



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 03:26 PM EST

PDB ID : 3FBT
Title : Crystal structure of a chorismate mutase/shikimate 5-dehydrogenase fusion protein from *Clostridium acetobutylicum*
Authors : Bonanno, J.B.; Gilmore, M.; Bain, K.T.; Hu, S.; Romero, R.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-11-19
Resolution : 2.10 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

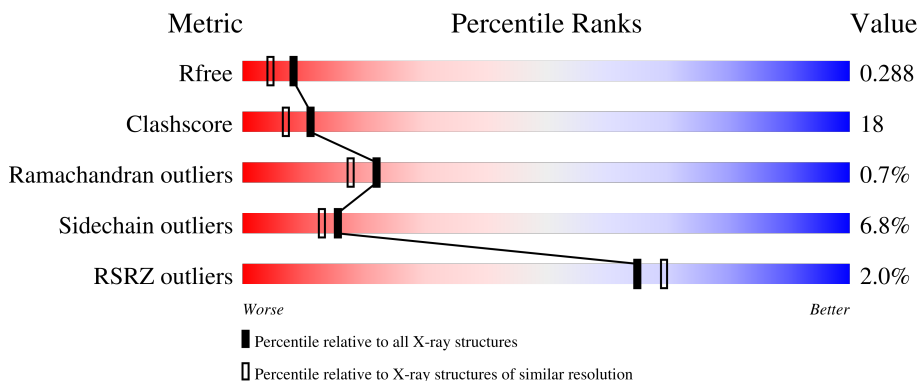
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



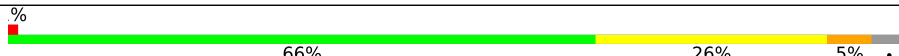
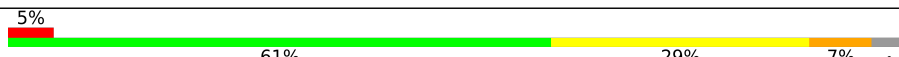
The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	
1	B	282	
1	C	282	
1	D	282	

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	A	4	-	-	X	-
2	SO4	B	8	-	-	X	-
2	SO4	C	6	-	-	X	-

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 8589 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 chorismate mutase and shikimate 5-dehydrogenase fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	Total 2128	C 1375	N 336	O 410	S 7	0	1	0
1	B	267	Total 2081	C 1347	N 331	O 396	S 7	0	0	0
1	C	270	Total 2090	C 1350	N 330	O 403	S 7	0	0	0
1	D	272	Total 2092	C 1355	N 334	O 396	S 7	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

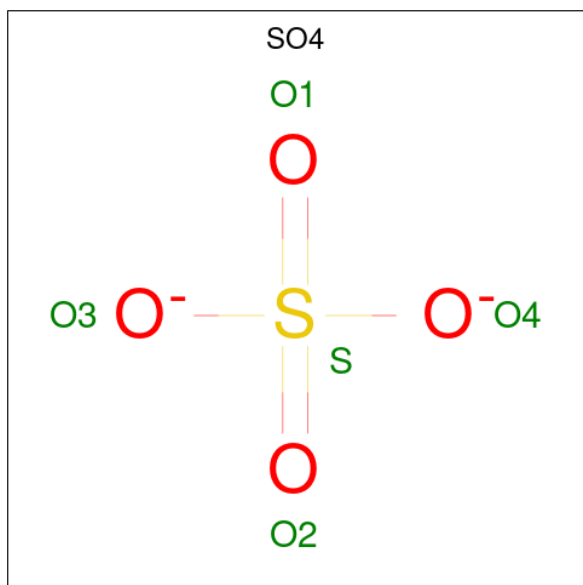
Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MET	-	expression tag	UNP Q97KM0
A	95	SER	-	expression tag	UNP Q97KM0
A	96	LEU	-	expression tag	UNP Q97KM0
A	368	GLU	-	expression tag	UNP Q97KM0
A	369	GLY	-	expression tag	UNP Q97KM0
A	370	HIS	-	expression tag	UNP Q97KM0
A	371	HIS	-	expression tag	UNP Q97KM0
A	372	HIS	-	expression tag	UNP Q97KM0
A	373	HIS	-	expression tag	UNP Q97KM0
A	374	HIS	-	expression tag	UNP Q97KM0
A	375	HIS	-	expression tag	UNP Q97KM0
B	94	MET	-	expression tag	UNP Q97KM0
B	95	SER	-	expression tag	UNP Q97KM0
B	96	LEU	-	expression tag	UNP Q97KM0
B	368	GLU	-	expression tag	UNP Q97KM0
B	369	GLY	-	expression tag	UNP Q97KM0
B	370	HIS	-	expression tag	UNP Q97KM0
B	371	HIS	-	expression tag	UNP Q97KM0
B	372	HIS	-	expression tag	UNP Q97KM0
B	373	HIS	-	expression tag	UNP Q97KM0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	374	HIS	-	expression tag	UNP Q97KM0
B	375	HIS	-	expression tag	UNP Q97KM0
C	94	MET	-	expression tag	UNP Q97KM0
C	95	SER	-	expression tag	UNP Q97KM0
C	96	LEU	-	expression tag	UNP Q97KM0
C	368	GLU	-	expression tag	UNP Q97KM0
C	369	GLY	-	expression tag	UNP Q97KM0
C	370	HIS	-	expression tag	UNP Q97KM0
C	371	HIS	-	expression tag	UNP Q97KM0
C	372	HIS	-	expression tag	UNP Q97KM0
C	373	HIS	-	expression tag	UNP Q97KM0
C	374	HIS	-	expression tag	UNP Q97KM0
C	375	HIS	-	expression tag	UNP Q97KM0
D	94	MET	-	expression tag	UNP Q97KM0
D	95	SER	-	expression tag	UNP Q97KM0
D	96	LEU	-	expression tag	UNP Q97KM0
D	368	GLU	-	expression tag	UNP Q97KM0
D	369	GLY	-	expression tag	UNP Q97KM0
D	370	HIS	-	expression tag	UNP Q97KM0
D	371	HIS	-	expression tag	UNP Q97KM0
D	372	HIS	-	expression tag	UNP Q97KM0
D	373	HIS	-	expression tag	UNP Q97KM0
D	374	HIS	-	expression tag	UNP Q97KM0
D	375	HIS	-	expression tag	UNP Q97KM0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

