Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:41 pm BST

PDB ID	:	2EUA
Title	:	Structure and Mechanism of MenF, the Menaquinone-Specific Isochorismate Synthase from Escherichia Coli
Authors	:	Kolappan, S.; Kisker, C.; Zwahlen, J.; Zhou, R.; Tonge, P.J.
Deposited on	:	2005-10-28
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

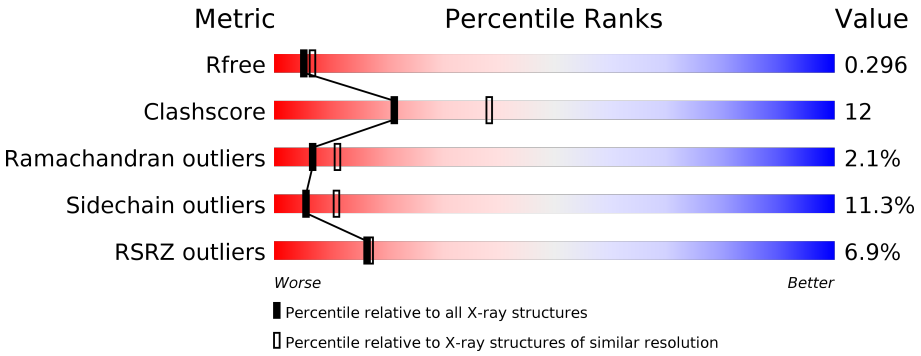
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 <=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	431	3% 74% 19% 6%
1	B	431	11% 76% 18% 5%

2 Entry composition

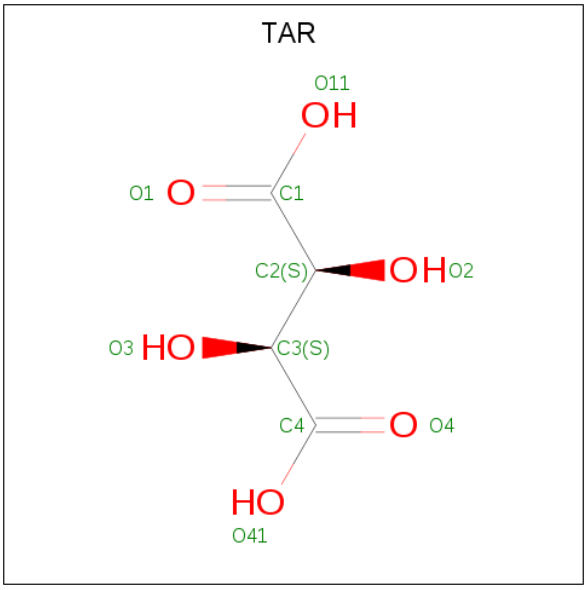
There are 3 unique types of molecules in this entry. The entry contains 6863 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Menaquinone-specific isochorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	1	0
			3353	2117	610	615	11			
1	B	428	Total	C	N	O	S	0	0	0
			3340	2110	605	614	11			

- Molecule 2 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is water.

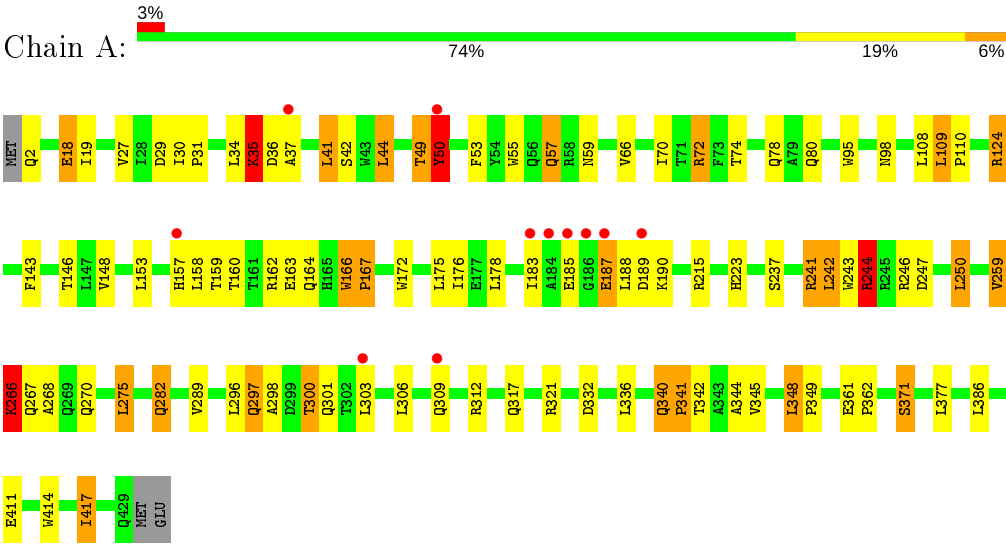
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	80	Total O 80 80	0	0
3	B	70	Total O 70 70	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

