



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 05:27 PM BST

PDB ID : 6K5V
Title : Structure of CSY4 Apo-form
Authors : Nishio, K.; Mizushima, T.
Deposited on : 2019-05-31
Resolution : 2.69 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
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

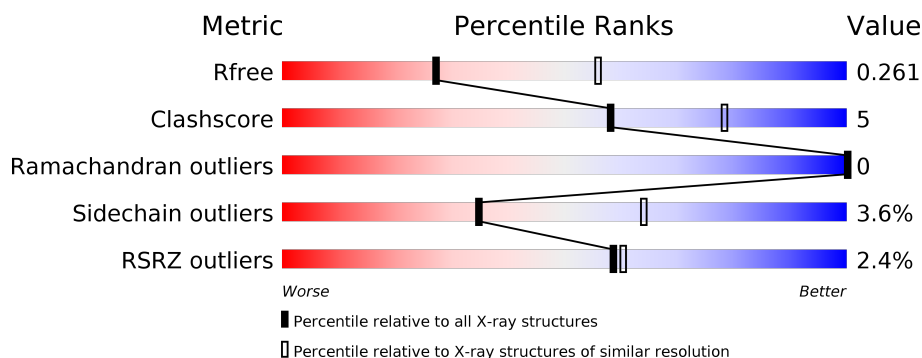
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. 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	458	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	B	458	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>6%</div> </div> </div>
1	C	458	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>5%</div> </div> </div>
1	D	458	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	E	458	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 6%</div> </div> </div>
1	F	458	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 6%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20387 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 Citrate synthase 4, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3394	2169	577	633	15			
1	B	430	Total	C	N	O	S	0	0	0
			3368	2153	572	628	15			
1	C	433	Total	C	N	O	S	0	0	0
			3394	2169	577	633	15			
1	D	430	Total	C	N	O	S	0	0	0
			3368	2153	572	628	15			
1	E	430	Total	C	N	O	S	0	0	0
			3368	2153	572	628	15			
1	F	432	Total	C	N	O	S	0	0	0
			3386	2165	576	630	15			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		
2	E	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	F	1	Total	Cl	0	0
			1	1		

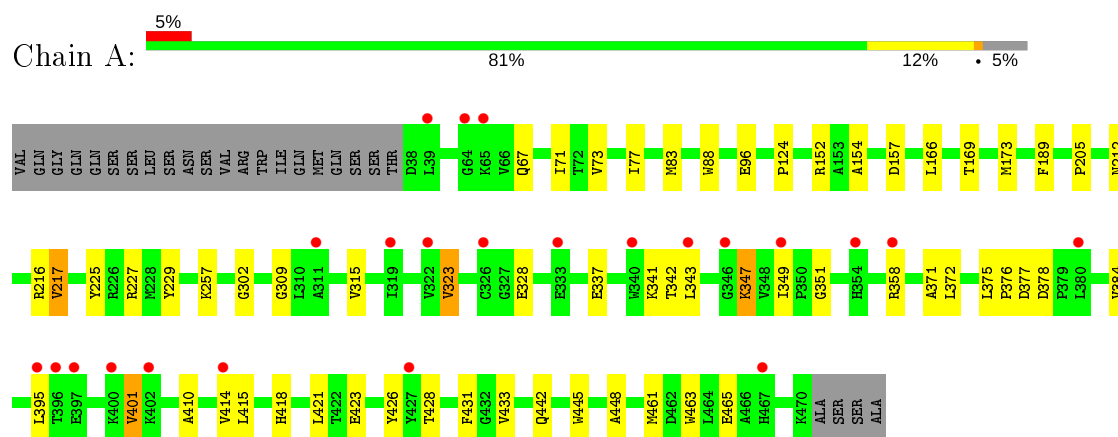
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0
3	B	23	Total 23	O 23	0	0
3	C	11	Total 11	O 11	0	0
3	D	9	Total 9	O 9	0	0
3	E	24	Total 24	O 24	0	0
3	F	14	Total 14	O 14	0	0