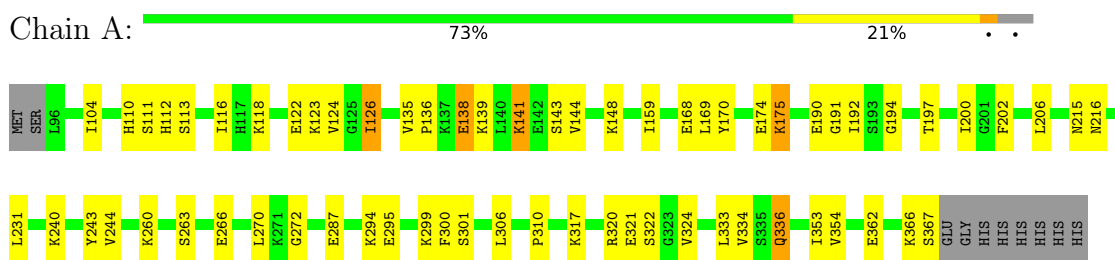
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	62	Total O 62 62	0	0
3	B	50	Total O 50 50	0	0
3	C	20	Total O 20 20	0	0
3	D	21	Total O 21 21	0	0

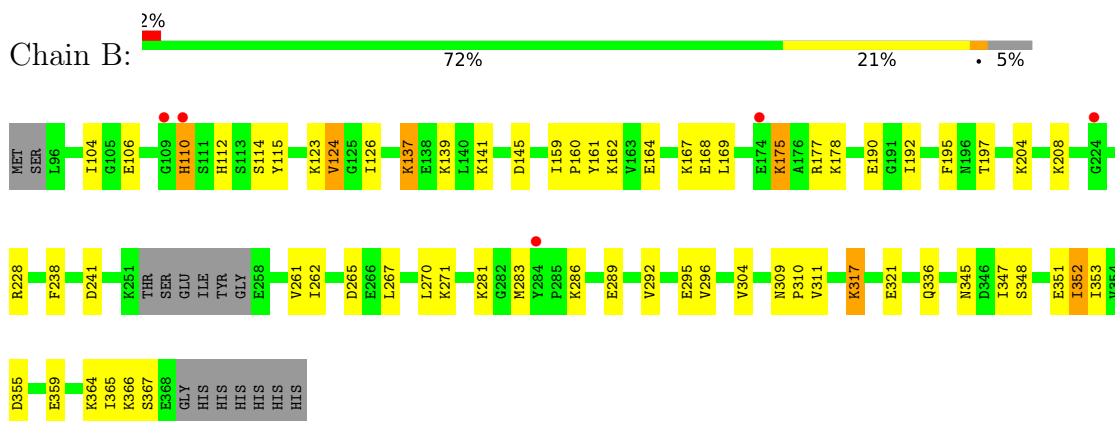
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

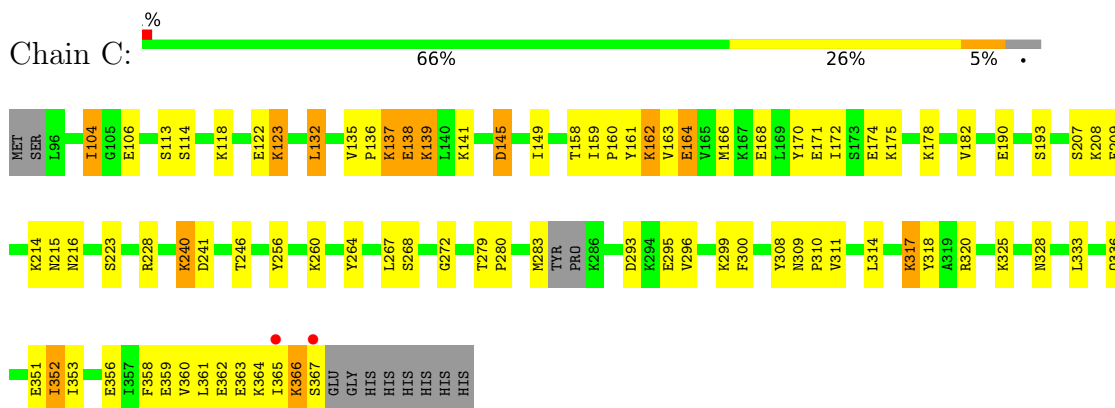
- Molecule 1: chorismate mutase and shikimate 5-dehydrogenase fusion protein



