MTE	C10-C9-N5	-2.10	116.20	118.85
3	B	302	MTE	C10-C9-N5	-2.09	116.21	118.85
3	B	302	MTE	N2-C2-N1	2.06	120.61	117.20
3	C	303	MTE	N2-C2-N1	2.08	120.64	117.20
3	J	310	MTE	N2-C2-N3	2.13	120.72	117.20
3	F	306	MTE	N2-C2-N1	2.14	120.74	117.20
3	H	308	MTE	N2-C2-N1	2.20	120.84	117.20
3	A	301	MTE	N2-C2-N3	2.21	120.86	117.20
3	I	309	MTE	N2-C2-N3	2.27	120.95	117.20
3	J	310	MTE	O3P-P-O2P	2.30	116.15	107.38
3	A	301	MTE	N2-C2-N1	2.30	121.02	117.20
3	A	301	MTE	O3P-P-O2P	2.31	116.19	107.38
3	H	308	MTE	N2-C2-N3	2.36	121.11	117.20
3	B	302	MTE	N2-C2-N3	2.39	121.16	117.20
3	C	303	MTE	N2-C2-N3	2.41	121.19	117.20
3	C	303	MTE	O3P-P-O2P	2.42	116.58	107.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	310	MTE	N2-C2-N1	2.42	121.21	117.20
3	A	301	MTE	O4'-P-O1P	2.49	113.47	107.14
3	E	305	MTE	N2-C2-N3	2.51	121.35	117.20
3	F	306	MTE	N2-C2-N3	2.54	121.40	117.20
3	D	304	MTE	N2-C2-N3	2.60	121.50	117.20
3	C	303	MTE	C4-N3-C2	2.65	119.61	115.94
3	D	304	MTE	O4'-P-O1P	2.67	113.95	107.14
3	I	309	MTE	N2-C2-N1	2.69	121.66	117.20
3	A	301	MTE	C4-N3-C2	2.70	119.68	115.94
3	F	306	MTE	C4-N3-C2	2.76	119.77	115.94
3	J	310	MTE	O4'-P-O1P	2.80	114.27	107.14
3	D	304	MTE	O3P-P-O2P	2.81	118.07	107.38
3	B	302	MTE	C4-N3-C2	2.83	119.87	115.94
3	H	308	MTE	O3P-P-O2P	2.90	118.42	107.38
3	F	306	MTE	O3P-P-O2P	2.93	118.53	107.38
3	E	305	MTE	C4-N3-C2	2.99	120.09	115.94
3	G	307	MTE	N2-C2-N1	3.02	122.20	117.20
3	J	310	MTE	C4-N3-C2	3.05	120.17	115.94
3	E	305	MTE	O3P-P-O2P	3.08	119.09	107.38
3	J	310	MTE	C9-N5-C6	3.09	126.95	118.65
3	C	303	MTE	C9-N5-C6	3.12	127.05	118.65
3	G	307	MTE	O3P-P-O2P	3.13	119.29	107.38
3	I	309	MTE	C9-N5-C6	3.16	127.14	118.65
3	I	309	MTE	O4'-P-O1P	3.17	115.22	107.14
3	H	308	MTE	C9-N5-C6	3.18	127.19	118.65
3	I	309	MTE	O3P-P-O2P	3.19	119.52	107.38
3	F	306	MTE	O4'-P-O1P	3.19	115.26	107.14
3	A	301	MTE	C9-N5-C6	3.19	127.23	118.65
3	D	304	MTE	C4-N3-C2	3.19	120.37	115.94
3	E	305	MTE	O4'-P-O1P	3.21	115.30	107.14
3	H	308	MTE	C4-N3-C2	3.24	120.43	115.94
3	B	302	MTE	C9-N5-C6	3.25	127.37	118.65
3	D	304	MTE	C9-N5-C6	3.28	127.47	118.65
3	F	306	MTE	C9-N5-C6	3.30	127.52	118.65
3	I	309	MTE	C4-N3-C2	3.32	120.54	115.94
3	B	302	MTE	O3P-P-O2P	3.35	120.16	107.38
3	C	303	MTE	O4'-P-O1P	3.36	115.68	107.14
3	H	308	MTE	O4'-P-O1P	3.46	115.94	107.14
3	C	303	MTE	C10-N8-C7	3.46	130.46	123.67
