WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 04:07 PM JST

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PDB ID	:	6JKQ
Title	:	Crystal structure of aspartate transcarbamoylase from Trypanosoma cruzi (Ligand-free form)
Authors	:	Matoba, K.; Shiba, T.; Nara, T.; Aoki, T.; Nagasaki, S.; Hayamizu, R.; Honma, T.; Tanaka, A.; Inoue, M.; Matsuoka, S.; Balogun, E.O.; Inaoka, D.K.; Kita, K.; Harada, S.
Deposited on	:	2019-03-01
Resolution	:	2.81 Å(reported)

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 2.81 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.
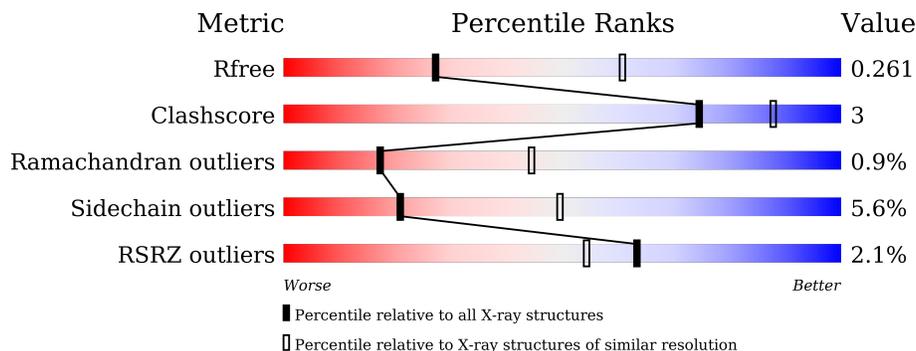
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 <=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	327	2% / 82% / 8% · 8%
1	B	327	3% / 78% / 11% · 10%
1	C	327	% / 84% / 11% 5%
1	D	327	3% / 81% / 9% 9%
1	E	327	2% / 71% / 17% · 10%
1	F	327	% / 83% / 9% · 7%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 13949 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 Aspartate carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2328	1471	409	431	17			
1	B	295	Total	C	N	O	S	0	0	0
			2289	1447	402	424	16			
1	C	312	Total	C	N	O	S	0	0	0
			2402	1519	422	444	17			
1	D	297	Total	C	N	O	S	0	0	0
			2295	1453	404	421	17			
1	E	294	Total	C	N	O	S	0	0	0
			2280	1442	400	422	16			
1	F	304	Total	C	N	O	S	0	0	0
			2355	1490	412	436	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O15636
B	0	SER	-	expression tag	UNP O15636
C	0	SER	-	expression tag	UNP O15636
D	0	SER	-	expression tag	UNP O15636
E	0	SER	-	expression tag	UNP O15636
F	0	SER	-	expression tag	UNP O15636

3 Residue-property plots ⓘ

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: Aspartate carbamoyltransferase
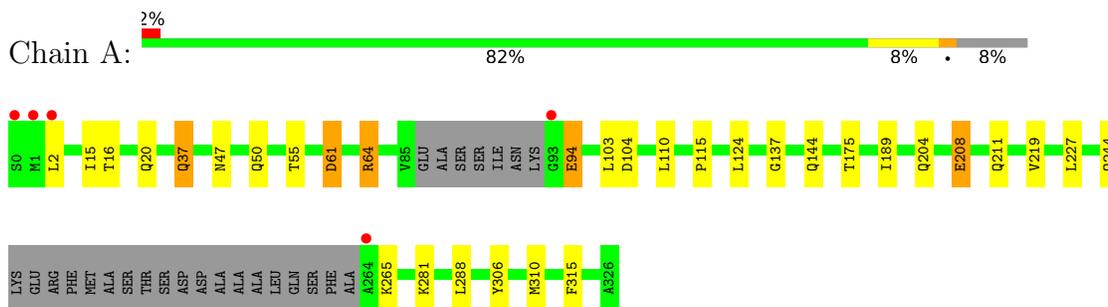
Chain A:

- Molecule 1: Aspartate carbamoyltransferase

Chain B:

- Molecule 1: Aspartate carbamoyltransferase

Chain C:

- Molecule 1: Aspartate carbamoyltransferase

Chain D:
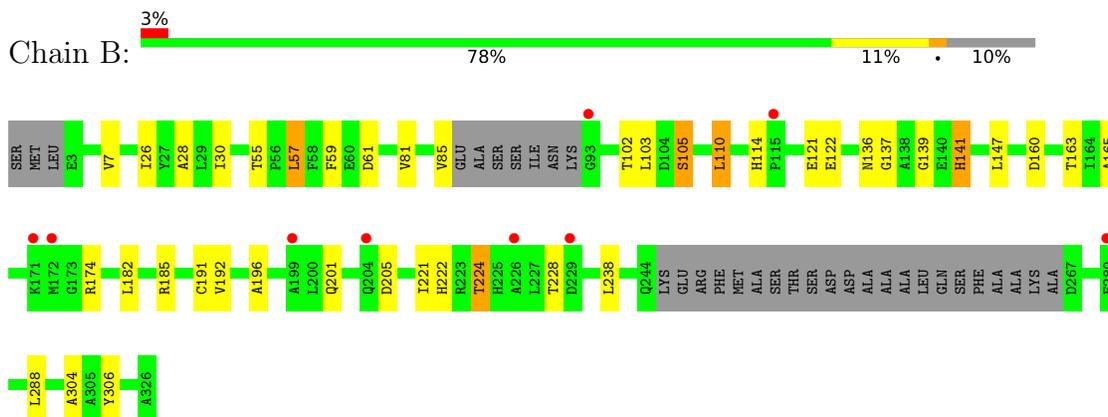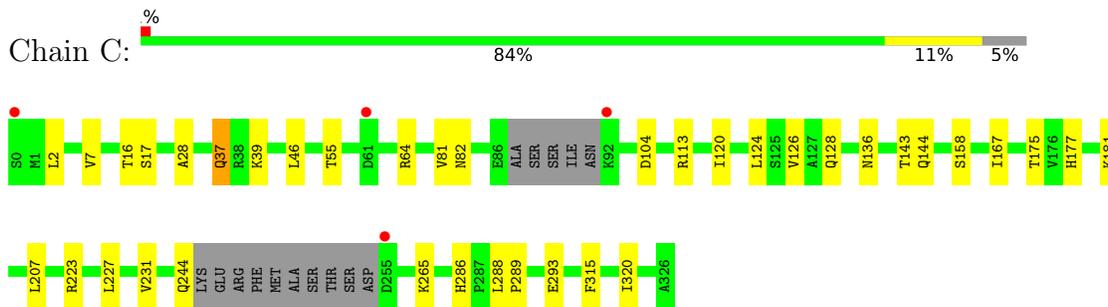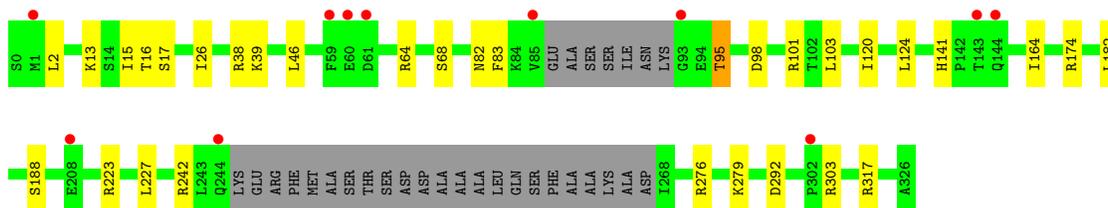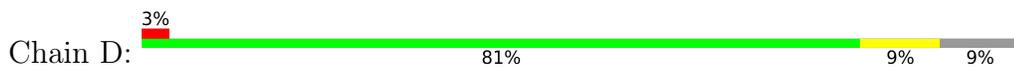
• Molecule 1: Aspartate carbamoyltransferase

Chain E:

• Molecule 1: Aspartate carbamoyltransferase

Chain F:
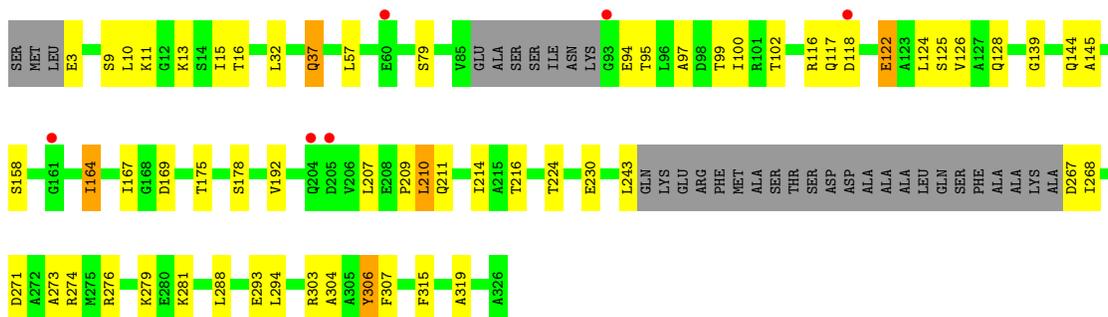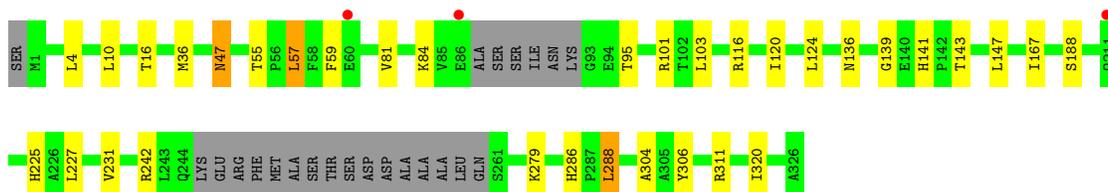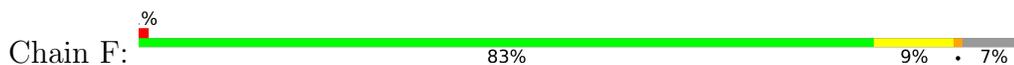
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.42Å 79.28Å 92.02Å 69.56° 82.90° 63.25°	Depositor
Resolution (Å)	29.51 – 2.81 29.51 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.51-2.81) 96.5 (29.51-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.65 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.178 , 0.265 0.181 , 0.261	Depositor DCC
R_{free} test set	2205 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.3	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13949	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

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	0.56	0/2364	0.80	1/3194 (0.0%)
1	B	0.57	0/2325	0.81	1/3143 (0.0%)
1	C	0.62	0/2439	0.82	1/3296 (0.0%)
1	D	0.56	0/2331	0.79	2/3151 (0.1%)
1	E	0.54	0/2316	0.77	0/3131
1	F	0.58	0/2392	0.80	2/3232 (0.1%)
All	All	0.57	0/14167	0.80	7/19147 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	160	ASP	CB-CG-OD1	5.57	123.31	118.30
1	D	101	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	C	113	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	64	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	F	311	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	F	116	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	242	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2328	0	2388	14	0
1	B	2289	0	2344	24	0
1	C	2402	0	2463	15	0
1	D	2295	0	2360	10	0
1	E	2280	0	2336	20	0
1	F	2355	0	2415	13	0
All	All	13949	0	14306	90	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 3.