- Molecule 1: chorismate mutase and shikimate 5-dehydrogenase fusion protein

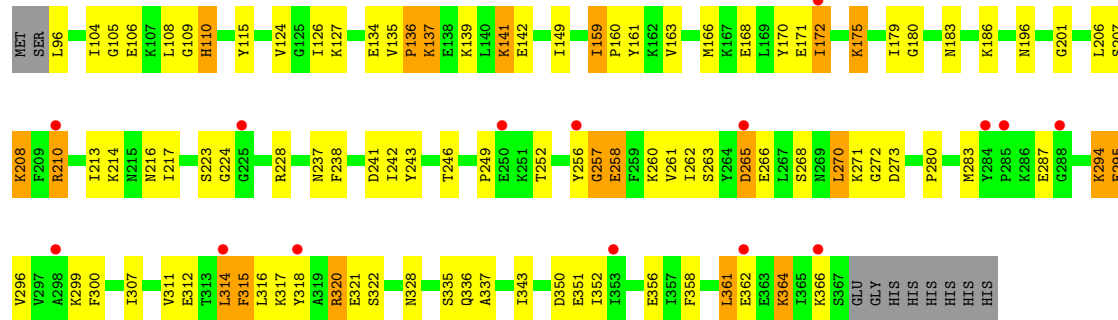


- Molecule 1: chorismate mutase and shikimate 5-dehydrogenase fusion protein



- Molecule 1: chorismate mutase and shikimate 5-dehydrogenase fusion protein

Chain D:  5% 61% 29% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.13Å 135.34Å 67.14Å 90.00° 102.14° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 48.07 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-2.10) 94.2 (48.07-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.10Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.233 , 0.299 0.230 , 0.288	Depositor DCC
R_{free} test set	3157 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtrriage
Anisotropy	0.156	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.019 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8589	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.03	0/2168	0.93	1/2922 (0.0%)
1	B	1.00	1/2116 (0.0%)	0.92	0/2850
1	C	0.88	0/2123	0.85	0/2861
1	D	0.84	1/2128 (0.0%)	0.86	1/2872 (0.0%)
All	All	0.94	2/8535 (0.0%)	0.89	2/11505 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	VAL	CB-CG1	6.48	1.66	1.52
1	D	337	ALA	CA-CB	5.23	1.63	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	ILE	CB-CA-C	-5.45	100.69	111.60
1	A	306	LEU	CB-CG-CD2	-5.21	102.15	111.00

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	2128	0	2151	58	0
1	B	2081	0	2112	61	0
1	C	2090	0	2108	91	0
1	D	2092	0	2104	97	0
2	A	15	0	0	3	0
2	B	10	0	0	6	0
2	C	10	0	0	4	0
2	D	10	0	0	0	0
3	A	62	0	0	8	0
3	B	50	0	0	3	0
3	C	20	0	0	0	0
3	D	21	0	0	1	0
All	All	8589	0	8475	302	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 18.