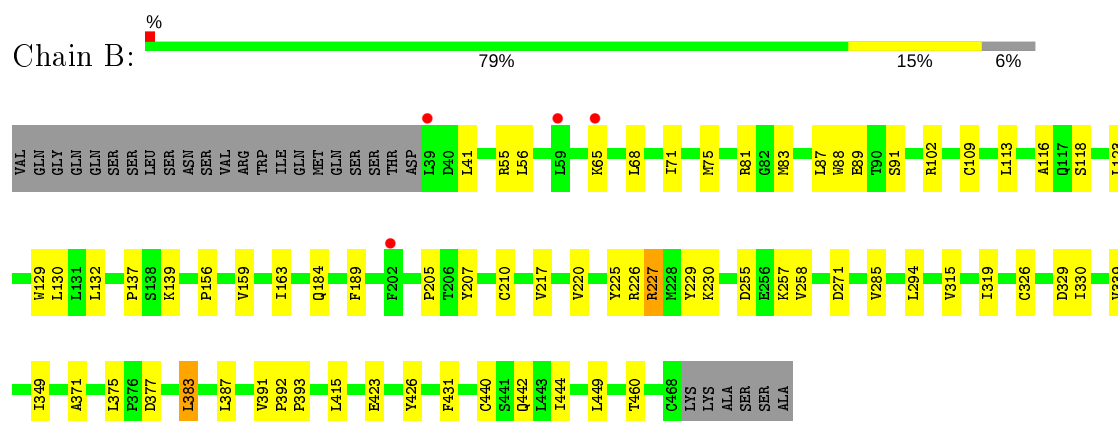
3 Residue-property plots [i](#)

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.

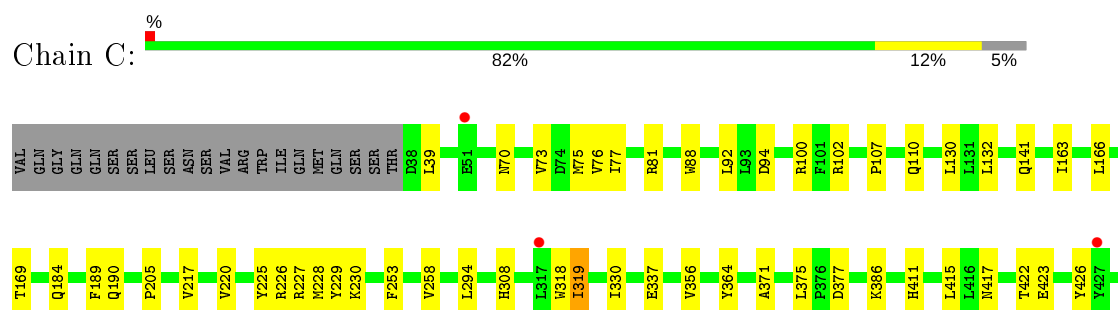
- Molecule 1: Citrate synthase 4, mitochondrial