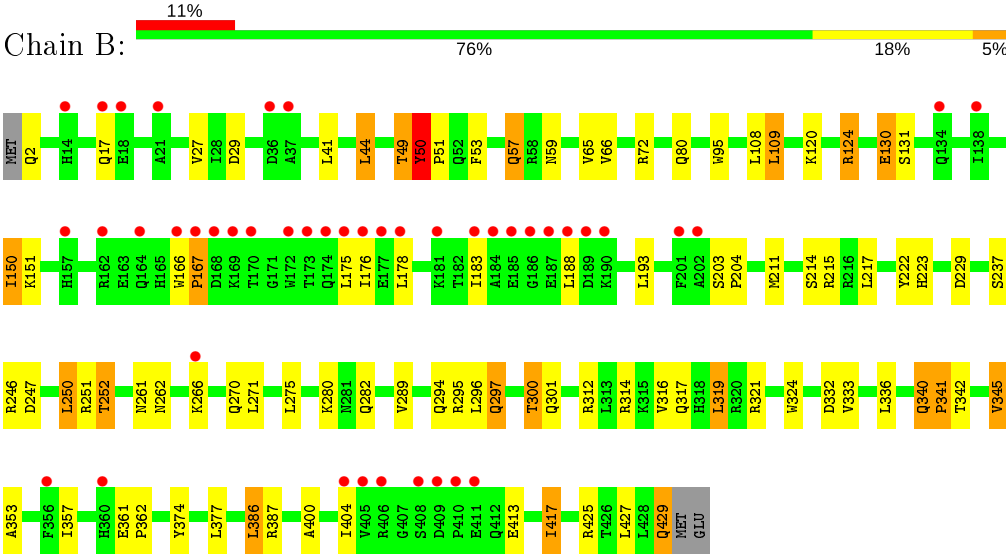
- Molecule 1: Menaquinone-specific isochorismate synthase

Chain A:



- Molecule 1: Menaquinone-specific isochorismate synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	146.41Å 146.41Å 125.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 47.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (25.00-2.50) 98.6 (47.86-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.276 0.259 , 0.296	Depositor DCC
R_{free} test set	2393 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6863	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: TAR

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	0.77	10/3431 (0.3%)	0.83	11/4669 (0.2%)
1	B	0.57	3/3413 (0.1%)	0.73	3/4645 (0.1%)
All	All	0.68	13/6844 (0.2%)	0.78	14/9314 (0.2%)

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	4
1	B	0	4
All	All	0	8

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	LYS	CE-NZ	12.75	1.80	1.49
1	A	264	ASP	C-O	11.61	1.45	1.23
1	A	266	LYS	CG-CD	10.84	1.89	1.52
1	A	266	LYS	CD-CE	9.71	1.75	1.51
1	A	267	GLN	CD-NE2	7.85	1.52	1.32
1	B	266	LYS	C-N	7.59	1.51	1.34
1	B	270	GLN	CG-CD	7.33	1.67	1.51
1	A	267	GLN	CD-OE1	6.74	1.38	1.24
1	A	268	ALA	C-O	6.35	1.35	1.23
1	A	268	ALA	C-N	5.90	1.47	1.34
1	A	266	LYS	CB-CG	5.69	1.68	1.52
1	B	266	LYS	C-O	5.60	1.33	1.23
1	A	270	GLN	CD-NE2	5.04	1.45	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	TRP	C-N-CD	-11.37	95.58	120.60
1	A	264	ASP	CB-CG-OD2	-9.79	109.49	118.30
1	A	266	LYS	CB-CG-CD	-7.41	92.32	111.60
1	A	166	TRP	C-N-CA	6.98	151.32	122.00
1	A	244	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	50	TYR	N-CA-C	6.09	127.44	111.00
1	B	50	TYR	N-CA-C	5.90	126.92	111.00
1	B	244	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	44	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	264	ASP	OD1-CG-OD2	5.53	133.81	123.30
1	A	270	GLN	OE1-CD-NE2	5.53	134.61	121.90
1	A	250	LEU	CA-CB-CG	5.49	127.93	115.30
1	B	271	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	A	266	LYS	CD-CE-NZ	-5.01	100.17	111.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	TRP	Peptide
1	A	340	GLN	Peptide
1	A	49	THR	Peptide
1	A	50	TYR	Peptide
1	B	166	TRP	Peptide
1	B	340	GLN	Peptide
1	B	49	THR	Peptide
1	B	50	TYR	Peptide