All (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:GLU:OE1	1:C:137:LYS:HD2	1.27	1.35
1:A:112:HIS:O	1:A:116:ILE:HD12	1.22	1.34
1:D:170:TYR:CE2	1:D:171:GLU:HG3	1.64	1.31
1:C:314:LEU:HD12	1:C:317:LYS:HZ3	1.08	1.19
1:C:106:GLU:OE1	1:C:137:LYS:CD	1.94	1.15
1:B:352:ILE:H	1:B:352:ILE:HD13	1.08	1.09
1:C:162:LYS:HB2	2:C:6:SO4:O1	1.56	1.04
1:A:175:LYS:HE2	1:A:175:LYS:CA	1.87	1.02
1:D:170:TYR:HE2	1:D:171:GLU:HG3	1.25	0.99
1:C:314:LEU:HD12	1:C:317:LYS:NZ	1.75	0.99
1:B:238:PHE:CE1	1:D:366:LYS:HD3	1.98	0.98
1:B:106:GLU:OE1	1:B:137:LYS:HD3	1.63	0.98
1:A:104:ILE:HD11	1:A:135:VAL:HG21	1.44	0.96
1:A:104:ILE:CD1	1:A:135:VAL:HG21	1.94	0.96
1:B:352:ILE:N	1:B:352:ILE:HD13	1.80	0.96
1:A:112:HIS:O	1:A:116:ILE:CD1	2.15	0.95
1:C:159:ILE:CG2	1:C:160:PRO:CA	2.47	0.93
1:B:352:ILE:CD1	1:B:352:ILE:H	1.81	0.92
1:C:159:ILE:HG23	1:C:160:PRO:HA	1.49	0.92
1:C:352:ILE:HD12	1:C:353:ILE:HG13	1.51	0.91
1:A:118:LYS:NZ	1:A:122:GLU:OE2	2.03	0.91
1:C:141:LYS:HG3	1:C:168:GLU:OE1	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ILE:CG2	1:C:160:PRO:HA	2.01	0.91
1:C:159:ILE:HG22	1:C:160:PRO:CA	2.00	0.90
1:C:317:LYS:HG3	1:C:320:ARG:HH21	1.36	0.90
1:D:170:TYR:CE2	1:D:171:GLU:CG	2.54	0.89
1:C:159:ILE:HG22	1:C:160:PRO:CB	2.03	0.88
1:C:159:ILE:HG22	1:C:160:PRO:HB3	1.54	0.88
1:B:106:GLU:OE1	1:B:137:LYS:CD	2.22	0.87
1:C:314:LEU:CD1	1:C:317:LYS:NZ	2.39	0.86
1:A:112:HIS:C	1:A:116:ILE:HD12	1.97	0.85
1:C:361:LEU:O	1:C:365:ILE:HG12	1.77	0.84
1:D:210:ARG:HH11	1:D:210:ARG:HG3	1.40	0.84
1:D:263:SER:OG	1:D:266:GLU:HG3	1.79	0.82
1:D:261:VAL:O	1:D:262:ILE:HG22	1.80	0.81
1:B:112:HIS:N	3:B:19:HOH:O	2.07	0.81
1:B:159:ILE:CD1	2:B:8:SO4:O3	2.30	0.80
1:A:334:VAL:HG12	1:A:354:VAL:HG13	1.64	0.80
1:D:311:VAL:O	1:D:328:ASN:ND2	2.15	0.80
1:B:352:ILE:CD1	1:B:352:ILE:N	2.44	0.78
1:A:148:LYS:HD3	1:A:192:ILE:HG13	1.64	0.78
1:A:141:LYS:HG3	1:A:168:GLU:OE2	1.84	0.78
1:D:179:ILE:HG23	1:D:228:ARG:HB3	1.65	0.78
1:C:317:LYS:HG3	1:C:320:ARG:NH2	1.98	0.78
1:D:170:TYR:CD2	1:D:171:GLU:HG3	2.20	0.77
1:A:175:LYS:N	1:A:175:LYS:HE2	2.00	0.77
1:A:299:LYS:HD2	3:A:377:HOH:O	1.85	0.77
1:A:294:LYS:HE2	1:A:322:SER:OG	1.86	0.76
1:C:104:ILE:HD11	1:C:135:VAL:HB	1.66	0.76
1:B:311:VAL:HG13	1:B:365:ILE:CG2	2.15	0.76
1:D:109:GLY:O	1:D:110:HIS:C	2.24	0.76
1:B:162:LYS:NZ	3:B:409:HOH:O	2.17	0.75
1:D:287:GLU:O	1:D:287:GLU:HG2	1.84	0.75
1:D:261:VAL:O	1:D:262:ILE:CG2	2.34	0.75
1:A:104:ILE:HD11	1:A:135:VAL:CG2	2.16	0.75
1:C:159:ILE:CG2	1:C:160:PRO:HB3	2.18	0.74
1:A:174:GLU:HB3	3:A:31:HOH:O	1.86	0.74
1:B:159:ILE:HD13	2:B:8:SO4:S	2.28	0.74
1:A:124:VAL:CG2	1:A:126:ILE:HG13	2.18	0.74
1:C:308:TYR:CZ	1:C:333:LEU:HD22	2.23	0.73
1:D:210:ARG:HH11	1:D:210:ARG:CG	2.01	0.73
1:A:362:GLU:O	1:A:366:LYS:HG3	1.88	0.73
1:D:170:TYR:CD2	1:D:171:GLU:CG	2.72	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:LYS:HE2	1:D:322:SER:OG	1.90	0.72
1:C:314:LEU:CD1	1:C:317:LYS:HZ3	1.93	0.72
1:C:364:LYS:O	1:C:367:SER:HB2	1.90	0.71
1:D:294:LYS:CE	1:D:322:SER:OG	2.39	0.71
1:A:175:LYS:HA	1:A:175:LYS:HE2	1.73	0.70
1:B:281:LYS:HG2	1:B:289:GLU:OE1	1.92	0.70
1:A:104:ILE:CD1	1:A:135:VAL:CG2	2.70	0.69
1:B:164:GLU:OE1	1:B:167:LYS:HE2	1.92	0.69
1:B:311:VAL:HG13	1:B:365:ILE:HG22	1.74	0.69
1:B:169:LEU:HD22	1:B:192:ILE:HG22	1.75	0.68
1:D:106:GLU:OE1	1:D:137:LYS:HE3	1.94	0.67
1:A:148:LYS:HD2	1:A:191:GLY:HA2	1.77	0.67
1:B:159:ILE:HD13	2:B:8:SO4:O3	1.95	0.67
1:C:106:GLU:OE1	1:C:137:LYS:NZ	2.28	0.67
1:C:159:ILE:CG2	1:C:160:PRO:CB	2.70	0.66
1:A:299:LYS:CE	3:A:377:HOH:O	2.44	0.66
1:C:163:VAL:HG23	2:C:6:SO4:O3	1.96	0.66
1:C:123:LYS:HE2	1:C:356:GLU:OE1	1.95	0.66
1:C:159:ILE:HG22	1:C:160:PRO:N	2.08	0.66
1:D:261:VAL:C	1:D:262:ILE:CG2	2.65	0.66
1:C:137:LYS:HG3	1:C:161:TYR:OH	1.97	0.65
1:A:104:ILE:HD12	1:A:135:VAL:HG21	1.76	0.65
1:D:243:TYR:CE1	1:D:260:LYS:HD3	2.32	0.64
1:D:295:GLU:HG3	1:D:296:VAL:N	2.09	0.64
1:A:123:LYS:HD2	1:A:353:ILE:HG23	1.78	0.64
1:A:317:LYS:O	1:A:320:ARG:N	2.31	0.64
1:B:124:VAL:HG22	1:B:126:ILE:HD12	1.79	0.64
1:C:314:LEU:CD1	1:C:317:LYS:HZ1	2.10	0.63
1:A:110:HIS:ND1	1:A:111:SER:N	2.47	0.62
1:B:137:LYS:HG3	1:B:161:TYR:HE1	1.64	0.62
1:B:317:LYS:O	1:B:321:GLU:HG3	1.99	0.62
1:C:106:GLU:CD	1:C:137:LYS:HD2	2.18	0.62
1:C:293:ASP:HB2	1:C:295:GLU:HG2	1.81	0.62
1:C:162:LYS:HB2	2:C:6:SO4:S	2.40	0.61
1:D:261:VAL:C	1:D:262:ILE:HG23	2.19	0.61
1:A:136:PRO:HG2	1:A:139:LYS:HG3	1.83	0.61
1:B:104:ILE:O	1:B:104:ILE:HG23	2.01	0.60
1:B:311:VAL:HG13	1:B:365:ILE:HG21	1.82	0.60
1:B:123:LYS:HB3	1:B:353:ILE:HD12	1.81	0.60
1:B:164:GLU:OE1	1:B:167:LYS:CE	2.49	0.60