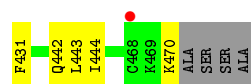


- Molecule 1: Citrate synthase 4, mitochondrial

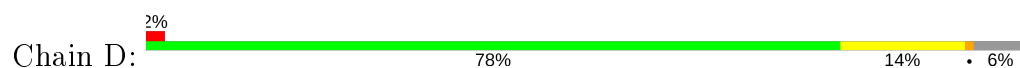


- Molecule 1: Citrate synthase 4, mitochondrial

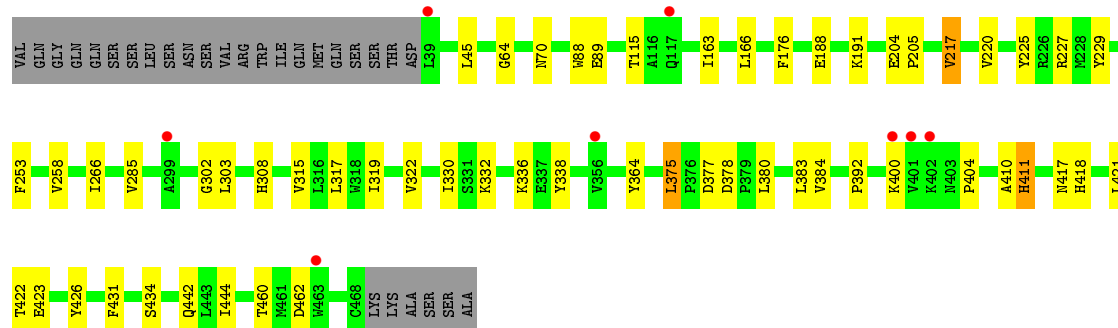
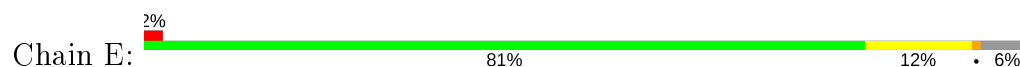




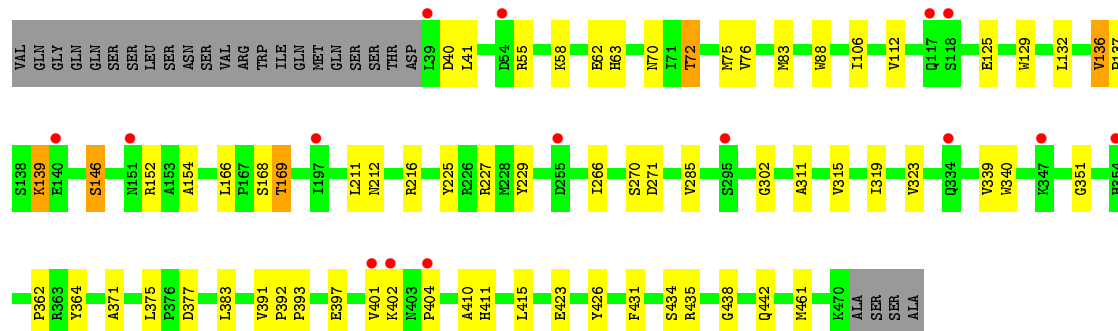
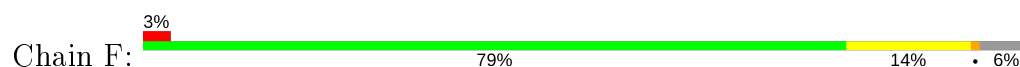
- Molecule 1: Citrate synthase 4, mitochondrial



- Molecule 1: Citrate synthase 4, mitochondrial



- Molecule 1: Citrate synthase 4, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.35Å 67.94Å 317.82Å 90.00° 100.86° 90.00°	Depositor
Resolution (Å)	46.85 – 2.69 46.85 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.85-2.69) 99.1 (46.85-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.227 , 0.261 0.227 , 0.261	Depositor DCC
R_{free} test set	4001 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20387	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7805e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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:
CL

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	0.24	0/3474	0.43	0/4716
1	B	0.24	0/3448	0.43	0/4683
1	C	0.25	0/3474	0.43	0/4716
1	D	0.25	0/3448	0.44	0/4683
1	E	0.25	0/3448	0.43	0/4683
1	F	0.24	0/3466	0.42	0/4705
All	All	0.25	0/20758	0.43	0/28186

There are no bond length outliers.

There are no bond angle outliers.

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	3394	0	3393	40	0
1	B	3368	0	3363	41	0
1	C	3394	0	3393	27	1
1	D	3368	0	3363	39	0
1	E	3368	0	3363	30	0
1	F	3386	0	3389	37	1
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	22	0	0	1	0
3	B	23	0	0	0	0
3	C	11	0	0	0	0
3	D	9	0	0	0	0
3	E	24	0	0	0	0
3	F	14	0	0	0	0
All	All	20387	0	20264	195	1

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 5.