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	3353	0	3294	91	0
1	B	3340	0	3271	69	0
2	A	10	0	4	3	0
2	B	10	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	80	0	0	11	0
3	B	70	0	0	10	0
All	All	6863	0	6573	160	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 12.

All (160) 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:A:266:LYS:CD	1:A:266:LYS:CE	1.75	1.59
1:A:266:LYS:CD	1:A:266:LYS:CG	1.89	1.48
1:A:266:LYS:CE	1:A:266:LYS:NZ	1.80	1.43
1:B:51:PRO:HD3	3:B:1071:HOH:O	1.46	1.14
1:B:51:PRO:CD	3:B:1071:HOH:O	1.96	1.10
1:A:259:VAL:HG22	1:A:275:LEU:HG	1.49	0.92
1:B:348:LEU:CB	1:B:349:PRO:HD2	1.99	0.91
1:A:261:ASN:ND2	1:A:312:ARG:HD2	1.88	0.89
1:A:296:LEU:HD11	1:A:303:LEU:HD21	1.54	0.89
1:A:246:ARG:HH11	1:A:246:ARG:HG2	1.40	0.86
1:B:29:ASP:OD2	1:B:124:ARG:HG2	1.75	0.85
1:B:57:GLN:NE2	1:B:59:ASN:H	1.75	0.84
1:A:348:LEU:CB	1:A:349:PRO:CD	2.56	0.84
1:A:266:LYS:CD	1:A:266:LYS:CB	2.57	0.82
1:A:340:GLN:HE22	1:A:371:SER:HB2	1.40	0.82
1:A:241:ARG:HH22	2:A:1000:TAR:C4	1.93	0.81
1:B:242:LEU:O	1:B:252:THR:CG2	2.28	0.81
1:A:189:ASP:H	1:A:348:LEU:CB	1.93	0.81
1:A:342:THR:HG22	1:A:344:ALA:H	1.45	0.80
1:B:80:GLN:HE22	1:B:332:ASP:H	1.29	0.79
1:A:35:LYS:HB3	3:A:1044:HOH:O	1.83	0.79
1:B:27:VAL:HG13	1:B:124:ARG:HD3	1.65	0.77
1:B:342:THR:HG21	3:B:1068:HOH:O	1.84	0.77
1:B:242:LEU:O	1:B:252:THR:HG22	1.87	0.74
1:A:80:GLN:HE22	1:A:332:ASP:H	1.35	0.74
1:A:247:ASP:HB3	3:B:1036:HOH:O	1.88	0.74
1:A:246:ARG:HH11	1:A:246:ARG:CG	2.01	0.73
1:A:167:PRO:HD3	1:A:362:PRO:HG2	1.72	0.71
1:A:34:LEU:C	1:A:36:ASP:N	2.44	0.71
1:A:296:LEU:CD1	1:A:303:LEU:HD21	2.20	0.70
1:A:190:LYS:H	1:A:348:LEU:CB	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:HB3	1:A:66:VAL:HG22	1.74	0.70
1:B:348:LEU:CB	1:B:349:PRO:CD	2.69	0.70
1:B:150:ILE:H	1:B:150:ILE:HD12	1.57	0.69
1:B:342:THR:HG22	1:B:345:VAL:HB	1.74	0.69
1:A:160:THR:HG21	1:A:163:GLU:HG3	1.75	0.69
1:A:261:ASN:HD21	1:A:312:ARG:HD2	1.57	0.69
1:A:340:GLN:HE22	1:A:371:SER:CB	2.06	0.68
1:A:27:VAL:HG13	1:A:124:ARG:HD3	1.75	0.68
1:A:34:LEU:C	1:A:36:ASP:H	1.95	0.68
1:A:29:ASP:OD1	1:A:124:ARG:HG2	1.95	0.67
1:A:282:GLN:NE2	1:A:282:GLN:HA	2.10	0.67
1:A:282:GLN:HA	1:A:282:GLN:HE21	1.59	0.66
1:A:18:GLU:HA	3:A:1038:HOH:O	1.95	0.65
1:B:321:ARG:HD2	3:B:1024:HOH:O	1.95	0.65
1:B:340:GLN:HG2	1:B:341:PRO:CD	2.27	0.65
1:A:265:ASP:HB2	1:A:312:ARG:NH2	2.10	0.65
1:B:223:HIS:HD2	1:B:237:SER:OG	1.80	0.65
1:A:266:LYS:CE	1:A:266:LYS:CG	2.75	0.64
1:A:241:ARG:NH2	2:A:1000:TAR:C4	2.60	0.64
3:A:1029:HOH:O	1:B:247:ASP:HB3	2.00	0.62