1:D:108:LEU:N	1:D:134:GLU:OE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:PRO:HD2	1:D:139:LYS:HB2	1.84	0.59
1:C:159:ILE:HG23	1:C:160:PRO:CA	2.21	0.59
1:B:106:GLU:OE1	1:B:137:LYS:NZ	2.31	0.59
1:B:124:VAL:CG2	1:B:126:ILE:HD12	2.33	0.59
1:D:109:GLY:O	1:D:110:HIS:O	2.21	0.59
1:A:299:LYS:HE3	3:A:377:HOH:O	2.02	0.59
1:D:106:GLU:OE1	1:D:137:LYS:CE	2.51	0.58
1:D:217:ILE:N	1:D:273:ASP:OD2	2.24	0.58
1:B:175:LYS:HD3	1:B:178:LYS:NZ	2.19	0.58
1:A:299:LYS:CD	3:A:377:HOH:O	2.49	0.57
1:C:106:GLU:OE1	1:C:137:LYS:CE	2.52	0.57
1:C:365:ILE:C	1:C:367:SER:H	2.07	0.57
1:D:311:VAL:HG23	1:D:312:GLU:N	2.19	0.57
1:D:208:LYS:HB2	1:D:208:LYS:NZ	2.20	0.57
1:C:209:PHE:O	1:C:325:LYS:HE2	2.05	0.57
1:C:164:GLU:OE2	1:C:164:GLU:HA	2.03	0.57
1:D:280:PRO:O	1:D:283:MET:HG2	2.05	0.56
1:A:141:LYS:CG	1:A:168:GLU:OE2	2.52	0.56
1:B:238:PHE:CE1	1:D:366:LYS:CD	2.82	0.56
1:D:314:LEU:HD12	1:D:317:LYS:HG2	1.86	0.56
1:C:358:PHE:O	1:C:362:GLU:HB2	2.06	0.56
1:B:345:ASN:O	1:B:347:ILE:HG23	2.05	0.55
1:C:241:ASP:OD2	1:C:260:LYS:NZ	2.36	0.55
1:C:139:LYS:HG3	1:D:149:ILE:HD11	1.87	0.55
1:C:280:PRO:O	1:C:283:MET:HG2	2.07	0.55
1:C:166:MET:CE	1:C:172:ILE:CD1	2.86	0.54
1:A:200:ILE:HD11	2:A:9:SO4:O3	2.06	0.54
1:C:314:LEU:HD13	1:C:317:LYS:HZ1	1.71	0.54
1:D:179:ILE:CG2	1:D:228:ARG:HB3	2.37	0.54
1:D:352:ILE:O	1:D:356:GLU:HG3	2.08	0.54
1:D:166:MET:HE3	1:D:172:ILE:HD13	1.91	0.53
1:D:137:LYS:HD2	1:D:161:TYR:CE1	2.44	0.53
1:B:295:GLU:HG3	1:B:296:VAL:N	2.22	0.53
1:A:159:ILE:HD13	2:A:4:SO4:S	2.48	0.53
1:D:137:LYS:HD2	1:D:161:TYR:HE1	1.74	0.53
1:D:317:LYS:O	1:D:321:GLU:HG3	2.08	0.53
1:C:166:MET:HE2	1:C:172:ILE:HD12	1.90	0.53
1:D:256:TYR:O	1:D:257:GLY:C	2.48	0.52
1:D:317:LYS:HB2	1:D:320:ARG:HH21	1.73	0.52
1:C:174:GLU:O	1:C:178:LYS:HG3	2.10	0.52
1:B:124:VAL:CG2	1:B:126:ILE:CD1	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ASP:O	1:C:149:ILE:HG12	2.10	0.52
1:C:293:ASP:CB	1:C:295:GLU:HG2	2.39	0.52
1:C:309:ASN:HA	1:C:310:PRO:C	2.28	0.52
1:D:163:VAL:HG22	1:D:180:GLY:O	2.09	0.52
1:A:118:LYS:CE	1:A:122:GLU:OE2	2.57	0.52
1:A:138:GLU:H	1:A:138:GLU:CD	2.12	0.52
1:A:287:GLU:OE2	1:A:310:PRO:HG3	2.11	0.51
1:D:270:LEU:HD12	1:D:271:LYS:O	2.10	0.51
1:D:287:GLU:O	1:D:287:GLU:CG	2.55	0.51
1:B:159:ILE:HD11	2:B:8:SO4:O3	2.10	0.51
1:D:362:GLU:OE1	1:D:366:LYS:HE3	2.10	0.51
1:D:314:LEU:O	1:D:315:PHE:C	2.47	0.51
1:D:268:SER:O	1:D:299:LYS:NZ	2.44	0.51
1:C:208:LYS:NZ	1:C:351:GLU:OE2	2.28	0.51
1:D:243:TYR:CE1	1:D:260:LYS:CD	2.94	0.51
1:B:160:PRO:HA	2:B:8:SO4:O4	2.11	0.50
1:B:283:MET:O	1:B:286:LYS:N	2.43	0.50
1:C:170:TYR:O	1:C:170:TYR:CD2	2.64	0.50
1:C:228:ARG:HG3	1:C:256:TYR:OH	2.12	0.50
1:B:141:LYS:HD2	1:B:145:ASP:OD2	2.11	0.50
1:C:118:LYS:O	1:C:122:GLU:HG3	2.12	0.50
1:D:223:SER:HB2	1:D:256:TYR:CE2	2.47	0.50
1:D:246:THR:HG21	1:D:252:THR:CB	2.42	0.49
1:A:317:LYS:HG3	1:A:320:ARG:NH2	2.27	0.49
1:D:256:TYR:O	1:D:258:GLU:N	2.45	0.49
1:C:352:ILE:CD1	1:C:353:ILE:HG13	2.34	0.49
1:C:170:TYR:CE2	1:C:171:GLU:HB2	2.48	0.49
1:D:141:LYS:HG2	1:D:168:GLU:OE1	2.12	0.49
1:D:246:THR:HG21	1:D:252:THR:OG1	2.12	0.49
1:C:308:TYR:CE2	1:C:333:LEU:HD22	2.47	0.48
1:C:268:SER:O	1:C:299:LYS:NZ	2.45	0.48
1:D:243:TYR:CZ	1:D:260:LYS:HD2	2.48	0.48
1:C:214:LYS:O	1:C:215:ASN:HB2	2.13	0.48
1:D:358:PHE:O	1:D:362:GLU:HB2	2.14	0.48
1:A:333:LEU:HD12	3:A:65:HOH:O	2.14	0.48
1:A:148:LYS:HD3	1:A:192:ILE:CG1	2.40	0.48
1:C:137:LYS:HG3	1:C:161:TYR:CZ	2.49	0.48
1:A:159:ILE:HD13	2:A:4:SO4:O3	2.14	0.47
1:D:362:GLU:OE2	1:D:366:LYS:HE3	2.13	0.47
1:A:202:PHE:CE2	1:A:206:LEU:HD11	2.50	0.47
1:D:228:ARG:HG3	1:D:256:TYR:OH	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:LYS:HD3	1:D:364:LYS:C	2.34	0.47
1:D:186:LYS:NZ	1:D:343:ILE:O	2.43	0.47
1:B:238:PHE:HE1	1:D:366:LYS:HD3	1.69	0.47
1:A:243:TYR:CE1	1:A:260:LYS:HD3	2.50	0.47
1:C:132:LEU:N	1:C:132:LEU:HD23	2.30	0.47
1:B:175:LYS:HD3	1:B:178:LYS:HZ1	1.79	0.47
1:D:183:ASN:OD1	1:D:196:ASN:HA	2.15	0.46
1:D:272:GLY:HA3	1:D:300:PHE:CE1	2.49	0.46
1:B:281:LYS:CG	1:B:289:GLU:OE1	2.63	0.46
1:A:175:LYS:CE	1:A:175:LYS:HA	2.39	0.46
1:C:162:LYS:HG3	1:C:182:VAL:O	2.15	0.46
1:D:307:ILE:O	1:D:328:ASN:HB2	2.14	0.46
1:C:137:LYS:HG3	1:C:161:TYR:CE1	2.50	0.46
1:D:210:ARG:NH1	1:D:210:ARG:CG	2.69	0.46
1:A:231:LEU:HD21	1:A:244:VAL:HG22	1.98	0.46
1:D:208:LYS:HE3	1:D:208:LYS:CA	2.45	0.46
1:A:263:SER:OG	1:A:266:GLU:HG3	2.16	0.46
1:B:104:ILE:O	1:B:104:ILE:CG2	2.62	0.46
1:B:355:ASP:O	1:B:359:GLU:HG3	2.16	0.46
1:D:265:ASP:O	1:D:266:GLU:C	2.55	0.46
1:C:170:TYR:C	1:C:170:TYR:CD2	2.89	0.46