All (195) 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:B:339:VAL:HG13	1:B:349:ILE:HD11	1.70	0.73
1:D:319:ILE:HG23	1:D:383:LEU:HD23	1.72	0.71
1:A:212:ASN:HB3	1:A:216:ARG:HH12	1.57	0.69
1:F:212:ASN:HB3	1:F:216:ARG:NH1	2.08	0.69
1:E:70:ASN:ND2	1:F:70:ASN:OD1	2.26	0.69
1:E:166:LEU:O	1:E:227:ARG:NH2	2.26	0.68
1:F:166:LEU:O	1:F:227:ARG:NH2	2.21	0.68
1:A:212:ASN:HB3	1:A:216:ARG:NH1	2.09	0.68
1:A:309:GLY:O	1:A:428:THR:OG1	2.14	0.65
1:C:166:LEU:O	1:C:227:ARG:NH2	2.29	0.64
1:E:378:ASP:OD1	1:E:418:HIS:ND1	2.30	0.63
1:D:166:LEU:O	1:D:227:ARG:NH2	2.27	0.62
1:B:387:LEU:O	1:B:391:VAL:HG13	2.00	0.61
1:C:184:GLN:NE2	1:C:190:GLN:OE1	2.34	0.60
1:A:154:ALA:O	1:A:216:ARG:NE	2.30	0.59
1:C:77:ILE:HD11	1:D:59:LEU:HD13	1.84	0.59
1:F:154:ALA:O	1:F:216:ARG:NE	2.31	0.59
1:A:96:GLU:OE1	1:A:358:ARG:NE	2.26	0.59
1:F:212:ASN:HB3	1:F:216:ARG:HH12	1.67	0.58
1:B:116:ALA:HB2	1:B:123:LEU:HD21	1.86	0.58
1:A:166:LEU:O	1:A:227:ARG:NH2	2.37	0.58
1:A:347:LYS:HB3	1:A:347:LYS:NZ	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:TRP:HE3	1:C:319:ILE:HD12	1.69	0.57
1:E:188:GLU:HA	1:E:191:LYS:HE2	1.86	0.56
1:D:400:LYS:O	1:D:400:LYS:HD2	2.05	0.56
1:A:378:ASP:OD2	1:A:418:HIS:ND1	2.36	0.56
1:E:315:VAL:HG11	1:E:410:ALA:HA	1.87	0.56
1:D:353:GLY:HA2	1:D:401:VAL:HG21	1.87	0.56
1:B:319:ILE:HG23	1:B:383:LEU:HD12	1.87	0.56
1:D:253:PHE:HB3	1:D:258:VAL:HG11	1.89	0.54
1:E:462:ASP:OD1	1:F:55:ARG:NH2	2.39	0.54
1:F:392:PRO:HA	1:F:404:PRO:HB2	1.90	0.54
1:F:62:GLU:HG3	1:F:63:HIS:CD2	2.43	0.53
1:B:163:ILE:O	1:B:227:ARG:NH2	2.41	0.53
1:F:229:TYR:CD1	1:F:423:GLU:HG2	2.44	0.53
1:C:184:GLN:HG3	1:C:294:LEU:HG	1.91	0.52
1:A:217:VAL:HG13	1:A:433:VAL:HG22	1.91	0.52
1:C:73:VAL:HG11	1:D:59:LEU:HD22	1.91	0.52
1:B:129:TRP:CG	1:B:137:PRO:HB3	2.45	0.52
1:C:229:TYR:CD1	1:C:423:GLU:HG2	2.45	0.52
1:E:332:LYS:O	1:E:336:LYS:HG3	2.10	0.52
1:B:315:VAL:O	1:B:319:ILE:HG12	2.09	0.52
1:D:336:LYS:HG2	1:D:390:VAL:HG23	1.92	0.52
1:B:88:TRP:CE3	1:B:442:GLN:HG2	2.45	0.52
1:B:91:SER:OG	1:B:271:ASP:OD2	2.25	0.51