All (90) 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:144:GLN:HG2	1:A:175:THR:HG22	1.71	0.73
1:C:16:THR:HG21	1:C:124:LEU:HD11	1.73	0.70
1:C:55:THR:HG22	1:C:81:VAL:O	1.90	0.70
1:A:16:THR:HG21	1:A:124:LEU:HD11	1.78	0.66
1:C:144:GLN:HG2	1:C:175:THR:HG22	1.77	0.65
1:D:64:ARG:NH2	1:E:102:THR:OG1	2.30	0.65
1:B:26:ILE:HD11	1:B:182:LEU:HD11	1.80	0.63
1:B:59:PHE:CE1	1:B:85:VAL:HG11	2.35	0.62
1:B:55:THR:HG23	1:B:81:VAL:O	2.02	0.60
1:A:55:THR:CG2	1:A:103:LEU:HD13	2.33	0.59
1:B:196:ALA:HB3	1:B:201:GLN:HE21	1.67	0.59
1:A:37:GLN:HG3	1:A:315:PHE:CE2	2.37	0.58
1:B:224:THR:HG21	1:B:228:THR:HG21	1.84	0.58
1:E:10:LEU:HD23	1:E:15:ILE:HD11	1.87	0.56
1:B:163:THR:HG23	1:B:191:CYS:HB3	1.86	0.56
1:C:37:GLN:HA	1:C:315:PHE:CE1	2.40	0.56
1:E:116:ARG:NH1	1:E:118:ASP:OD1	2.39	0.55
1:C:177:HIS:O	1:C:181:LYS:HG3	2.07	0.54
1:E:100:ILE:HG21	1:E:126:VAL:HG23	1.91	0.53
1:F:57:LEU:HD22	1:F:59:PHE:CE2	2.43	0.53
1:F:16:THR:HG21	1:F:124:LEU:HD11	1.91	0.53
1:B:224:THR:HG21	1:B:228:THR:CG2	2.39	0.53
1:A:55:THR:HG22	1:A:103:LEU:HD13	1.92	0.52
1:B:26:ILE:HD11	1:B:182:LEU:CD1	2.40	0.52
1:B:196:ALA:HB3	1:B:201:GLN:NE2	2.26	0.51
1:A:189:ILE:O	1:A:219:VAL:HG22	2.11	0.51
1:B:110:LEU:HD23	1:B:110:LEU:N	2.26	0.51
1:B:221:ILE:HG22	1:B:221:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:MET:HB3	1:B:105:SER:OG	2.11	0.50
1:B:102:THR:O	1:B:105:SER:HB2	2.11	0.50
1:E:279:LYS:O	1:E:303:ARG:NH1	2.44	0.50
1:E:304:ALA:HB1	1:E:306:TYR:CE2	2.47	0.50
1:A:94:GLU:HG3	1:C:289:PRO:HB3	1.93	0.50
1:D:16:THR:HG21	1:D:124:LEU:HD11	1.94	0.50
1:B:57:LEU:HD22	1:B:59:PHE:CE2	2.46	0.50
1:E:210:LEU:HD12	1:E:214:ILE:HD11	1.94	0.50
1:E:294:LEU:HD21	1:E:306:TYR:CZ	2.47	0.50
1:F:57:LEU:HG	1:F:103:LEU:HD11	1.93	0.49
1:C:39:LYS:HE2	1:C:46:LEU:HD21	1.94	0.49
1:D:26:ILE:HD11	1:D:182:LEU:HD11	1.95	0.49
1:D:16:THR:HG22	1:D:120:ILE:HG21	1.95	0.48
1:D:68:SER:OG	1:D:317:ARG:NH1	2.45	0.48
1:D:279:LYS:O	1:D:303:ARG:NH1	2.47	0.47
1:F:143:THR:HG22	1:F:320:ILE:HD13	1.96	0.47
1:F:227:LEU:HD23	1:F:231:VAL:HG11	1.96	0.47
1:A:115:PRO:O	1:A:137:GLY:HA2	2.15	0.47
1:E:97:ALA:HB1	1:E:126:VAL:HG11	1.97	0.46
1:A:310:MET:CB	1:B:105:SER:OG	2.63	0.46
1:A:64:ARG:NH2	1:B:102:THR:OG1	2.49	0.46