3	G	307	MTE	C9-N5-C6	3.51	128.07	118.65
3	D	304	MTE	C10-N8-C7	3.61	130.75	123.67
3	H	308	MTE	C10-N8-C7	3.71	130.94	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	MTE	O4'-P-O1P	3.73	116.63	107.14
3	E	305	MTE	C9-N5-C6	3.83	128.95	118.65
3	E	305	MTE	C10-N8-C7	3.87	131.26	123.67
3	G	307	MTE	C4-N3-C2	3.89	121.34	115.94
3	A	301	MTE	C10-N8-C7	3.92	131.35	123.67
3	G	307	MTE	C10-N8-C7	3.93	131.37	123.67
3	F	306	MTE	C10-N8-C7	4.03	131.57	123.67
3	B	302	MTE	C10-N8-C7	4.10	131.70	123.67
3	J	310	MTE	C10-N8-C7	4.15	131.80	123.67
3	I	309	MTE	C10-N8-C7	4.16	131.83	123.67
3	B	302	MTE	C2-N1-C10	7.14	130.59	114.54
3	J	310	MTE	C2-N1-C10	7.26	130.87	114.54
3	E	305	MTE	C2-N1-C10	7.27	130.89	114.54
3	H	308	MTE	C2-N1-C10	7.30	130.96	114.54
3	F	306	MTE	C2-N1-C10	7.33	131.01	114.54
3	G	307	MTE	C2-N1-C10	7.42	131.23	114.54
3	I	309	MTE	C2-N1-C10	7.43	131.25	114.54
3	A	301	MTE	C2-N1-C10	7.56	131.54	114.54
3	D	304	MTE	C2-N1-C10	7.57	131.56	114.54
3	C	303	MTE	C2-N1-C10	7.60	131.64	114.54
3	H	308	MTE	N8-C10-N1	9.84	132.27	116.62
3	D	304	MTE	N8-C10-N1	9.90	132.38	116.62
3	A	301	MTE	N8-C10-N1	9.91	132.39	116.62
3	F	306	MTE	N8-C10-N1	9.95	132.45	116.62
3	E	305	MTE	N8-C10-N1	9.99	132.52	116.62
3	J	310	MTE	N8-C10-N1	9.99	132.52	116.62
3	I	309	MTE	N8-C10-N1	10.04	132.59	116.62
3	C	303	MTE	N8-C10-N1	10.06	132.62	116.62
3	B	302	MTE	N8-C10-N1	10.15	132.77	116.62
3	G	307	MTE	N8-C10-N1	10.56	133.43	116.62

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	309	MTE	C6
3	C	303	MTE	C6
3	G	307	MTE	C6
3	B	302	MTE	C6
3	E	305	MTE	C6
3	A	301	MTE	C6
3	J	310	MTE	C6
3	D	304	MTE	C6

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Mol	Chain	Res	Type	Atom
3	H	308	MTE	C6
3	F	306	MTE	C6

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	263/298 (88%)	0.22	9 (3%) 49 47	22, 46, 78, 95	0
1	B	262/298 (87%)	0.73	33 (12%) 5 5	33, 68, 94, 106	0
1	C	264/298 (88%)	0.25	12 (4%) 37 36	22, 49, 78, 90	0
1	D	263/298 (88%)	0.26	6 (2%) 64 63	24, 46, 76, 92	0
1	E	262/298 (87%)	0.25	10 (3%) 44 43	25, 46, 80, 97	0
1	F	262/298 (87%)	1.09	53 (20%) 1 1	36, 64, 88, 94	1 (0%)
1	G	261/298 (87%)	0.48	18 (6%) 20 19	21, 49, 84, 100	0
1	H	263/298 (88%)	0.73	26 (9%) 9 8	36, 68, 95, 102	0
1	I	262/298 (87%)	0.79	26 (9%) 9 8	34, 61, 90, 106	0
1	J	262/298 (87%)	0.22	8 (3%) 52 51	20, 44, 73, 91	0