1:C:328:ASN:C	1:C:328:ASN:OD1	2.55	0.46
1:D:207:SER:O	1:D:210:ARG:HD2	2.15	0.46
1:B:115:TYR:CD2	1:B:364:LYS:HE3	2.51	0.46
1:C:175:LYS:HA	1:C:175:LYS:HD3	1.61	0.45
1:D:270:LEU:HD12	1:D:271:LYS:N	2.31	0.45
1:D:104:ILE:HD11	1:D:135:VAL:HG21	1.98	0.45
1:B:270:LEU:HG	1:B:271:LYS:N	2.30	0.45
1:D:314:LEU:O	1:D:317:LYS:N	2.32	0.45
1:D:96:LEU:HA	3:D:8:HOH:O	2.16	0.45
1:B:110:HIS:CD2	1:B:110:HIS:C	2.90	0.45
1:B:195:PHE:CD2	1:B:195:PHE:N	2.84	0.45
1:D:223:SER:HB2	1:D:256:TYR:HE2	1.82	0.45
1:B:228:ARG:HB2	3:B:376:HOH:O	2.17	0.45
1:C:214:LYS:O	1:C:216:ASN:ND2	2.49	0.45
1:D:294:LYS:HE3	1:D:322:SER:OG	2.13	0.45
1:D:141:LYS:HG2	1:D:168:GLU:CD	2.38	0.44
1:D:170:TYR:CD2	1:D:171:GLU:HG2	2.51	0.44
1:D:311:VAL:CG2	1:D:312:GLU:N	2.80	0.44
1:C:308:TYR:CZ	1:C:333:LEU:CD2	2.97	0.44
1:C:139:LYS:HG3	1:D:149:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:GLY:HA2	1:D:335:SER:HB2	1.98	0.44
1:D:350:ASP:OD2	1:D:352:ILE:HG12	2.17	0.44
1:D:362:GLU:CD	1:D:366:LYS:HE3	2.38	0.44
1:C:139:LYS:HD2	1:C:139:LYS:HA	1.44	0.44
1:B:309:ASN:HA	1:B:310:PRO:C	2.38	0.44
1:A:144:VAL:HG13	1:A:192:ILE:HD13	2.00	0.44
1:B:141:LYS:HE3	1:B:141:LYS:HB3	1.77	0.44
1:D:314:LEU:O	1:D:316:LEU:N	2.51	0.44
1:C:166:MET:HE3	1:C:172:ILE:CD1	2.47	0.44
1:C:216:ASN:N	1:C:216:ASN:HD22	2.16	0.44
1:D:159:ILE:HA	1:D:160:PRO:HA	1.87	0.44
1:D:364:LYS:O	1:D:364:LYS:HD3	2.18	0.44
1:A:272:GLY:O	1:A:300:PHE:HA	2.18	0.44
1:C:223:SER:HB2	1:C:256:TYR:HE2	1.83	0.44
1:D:175:LYS:HD3	1:D:175:LYS:HA	1.41	0.44
1:A:334:VAL:CG1	1:A:354:VAL:HG13	2.44	0.43
1:D:124:VAL:HG23	1:D:124:VAL:O	2.18	0.43
1:D:105:GLY:HA3	1:D:108:LEU:HD21	2.00	0.43
1:A:174:GLU:N	3:A:31:HOH:O	2.51	0.43
1:D:216:ASN:HB3	1:D:273:ASP:HB2	2.01	0.43
1:A:216:ASN:O	1:A:240:LYS:N	2.44	0.43
1:A:197:THR:OG1	1:A:336:GLN:HG2	2.18	0.43
1:B:175:LYS:HA	1:B:175:LYS:HD3	1.79	0.43
1:B:177:ARG:O	1:B:177:ARG:HG2	2.18	0.43
1:C:314:LEU:HD11	1:C:318:TYR:CE1	2.54	0.43
1:C:279:THR:HB	1:C:280:PRO:HD2	2.00	0.43
1:C:365:ILE:C	1:C:367:SER:N	2.72	0.43
1:D:106:GLU:OE1	1:D:137:LYS:CD	2.66	0.43
1:B:204:LYS:HD3	1:B:204:LYS:HA	1.81	0.43
1:B:208:LYS:NZ	1:B:351:GLU:OE2	2.44	0.43
1:A:104:ILE:HD11	1:A:135:VAL:CB	2.49	0.42
1:B:261:VAL:O	1:B:262:ILE:CG2	2.67	0.42
1:B:317:LYS:HB2	1:B:317:LYS:HE2	1.56	0.42
1:C:208:LYS:HA	1:C:208:LYS:HD3	1.84	0.42
1:B:267:LEU:HD21	1:B:292:VAL:HG11	2.01	0.42
1:C:166:MET:HE3	1:C:172:ILE:HD11	2.01	0.42
1:C:352:ILE:HG13	1:C:352:ILE:H	1.65	0.42
1:A:169:LEU:HD13	1:A:194:GLY:HA3	2.01	0.42
1:C:359:GLU:O	1:C:363:GLU:HG2	2.20	0.42
1:D:246:THR:CG2	1:D:249:PRO:HA	2.50	0.42
1:B:139:LYS:HA	1:B:139:LYS:HD3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ILE:HD11	1:C:135:VAL:CB	2.43	0.42
1:C:159:ILE:CG2	1:C:160:PRO:N	2.77	0.42
1:A:124:VAL:HG23	1:A:126:ILE:HG13	2.00	0.42
1:D:126:ILE:HG22	1:D:127:LYS:N	2.35	0.42
1:A:124:VAL:O	1:A:124:VAL:HG23	2.20	0.41
1:A:333:LEU:CD1	3:A:65:HOH:O	2.67	0.41
1:D:237:ASN:O	1:D:238:PHE:HB2	2.19	0.41
1:A:301:SER:C	1:A:324:VAL:HG13	2.40	0.41
1:B:197:THR:OG1	1:B:336:GLN:HG2	2.19	0.41
1:C:295:GLU:CG	1:C:296:VAL:N	2.82	0.41
1:C:166:MET:HE2	1:C:172:ILE:CD1	2.49	0.41
1:C:366:LYS:HB3	1:C:366:LYS:HE3	1.79	0.41
1:D:317:LYS:HG3	1:D:318:TYR:N	2.35	0.41
1:A:113:SER:HA	1:A:116:ILE:CD1	2.51	0.41
1:A:170:TYR:CE1	1:A:190:GLU:HB2	2.55	0.41
1:C:240:LYS:HB2	1:C:240:LYS:HE2	1.59	0.41
1:C:158:THR:HG23	1:C:159:ILE:N	2.35	0.41
1:D:317:LYS:O	1:D:321:GLU:N	2.49	0.41
1:C:360:VAL:O	1:C:363:GLU:HB2	2.21	0.41
1:C:160:PRO:HA	2:C:6:SO4:O2	2.21	0.41
1:D:127:LYS:HB3	1:D:127:LYS:HE3	1.83	0.41
1:B:190:GLU:CG	1:B:190:GLU:O	2.69	0.41
1:D:166:MET:CE	1:D:172:ILE:HD13	2.50	0.41
1:B:175:LYS:HD3	1:B:178:LYS:HZ2	1.86	0.41
1:C:352:ILE:HD12	1:C:353:ILE:N	2.36	0.40
1:A:113:SER:HA	1:A:116:ILE:HD13	2.04	0.40
1:B:366:LYS:O	1:B:367:SER:C	2.59	0.40
1:C:136:PRO:HB3	1:C:138:GLU:OE2	2.21	0.40
1:C:264:TYR:O	1:C:267:LEU:HB3	2.22	0.40
1:B:190:GLU:O	1:B:190:GLU:HG2	2.21	0.40
1:D:206:LEU:HD13	1:D:213:ILE:HD11	2.04	0.40
1:D:115:TYR:CD2	1:D:361:LEU:HD21	2.57	0.40
1:B:159:ILE:CD1	2:B:8:SO4:S	3.01	0.40
1:C:272:GLY:O	1:C:300:PHE:HA	2.21	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	271/282 (96%)	263 (97%)	7 (3%)	1 (0%)	34	32
1	B	263/282 (93%)	255 (97%)	8 (3%)	0	100	100
1	C	266/282 (94%)	258 (97%)	8 (3%)	0	100	100
1	D	270/282 (96%)	241 (89%)	23 (8%)	6 (2%)	6	2
All	All	1070/1128 (95%)	1017 (95%)	46 (4%)	7 (1%)	22	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	315	PHE
1	D	110	HIS
1	D	257	GLY
1	D	314	LEU
1	D	351	GLU
1	A	321	GLU
1	D	224	GLY