1:A:261:ASN:HD21	1:A:312:ARG:HH11	1.45	0.62
1:A:265:ASP:CB	1:A:312:ARG:HH22	2.12	0.62
1:A:98:ASN:HD22	1:A:371:SER:HB3	1.64	0.62
1:B:53:PHE:HB3	1:B:66:VAL:HG22	1.81	0.62
1:A:57:GLN:NE2	1:A:59:ASN:H	1.97	0.62
1:B:413:GLU:O	1:B:417:ILE:HB	1.99	0.62
1:A:246:ARG:HD2	3:A:1057:HOH:O	2.00	0.61
1:B:342:THR:CG2	1:B:345:VAL:HB	2.29	0.61
1:B:66:VAL:HG11	1:B:95:TRP:CD1	2.36	0.61
1:B:242:LEU:O	1:B:252:THR:HG23	2.02	0.60
1:B:400:ALA:O	1:B:417:ILE:HD11	2.02	0.59
1:A:394:ASN:ND2	1:A:394:ASN:H	2.01	0.59
1:B:241:ARG:HH22	2:B:1001:TAR:C4	2.17	0.57
1:A:265:ASP:HB3	1:A:312:ARG:HH22	1.69	0.57
1:A:241:ARG:NH2	2:A:1000:TAR:O41	2.37	0.57
1:A:312:ARG:HA	1:A:317:GLN:HG2	1.86	0.57
1:A:348:LEU:CB	1:A:349:PRO:HD3	2.35	0.57
1:B:29:ASP:OD2	1:B:124:ARG:CG	2.48	0.57
1:A:80:GLN:HE22	1:A:332:ASP:N	2.02	0.57
1:A:394:ASN:N	1:A:394:ASN:ND2	2.53	0.56
1:B:340:GLN:HG2	1:B:341:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TRP:O	1:A:176:ILE:HG12	2.05	0.56
1:A:132:SER:OG	1:A:135:HIS:HD2	1.89	0.55
1:B:183:ILE:HG23	1:B:188:LEU:O	2.07	0.55
1:B:80:GLN:HE22	1:B:332:ASP:N	2.02	0.55
1:B:167:PRO:CD	1:B:362:PRO:HG2	2.38	0.54
1:A:297:GLN:HG2	1:A:298:ALA:N	2.22	0.54
1:B:353:ALA:O	1:B:357:ILE:HG12	2.08	0.54
1:A:42:SER:HB3	1:A:153:LEU:HD22	1.90	0.53
1:B:251:ARG:HG2	1:B:324:TRP:CD1	2.44	0.53
1:B:80:GLN:NE2	1:B:332:ASP:H	2.02	0.53
1:B:49:THR:HG21	1:B:143:PHE:HE1	1.73	0.53
1:A:167:PRO:HD3	1:A:362:PRO:CG	2.38	0.53
1:A:265:ASP:CB	1:A:312:ARG:NH2	2.71	0.53
1:A:266:LYS:CD	1:A:266:LYS:NZ	2.73	0.52
1:B:51:PRO:HD2	3:B:1071:HOH:O	1.81	0.52
1:B:282:GLN:NE2	1:B:321:ARG:HH12	2.06	0.52
1:B:44:LEU:HG	1:B:65:VAL:HB	1.92	0.51
1:A:312:ARG:HB2	1:A:317:GLN:HE21	1.75	0.51
1:A:66:VAL:HG11	1:A:95:TRP:CD1	2.45	0.51
1:B:167:PRO:CG	1:B:362:PRO:HG2	2.40	0.51
1:A:223:HIS:HD2	1:A:237:SER:OG	1.94	0.50
1:B:203:SER:HB2	1:B:204:PRO:HD2	1.92	0.50
1:A:109:LEU:HD22	3:A:1002:HOH:O	2.10	0.50
1:A:80:GLN:NE2	1:A:332:ASP:H	2.07	0.49
1:B:27:VAL:CG1	1:B:124:ARG:HD3	2.38	0.49
1:A:348:LEU:CB	1:A:349:PRO:HD2	2.39	0.49
1:A:55:TRP:CH2	1:A:57:GLN:HB3	2.47	0.49
1:B:167:PRO:HG3	1:B:362:PRO:HG2	1.93	0.49
1:B:215:ARG:HD2	3:B:1005:HOH:O	2.11	0.49
1:A:66:VAL:HB	1:A:110:PRO:HB3	1.95	0.48
1:B:261:ASN:ND2	1:B:262:ASN:H	2.10	0.48
1:B:296:LEU:O	1:B:300:THR:HB	2.13	0.48
1:A:390:LYS:HG2	3:A:1016:HOH:O	2.12	0.47
1:A:242:LEU:HD12	1:A:371:SER:OG	2.14	0.47
1:A:261:ASN:ND2	1:A:262:ASN:H	2.12	0.47
1:A:402:ALA:HB2	1:A:417:ILE:HD12	1.96	0.47
1:A:2:GLN:N	3:A:1034:HOH:O	2.47	0.47
1:A:306:LEU:O	1:A:321[B]:ARG:NH1	2.48	0.47
1:A:296:LEU:O	1:A:300:THR:HB	2.15	0.46