1:B:165:ALA:HB3	1:B:238:LEU:HD23	1.97	0.46
1:E:32:LEU:HD23	1:E:319:ALA:HB1	1.97	0.46
1:A:55:THR:HG21	1:A:103:LEU:HD13	1.99	0.45
1:E:16:THR:HG21	1:E:124:LEU:HD11	1.98	0.45
1:C:120:ILE:HD13	1:C:136:ASN:HB3	1.98	0.45
1:B:141:HIS:HB2	1:B:174:ARG:HD2	1.98	0.45
1:D:39:LYS:HD3	1:D:46:LEU:HD21	1.99	0.45
1:B:304:ALA:HB1	1:B:306:TYR:CE2	2.52	0.44
1:E:294:LEU:HD21	1:E:306:TYR:CE2	2.52	0.44
1:D:95:THR:HG23	1:D:98:ASP:HB2	1.99	0.44
1:B:191:CYS:SG	1:B:192:VAL:N	2.90	0.44
1:E:144:GLN:HG2	1:E:175:THR:HG22	1.98	0.44
1:B:26:ILE:HG22	1:B:30:ILE:HD12	1.99	0.44
1:F:4:LEU:HD22	1:F:36:MET:HG3	2.00	0.44
1:B:7:VAL:HG22	1:B:28:ALA:HB1	2.00	0.44
1:F:304:ALA:HB1	1:F:306:TYR:CE2	2.53	0.44
1:C:167:ILE:HD13	1:C:227:LEU:HD21	1.99	0.43
1:C:7:VAL:HG22	1:C:28:ALA:HB1	2.01	0.43
1:E:164:ILE:O	1:E:192:VAL:HA	2.18	0.43
1:D:141:HIS:HB2	1:D:174:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:ASN:HD22	1:F:47:ASN:H	1.67	0.42
1:C:143:THR:HG22	1:C:320:ILE:HD13	2.01	0.42
1:F:167:ILE:HD11	1:F:227:LEU:HD21	2.00	0.42
1:A:15:ILE:HA	1:A:20:GLN:HE22	1.84	0.42
1:E:307:PHE:CE1	1:F:101:ARG:HD3	2.55	0.42
1:F:55:THR:HG23	1:F:81:VAL:O	2.19	0.42
1:F:286:HIS:HD2	1:F:288:LEU:N	2.18	0.42
1:B:114:HIS:O	1:B:136:ASN:HA	2.19	0.42
1:E:145:ALA:HB2	1:E:178:SER:HB3	2.02	0.42
1:F:120:ILE:HD13	1:F:136:ASN:HB3	2.02	0.42
1:C:286:HIS:HE1	1:C:293:GLU:OE2	2.02	0.42
1:E:37:GLN:HG3	1:E:315:PHE:CE2	2.54	0.42
1:A:204:GLN:O	1:A:208:GLU:N	2.50	0.42
1:E:167:ILE:HG23	1:E:268:ILE:HD12	2.01	0.41
1:B:103:LEU:HD23	1:B:110:LEU:HD13	2.02	0.41
1:C:286:HIS:CD2	1:C:288:LEU:H	2.39	0.41
1:E:122:GLU:O	1:E:125:SER:OG	2.39	0.41
1:D:83:PHE:CD1	1:D:103:LEU:HD11	2.55	0.41
1:C:207:LEU:HD13	1:C:223:ARG:HH22	1.86	0.40
1:C:227:LEU:HD23	1:C:231:VAL:HG11	2.04	0.40
1:E:271:ASP:OD1	1:E:273:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/327 (90%)	274 (93%)	17 (6%)	4 (1%)	11	32
1	B	289/327 (88%)	262 (91%)	23 (8%)	4 (1%)	11	32
1	C	306/327 (94%)	293 (96%)	13 (4%)	0	100	100
1	D	291/327 (89%)	276 (95%)	14 (5%)	1 (0%)	41	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	288/327 (88%)	259 (90%)	24 (8%)	5 (2%)	9	27
1	F	298/327 (91%)	280 (94%)	16 (5%)	2 (1%)	22	51
All	All	1767/1962 (90%)	1644 (93%)	107 (6%)	16 (1%)	17	44