All	All	2624/2980 (88%)	0.50	201 (7%) 16 16	20, 54, 88, 106	1 (0%)

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	31	ASN	7.9
1	F	130	ALA	7.4
1	G	66	ASP	5.7
1	F	120	LEU	5.4
1	B	256	SER	4.8
1	H	26	ALA	4.7
1	J	263	GLN	4.6
1	E	256	SER	4.5
1	F	65	THR	4.5
1	B	89	ARG	4.5
1	B	125	GLU	4.4
1	F	88	THR	4.4
1	A	31	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	28	TRP	4.2
1	I	26	ALA	4.1
1	H	20	LEU	4.0
1	F	129	ASN	4.0
1	C	229	ASP	4.0
1	F	223	TRP	4.0
1	B	66	ASP	4.0
1	F	256	SER	4.0
1	I	229	ASP	3.9
1	H	91	PHE	3.9
1	B	255	GLY	3.9
1	I	263	GLN	3.8
1	F	31	ASN	3.8
1	F	206	ILE	3.8
1	E	263	GLN	3.8
1	B	61	GLY	3.8
1	A	26	ALA	3.8
1	I	150	ARG	3.8
1	I	89	ARG	3.7
1	H	256	SER	3.7
1	E	257	GLY	3.6
1	I	257	GLY	3.6
1	C	256	SER	3.6
1	G	22	PHE	3.6
1	J	151	PHE	3.6
1	H	86	ASP	3.6
1	F	156	LEU	3.6
1	I	66	ASP	3.5
1	F	166	LEU	3.5
1	I	64	LYS	3.5
1	F	203	PHE	3.5
1	F	253	PHE	3.5
1	I	55	ASP	3.4
1	F	28	TRP	3.4
1	B	58	ALA	3.4
1	I	20	LEU	3.4
1	B	264	ARG	3.4
1	F	205	GLY	3.4
1	B	85	ASP	3.4
1	H	70	LEU	3.3
1	G	30	ASN	3.3
1	H	85	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	160	TYR	3.3
1	I	58	ALA	3.3
1	F	66	ASP	3.3
1	G	90	ARG	3.3
1	B	87	LEU	3.2
1	A	285	ASP	3.2
1	B	263	GLN	3.2
1	F	64	LYS	3.2
1	F	124	ALA	3.1
1	A	256	SER	3.1
1	J	229	ASP	3.1
1	C	31	ASN	3.1
1	B	26	ALA	3.0
1	C	21	GLU	3.0
1	H	25	PRO	3.0
1	F	19	ALA	3.0
1	H	151	PHE	3.0
1	I	69	THR	3.0
1	F	103	VAL	3.0
1	B	21	GLU	3.0
1	H	75	GLU	2.9
1	H	263	GLN	2.9
1	F	89	ARG	2.9
1	F	257	GLY	2.9
1	F	51	LEU	2.9
1	H	69	THR	2.9
1	B	129	ASN	2.8
1	F	123	LEU	2.8
1	F	148	GLN	2.8
1	I	129	ASN	2.8
1	F	204	LYS	2.8
1	G	85	ASP	2.8
1	G	229	ASP	2.8
1	C	230	GLU	2.8
1	H	82	LEU	2.8
1	B	31	ASN	2.8
1	A	142	GLU	2.8
1	G	27	ALA	2.8
1	E	125	GLU	2.8
1	G	88	THR	2.7
1	I	185	LEU	2.7
1	F	195	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	217	GLU	2.7
1	I	70	LEU	2.6
1	G	256	SER	2.6
1	F	202	GLY	2.6
1	I	21	GLU	2.6
1	D	66	ASP	2.6
1	B	88	THR	2.6
1	I	193	VAL	2.6
1	H	32	LEU	2.6
1	F	232	GLY	2.6
1	I	77	ALA	2.6
1	C	255	GLY	2.6
1	G	20	LEU	2.6
1	E	244	PRO	2.6
1	I	139	TYR	2.6
1	F	197	VAL	2.6
1	H	18	LYS	2.5
1	F	254	ILE	2.5
1	F	201	TYR	2.5
1	D	31	ASN	2.5
1	E	129	ASN	2.5
1	B	20	LEU	2.5
1	H	65	THR	2.5
1	H	246	TRP	2.5
1	E	62	SER	2.5
1	F	128	SER	2.5
1	F	182	GLY	2.5
1	F	235	ALA	2.5
1	G	26	ALA	2.5
1	G	29	GLN	2.4
1	D	30	ASN	2.4
1	J	250	THR	2.4
1	A	286	LEU	2.4
1	B	92	PRO	2.4