1:B:282:GLN:NE2	1:B:321:ARG:HH22	2.14	0.46
1:B:282:GLN:HE21	1:B:321:ARG:HH22	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:THR:HG23	1:B:345:VAL:H	1.81	0.46
1:B:50:TYR:HB3	1:B:229:ASP:HA	1.98	0.46
1:A:146:THR:O	1:A:146:THR:HG22	2.15	0.45
1:B:243:TRP:HB2	1:B:250:LEU:HD21	1.99	0.45
1:B:386:LEU:O	1:B:387:ARG:C	2.54	0.45
1:A:70:ILE:HG21	1:A:128:PHE:HB3	1.98	0.45
1:B:214:SER:HA	1:B:427:LEU:HD22	1.98	0.45
1:A:246:ARG:NH1	1:A:246:ARG:CG	2.67	0.45
1:A:340:GLN:HG2	1:A:341:PRO:CD	2.47	0.45
1:A:215:ARG:HA	1:A:223:HIS:NE2	2.32	0.45
1:B:217:LEU:HD12	1:B:427:LEU:HD23	1.99	0.45
1:A:183:ILE:HG12	1:A:188:LEU:HG	2.00	0.44
1:B:300:THR:HG23	1:B:301:GLN:O	2.17	0.44
1:A:244:ARG:HD2	3:A:1005:HOH:O	2.17	0.44
1:A:41:LEU:HB2	1:A:215:ARG:HH12	1.82	0.44
1:B:130:GLU:HG2	1:B:130:GLU:H	1.69	0.44
1:B:244:ARG:HD2	3:B:1004:HOH:O	2.16	0.44
1:B:282:GLN:NE2	1:B:321:ARG:NH1	2.65	0.44
1:B:57:GLN:HE22	1:B:59:ASN:CG	2.21	0.44
1:A:312:ARG:HD3	1:A:317:GLN:NE2	2.33	0.43
1:A:167:PRO:CD	1:A:362:PRO:HG2	2.44	0.43
1:B:188:LEU:HD12	1:B:352:LEU:HB3	2.00	0.43
1:B:57:GLN:HE22	1:B:59:ASN:H	1.60	0.43
1:A:246:ARG:CD	3:A:1057:HOH:O	2.61	0.43
1:A:41:LEU:HB2	1:A:215:ARG:NH1	2.34	0.43
1:A:361:GLU:HA	1:A:362:PRO:HD3	1.68	0.43
1:A:72:ARG:HG2	1:A:72:ARG:H	1.73	0.43
1:B:297:GLN:HA	1:B:297:GLN:HE21	1.84	0.43
1:B:193:LEU:HD12	1:B:404:ILE:HD12	2.01	0.43
1:A:74:THR:H	1:A:78:GLN:NE2	2.17	0.43
1:B:109:LEU:HD22	3:B:1016:HOH:O	2.18	0.43
1:B:244:ARG:CD	3:B:1004:HOH:O	2.67	0.43
1:B:361:GLU:HA	1:B:362:PRO:HD3	1.69	0.43
1:B:425:ARG:O	1:B:429:GLN:NE2	2.52	0.43
1:A:309:GLN:HB2	3:A:1025:HOH:O	2.18	0.42
1:B:312:ARG:HA	1:B:317:GLN:HG2	2.01	0.42
1:A:34:LEU:O	1:A:36:ASP:N	2.51	0.42
1:B:222:TYR:OH	1:B:241:ARG:HD3	2.20	0.41
1:B:319:LEU:HA	1:B:319:LEU:HD12	1.94	0.41
1:A:30:ILE:HA	1:A:31:PRO:HD2	1.95	0.41
1:A:266:LYS:HD2	1:A:266:LYS:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASN:HB2	1:A:371:SER:HB2	2.03	0.41
1:B:282:GLN:HE21	1:B:321:ARG:HH12	1.68	0.41
1:B:95:TRP:CE3	1:B:374:TYR:HB3	2.56	0.40
1:A:244:ARG:CD	3:A:1005:HOH:O	2.69	0.40
1:A:394:ASN:N	1:A:394:ASN:HD22	2.17	0.40
1:A:49:THR:HG21	1:A:143:PHE:HE1	1.87	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	427/431 (99%)	396 (93%)	17 (4%)	14 (3%)	4 5
1	B	426/431 (99%)	396 (93%)	26 (6%)	4 (1%)	17 31
All	All	853/862 (99%)	792 (93%)	43 (5%)	18 (2%)	7 11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	37	ALA
1	A	167	PRO
1	A	341	PRO
1	A	348	LEU
1	B	167	PRO
1	B	341	PRO
1	B	348	LEU
1	A	301	GLN
1	A	35	LYS
1	A	157	HIS
1	A	187	GLU