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	169	ASP
1	A	306	TYR
1	B	137	GLY
1	D	292	ASP
1	E	293	GLU
1	A	2	LEU
1	B	139	GLY
1	B	222	HIS
1	F	139	GLY
1	A	288	LEU
1	A	61	ASP
1	E	139	GLY
1	E	209	PRO
1	F	288	LEU
1	E	288	LEU
1	B	288	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/275 (92%)	241 (95%)	13 (5%)	24	54
1	B	251/275 (91%)	240 (96%)	11 (4%)	28	60
1	C	260/275 (94%)	249 (96%)	11 (4%)	30	62
1	D	251/275 (91%)	239 (95%)	12 (5%)	25	56
1	E	250/275 (91%)	223 (89%)	27 (11%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	257/275 (94%)	246 (96%)	11 (4%)	29	60
All	All	1523/1650 (92%)	1438 (94%)	85 (6%)	21	49

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	47	ASN
1	A	50	GLN
1	A	61	ASP
1	A	94	GLU
1	A	104	ASP
1	A	110	LEU
1	A	208	GLU
1	A	211	GLN
1	A	227	LEU
1	A	244	GLN
1	A	265	LYS
1	A	281	LYS
1	B	57	LEU
1	B	61	ASP
1	B	105	SER
1	B	110	LEU
1	B	121	GLU
1	B	122	GLU
1	B	141	HIS
1	B	147	LEU
1	B	185	ARG
1	B	205	ASP
1	B	224	THR
1	C	2	LEU
1	C	17	SER
1	C	37	GLN
1	C	64	ARG
1	C	82	ASN
1	C	104	ASP
1	C	126	VAL
1	C	128	GLN
1	C	158	SER
1	C	244	GLN
1	C	265	LYS
1	D	2	LEU

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Mol	Chain	Res	Type
1	D	13	LYS
1	D	15	ILE
1	D	17	SER
1	D	38	ARG
1	D	82	ASN
1	D	95	THR
1	D	164	ILE
1	D	188	SER
1	D	223	ARG
1	D	227	LEU
1	D	276	ARG
1	E	3	GLU
1	E	9	SER
1	E	11	LYS
1	E	13	LYS
1	E	37	GLN
1	E	57	LEU
1	E	79	SER
1	E	94	GLU
1	E	95	THR
1	E	99	THR
1	E	117	GLN
1	E	122	GLU
1	E	128	GLN
1	E	158	SER
1	E	164	ILE
1	E	207	LEU
1	E	210	LEU
1	E	211	GLN
1	E	216	THR
1	E	224	THR
1	E	230	GLU
1	E	243	LEU
1	E	267	ASP
1	E	274	ARG
1	E	276	ARG
1	E	281	LYS
1	E	306	TYR
1	F	10	LEU
1	F	47	ASN
1	F	57	LEU
1	F	84	LYS

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Mol	Chain	Res	Type
1	F	95	THR
1	F	141	HIS
1	F	147	LEU
1	F	188	SER
1	F	225	HIS
1	F	242	ARG
1	F	279	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	211	GLN
1	A	244	GLN
1	A	291	ASN
1	B	31	HIS
1	B	117	GLN
1	B	153	HIS
1	B	201	GLN
1	C	37	GLN
1	C	128	GLN
1	C	211	GLN
1	C	286	HIS
1	D	153	HIS
1	E	212	HIS
1	F	31	HIS
1	F	47	ASN
1	F	117	GLN
1	F	153	HIS
1	F	286	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	301/327 (92%)	-0.38	5 (1%)	70	63	24, 48, 77, 112	0
1	B	295/327 (90%)	-0.27	9 (3%)	49	39	25, 50, 92, 106	0
1	C	312/327 (95%)	-0.47	4 (1%)	77	72	21, 40, 72, 105	1 (0%)
1	D	297/327 (90%)	-0.23	11 (3%)	41	31	27, 55, 86, 115	4 (1%)
1	E	294/327 (89%)	0.01	6 (2%)	65	56	29, 67, 102, 128	0
1	F	304/327 (92%)	-0.30	3 (0%)	82	77	27, 51, 81, 112	5 (1%)
All	All	1803/1962 (91%)	-0.27	38 (2%)	63	54	21, 51, 89, 128	10 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	GLY	4.4
1	C	92	LYS	4.0
1	B	199	ALA	3.8
1	D	208	GLU	3.8
1	D	85	VAL	3.7
1	C	61	ASP	3.6
1	D	1	MET	3.4
1	F	86	GLU	3.1
1	A	1	MET	3.1
1	D	61	ASP	3.0
1	F	211	GLN	2.8
1	B	229	ASP	2.7
1	C	255	ASP	2.7
1	D	93	GLY	2.7
1	A	0	SER	2.7
1	E	205	ASP	2.7
1	D	244	GLN	2.6
1	E	60	GLU	2.6
1	D	144	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	0	SER	2.5
1	A	2	LEU	2.5
1	D	143	THR	2.4
1	B	204	GLN	2.3
1	E	204	GLN	2.3
1	D	302	PRO	2.3
1	B	171	LYS	2.3
1	E	118	ASP	2.2
1	B	280	GLU	2.2
1	F	60	GLU	2.2
1	D	59	PHE	2.2
1	A	264	ALA	2.1
1	B	226	ALA	2.1
1	B	115	PRO	2.1
1	B	93	GLY	2.0
1	B	172	MET	2.0
1	D	60	GLU	2.0
1	E	161	GLY	2.0
1	E	93	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.