1	A	89	ARG	2.4
1	C	244	PRO	2.4
1	F	222	THR	2.4
1	I	128	SER	2.3
1	E	28	TRP	2.3
1	F	162	GLU	2.3
1	I	83	ASP	2.3
1	F	161	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	152	ILE	2.3
1	A	229	ASP	2.3
1	C	66	ASP	2.3
1	G	87	LEU	2.3
1	E	229	ASP	2.3
1	B	25	PRO	2.3
1	B	71	LYS	2.3
1	H	150	ARG	2.3
1	H	264	ARG	2.3
1	B	24	LYS	2.2
1	F	102	CYS	2.2
1	I	142	GLU	2.2
1	C	80	LEU	2.2
1	F	81	THR	2.2
1	F	76	VAL	2.2
1	H	84	HIS	2.2
1	G	21	GLU	2.2
1	H	229	ASP	2.2
1	C	60	ALA	2.2
1	H	68	TRP	2.2
1	I	27	ALA	2.2
1	F	75	GLU	2.2
1	H	66	ASP	2.2
1	B	90	ARG	2.2
1	B	150	ARG	2.2
1	E	128	SER	2.2
1	D	51	LEU	2.2
1	H	129	ASN	2.2
1	J	31	ASN	2.2
1	B	75	GLU	2.2
1	G	130	ALA	2.2
1	F	264	ARG	2.2
1	H	21	GLU	2.2
1	F	174	THR	2.2
1	B	266	PRO	2.1
1	B	268	LEU	2.1
1	I	102	CYS	2.1
1	B	142	GLU	2.1
1	B	244	PRO	2.1
1	B	182	GLY	2.1
1	F	155	GLY	2.1
1	J	155	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	83	ASP	2.1
1	A	250	THR	2.1
1	B	120	LEU	2.1
1	F	215	THR	2.1
1	B	84	HIS	2.1
1	F	231	TYR	2.1
1	F	21	GLU	2.1
1	I	216	ARG	2.1
1	C	38	ASP	2.1
1	F	229	ASP	2.1
1	F	45	ASN	2.1
1	H	83	ASP	2.1
1	J	51	LEU	2.0
1	B	60	ALA	2.0
1	C	18	LYS	2.0
1	B	72	ILE	2.0
1	I	161	VAL	2.0
1	G	228	PRO	2.0
1	D	29	GLN	2.0
1	D	19	ALA	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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
3	MTE	A	301	24/24	0.98	0.15	0.34	16,23,30,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MTE	G	307	24/24	0.97	0.16	0.19	17,26,32,36	0
3	MTE	J	310	24/24	0.97	0.15	0.15	8,22,28,29	0
2	W	D	404	1/1	1.00	0.14	0.06	32,32,32,32	0
3	MTE	H	308	24/24	0.95	0.15	-0.07	30,43,48,50	0
3	MTE	D	304	24/24	0.97	0.14	-0.26	18,28,35,38	0
3	MTE	F	306	24/24	0.96	0.19	-0.33	26,38,46,47	0
2	W	A	401	1/1	1.00	0.15	-0.38	28,28,28,28	0
3	MTE	B	302	24/24	0.97	0.14	-0.40	22,39,50,56	0
3	MTE	C	303	24/24	0.95	0.13	-0.44	15,32,39,42	0
2	W	C	403	1/1	1.00	0.15	-0.47	32,32,32,32	0
2	W	J	410	1/1	0.99	0.16	-0.49	30,30,30,30	0
3	MTE	E	305	24/24	0.98	0.13	-0.55	8,22,33,36	0
2	W	B	402	1/1	0.99	0.12	-0.74	43,43,43,43	0
2	W	E	405	1/1	1.00	0.14	-0.85	32,32,32,32	0
2	W	G	407	1/1	1.00	0.14	-0.92	29,29,29,29	0
3	MTE	I	309	24/24	0.94	0.14	-0.99	26,42,49,50	0
2	W	H	408	1/1	0.99	0.13	-1.29	41,41,41,41	0
2	W	F	406	1/1	0.98	0.14	-3.36	41,41,41,41	0
2	W	I	409	1/1	0.96	0.15	-4.91	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.