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Mol	Chain	Res	Type
1	A	264	ASP
1	A	19	ILE
1	A	266	LYS
1	B	17	GLN
1	A	158	LEU
1	A	50	TYR

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	346/363 (95%)	309 (89%)	37 (11%)	6 13
1	B	343/363 (94%)	302 (88%)	41 (12%)	5 9
All	All	689/726 (95%)	611 (89%)	78 (11%)	6 11

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	41	LEU
1	A	44	LEU
1	A	50	TYR
1	A	57	GLN
1	A	72	ARG
1	A	108	LEU
1	A	109	LEU
1	A	124	ARG
1	A	148	VAL
1	A	159	THR
1	A	162	ARG
1	A	164	GLN
1	A	175	LEU
1	A	178	LEU
1	A	185	GLU
1	A	187	GLU

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Mol	Chain	Res	Type
1	A	241	ARG
1	A	242	LEU
1	A	243	TRP
1	A	244	ARG
1	A	250	LEU
1	A	259	VAL
1	A	275	LEU
1	A	282	GLN
1	A	289	VAL
1	A	297	GLN
1	A	300	THR
1	A	336	LEU
1	A	345	VAL
1	A	371	SER
1	A	377	LEU
1	A	386	LEU
1	A	394	ASN
1	A	411	GLU
1	A	414	TRP
1	A	417	ILE
1	B	2	GLN
1	B	41	LEU
1	B	44	LEU
1	B	57	GLN
1	B	72	ARG
1	B	108	LEU
1	B	109	LEU
1	B	120	LYS
1	B	124	ARG
1	B	130	GLU
1	B	131	SER
1	B	148	VAL
1	B	149	SER
1	B	150	ILE
1	B	151	LYS
1	B	175	LEU
1	B	176	ILE
1	B	178	LEU
1	B	211	MET
1	B	242	LEU
1	B	244	ARG
1	B	246	ARG