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	234/247 (95%)	224 (96%)	10 (4%)	29	29
1	B	228/247 (92%)	217 (95%)	11 (5%)	25	24
1	C	228/247 (92%)	207 (91%)	21 (9%)	9	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	224/247 (91%)	204 (91%)	20 (9%)	9	6
All	All	914/988 (92%)	852 (93%)	62 (7%)	16	13

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ILE
1	A	138	GLU
1	A	141	LYS
1	A	143	SER
1	A	175	LYS
1	A	215	ASN
1	A	270	LEU
1	A	295	GLU
1	A	336	GLN
1	A	367	SER
1	B	110	HIS
1	B	114	SER
1	B	124	VAL
1	B	137	LYS
1	B	168	GLU
1	B	175	LYS
1	B	241	ASP
1	B	265	ASP
1	B	317	LYS
1	B	348	SER
1	B	352	ILE
1	C	104	ILE
1	C	113	SER
1	C	114	SER
1	C	123	LYS
1	C	132	LEU
1	C	137	LYS
1	C	138	GLU
1	C	139	LYS
1	C	145	ASP
1	C	162	LYS
1	C	164	GLU
1	C	190	GLU
1	C	193	SER
1	C	207	SER
1	C	240	LYS

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Mol	Chain	Res	Type
1	C	246	THR
1	C	311	VAL
1	C	317	LYS
1	C	336	GLN
1	C	352	ILE
1	C	366	LYS
1	D	136	PRO
1	D	137	LYS
1	D	141	LYS
1	D	142	GLU
1	D	159	ILE
1	D	172	ILE
1	D	175	LYS
1	D	208	LYS
1	D	210	ARG
1	D	214	LYS
1	D	241	ASP
1	D	258	GLU
1	D	265	ASP
1	D	270	LEU
1	D	294	LYS
1	D	295	GLU
1	D	320	ARG
1	D	336	GLN
1	D	361	LEU
1	D	364	LYS