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Mol	Chain	Res	Type
1	B	250	LEU
1	B	252	THR
1	B	275	LEU
1	B	280	LYS
1	B	289	VAL
1	B	294	GLN
1	B	295	ARG
1	B	297	GLN
1	B	300	THR
1	B	314	ARG
1	B	316	VAL
1	B	319	LEU
1	B	333	VAL
1	B	336	LEU
1	B	345	VAL
1	B	377	LEU
1	B	386	LEU
1	B	417	ILE
1	B	429	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	57	GLN
1	A	78	GLN
1	A	80	GLN
1	A	98	ASN
1	A	104	GLN
1	A	135	HIS
1	A	218	ASN
1	A	223	HIS
1	A	261	ASN
1	A	262	ASN
1	A	282	GLN
1	A	309	GLN
1	A	317	GLN
1	A	338	GLN
1	A	340	GLN
1	A	394	ASN
1	B	2	GLN
1	B	57	GLN

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Mol	Chain	Res	Type
1	B	80	GLN
1	B	164	GLN
1	B	174	GLN
1	B	223	HIS
1	B	261	ASN
1	B	262	ASN
1	B	282	GLN
1	B	297	GLN
1	B	317	GLN
1	B	340	GLN
1	B	429	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

2 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	TAR	A	1000	-	3,9,9	0.85	0	6,12,12	1.92	2 (33%)
2	TAR	B	1001	-	3,9,9	0.86	0	6,12,12	2.22	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TAR	A	1000	-	-	0/4/12/12	-
2	TAR	B	1001	-	-	0/4/12/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	TAR	C1-C2-C3	-3.98	104.55	113.11
2	A	1000	TAR	C1-C2-C3	-3.51	105.56	113.11
2	B	1001	TAR	C4-C3-C2	-2.94	106.77	113.11
2	A	1000	TAR	C4-C3-C2	-2.22	108.32	113.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	TAR	3	0
2	B	1001	TAR	1	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, 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	428/431 (99%)	0.42	11 (2%) 56 59	45, 56, 72, 77	0
1	B	428/431 (99%)	0.65	48 (11%) 5 4	45, 56, 72, 77	0
All	All	856/862 (99%)	0.54	59 (6%) 16 17	45, 56, 72, 77	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	ALA	7.1
1	B	189	ASP	4.9
1	B	181	LYS	4.8
1	B	178	LEU	4.8
1	A	184	ALA	4.7
1	B	18	GLU	4.6
1	B	174	GLN	4.6
1	A	186	GLY	4.3
1	A	189	ASP	4.3
1	B	170	THR	4.2
1	B	175	LEU	4.0
1	B	172	TRP	3.9
1	B	188	LEU	3.6
1	B	138	ILE	3.6
1	B	21	ALA	3.5
1	B	183	ILE	3.5
1	B	167	PRO	3.5
1	B	187	GLU	3.5
1	B	177	GLU	3.4
1	B	37	ALA	3.4
1	B	266	LYS	3.3
1	B	185	GLU	3.2
1	B	173	THR	3.2
1	B	360	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	411	GLU	3.1
1	B	356	PHE	3.1
1	B	157	HIS	3.0
1	A	183	ILE	3.0
1	B	406	ARG	3.0
1	B	166	TRP	2.9
1	B	202	ALA	2.7
1	A	187	GLU	2.7
1	B	410	PRO	2.6
1	B	164	GLN	2.6
1	A	185	GLU	2.6
1	B	176	ILE	2.6
1	B	409	ASP	2.6
1	B	405	VAL	2.5
1	B	346	ALA	2.5
1	A	157	HIS	2.5
1	B	352	LEU	2.5
1	B	404	ILE	2.4
1	A	37	ALA	2.4
1	B	169	LYS	2.4
1	B	17	GLN	2.3
1	B	36	ASP	2.3
1	A	50	TYR	2.3
1	B	190	LYS	2.3
1	B	186	GLY	2.2
1	A	303	LEU	2.2
1	B	201	PHE	2.2
1	B	142	GLU	2.2
1	B	408	SER	2.1
1	B	162	ARG	2.1
1	B	14	HIS	2.1
1	B	134	GLN	2.1
1	B	168	ASP	2.1
1	B	141	LYS	2.1
1	A	309	GLN	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. 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	B-factors(Å^2)	Q<0.9
2	TAR	B	1001	10/10	0.89	0.17	49,52,54,56	0
2	TAR	A	1000	10/10	0.91	0.15	44,49,52,54	0

6.5 Other polymers (i)

There are no such residues in this entry.