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

Mol	Chain	Res	Type
1	B	110	HIS
1	B	112	HIS
1	B	216	ASN
1	B	237	ASN
1	B	345	ASN
1	C	215	ASN
1	D	112	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	C	1	-	4,4,4	0.35	0	6,6,6	0.50	0
2	SO4	D	10	-	4,4,4	0.16	0	6,6,6	0.48	0
2	SO4	A	4	-	4,4,4	0.30	0	6,6,6	1.13	1 (16%)
2	SO4	A	9	-	4,4,4	0.27	0	6,6,6	1.30	1 (16%)
2	SO4	D	11	-	4,4,4	0.24	0	6,6,6	0.23	0
2	SO4	B	8	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	B	3	-	4,4,4	0.27	0	6,6,6	0.75	0
2	SO4	A	2	-	4,4,4	0.35	0	6,6,6	0.96	0
2	SO4	C	6	-	4,4,4	0.21	0	6,6,6	0.30	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4	SO4	O4-S-O3	2.39	119.25	109.06
2	A	9	SO4	O4-S-O3	-2.13	99.98	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4	SO4	2	0
2	A	9	SO4	1	0
2	B	8	SO4	6	0
2	C	6	SO4	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	272/282 (96%)	0.38	0 100 100	33, 47, 59, 74	0
1	B	267/282 (94%)	0.27	5 (1%) 66 71	34, 46, 60, 70	0
1	C	270/282 (95%)	0.26	2 (0%) 87 89	37, 50, 64, 71	0
1	D	272/282 (96%)	0.51	15 (5%) 25 31	37, 56, 73, 82	0
All	All	1081/1128 (95%)	0.36	22 (2%) 65 69	33, 49, 66, 82	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	256	TYR	6.6
1	D	288	GLY	5.5
1	B	109	GLY	3.5
1	D	314	LEU	3.1
1	D	284	TYR	2.9
1	D	362	GLU	2.8
1	D	265	ASP	2.7
1	D	285	PRO	2.6
1	C	365	ILE	2.5
1	B	110	HIS	2.5
1	C	367	SER	2.4
1	B	284	TYR	2.3
1	D	225	GLY	2.3
1	D	353	ILE	2.1
1	B	174	GLU	2.1
1	D	210	ARG	2.1
1	B	224	GLY	2.1
1	D	250	GLU	2.1
1	D	298	ALA	2.1
1	D	318	TYR	2.0
1	D	172	ILE	2.0
1	D	366	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	D	11	5/5	0.92	0.11	76,76,80,81	0
2	SO4	D	10	5/5	0.94	0.20	72,73,78,79	0
2	SO4	A	9	5/5	0.95	0.18	57,62,65,67	0
2	SO4	B	8	5/5	0.95	0.16	75,75,78,78	0
2	SO4	C	6	5/5	0.96	0.18	70,70,72,73	0
2	SO4	B	3	5/5	0.97	0.15	52,54,58,64	0
2	SO4	A	4	5/5	0.97	0.13	44,57,60,62	0
2	SO4	A	2	5/5	0.98	0.14	41,46,51,54	0
2	SO4	C	1	5/5	0.98	0.17	52,53,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.