1:B:326:CYS:HB3	1:B:330:ILE:HD12	1.92	0.51
1:C:330:ILE:O	1:C:386:LYS:NZ	2.39	0.51
1:D:255:ASP:HB3	1:D:258:VAL:HG12	1.91	0.51
1:F:351:GLY:HA3	1:F:410:ALA:HB2	1.92	0.51
1:F:58:LYS:O	1:F:62:GLU:HG2	2.11	0.51
1:A:323:VAL:HG22	1:A:328:GLU:HA	1.92	0.51
1:B:118:SER:O	1:B:118:SER:OG	2.29	0.51
1:E:204:GLU:HB2	1:E:205:PRO:HD3	1.92	0.50
1:C:163:ILE:HD11	1:C:220:VAL:HG13	1.93	0.50
1:C:107:PRO:HA	1:C:110:GLN:HE21	1.76	0.50
1:D:416:LEU:HD22	1:D:421:LEU:HD23	1.94	0.50
1:A:384:VAL:HG21	1:A:414:VAL:HG11	1.93	0.50
1:D:460:THR:HG23	1:D:463:TRP:H	1.77	0.50
1:D:56:LEU:HD22	1:D:449:LEU:HB3	1.94	0.49
1:E:45:LEU:HD21	1:E:444:ILE:HG21	1.93	0.49
1:E:302:GLY:HA2	1:F:285:VAL:HG13	1.94	0.49
1:F:72:THR:HG23	1:F:75:MET:HG3	1.95	0.49
1:E:225:TYR:HB2	1:E:426:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:TYR:HB2	1:A:426:TYR:CZ	2.48	0.49
1:A:302:GLY:HA2	1:B:285:VAL:HG13	1.95	0.49
1:D:371:ALA:HB2	1:D:415:LEU:HD21	1.95	0.48
1:A:351:GLY:HA3	1:A:410:ALA:HB2	1.95	0.48
1:B:255:ASP:HB3	1:B:258:VAL:HG23	1.95	0.48
1:C:92:LEU:HD22	1:D:460:THR:HG22	1.95	0.48
1:C:70:ASN:OD1	1:D:70:ASN:ND2	2.46	0.48
1:F:88:TRP:CE3	1:F:442:GLN:HG2	2.48	0.48
1:F:271:ASP:HB2	1:F:438:GLY:HA3	1.95	0.48
1:D:386:LYS:O	1:D:390:VAL:HG12	2.13	0.48
1:E:88:TRP:CE3	1:E:442:GLN:HG2	2.49	0.48
1:B:163:ILE:HD11	1:B:220:VAL:HG13	1.96	0.47
1:A:189:PHE:HD1	1:A:205:PRO:HG2	1.79	0.47
1:C:88:TRP:CE3	1:C:442:GLN:HG2	2.50	0.47
1:F:75:MET:SD	1:F:83:MET:HG3	2.54	0.47
1:B:109:CYS:HA	1:B:113:LEU:HD13	1.95	0.47
1:E:253:PHE:HB3	1:E:258:VAL:HG11	1.97	0.47
1:F:339:VAL:HG11	1:F:391:VAL:HG22	1.97	0.47
1:B:229:TYR:CD1	1:B:423:GLU:HG2	2.50	0.47
1:F:371:ALA:HB2	1:F:415:LEU:HD21	1.97	0.47
1:D:384:VAL:HA	1:D:387:LEU:HD22	1.96	0.47
1:F:129:TRP:CG	1:F:137:PRO:HB3	2.50	0.47
1:D:163:ILE:HD11	1:D:220:VAL:HG13	1.95	0.46
1:D:384:VAL:HG21	1:D:414:VAL:HG11	1.96	0.46
1:D:287:SER:HB2	1:D:453:LEU:HA	1.97	0.46
1:C:225:TYR:HB2	1:C:426:TYR:CZ	2.51	0.46
1:F:393:PRO:O	1:F:397:GLU:HG3	2.15	0.46
1:D:225:TYR:HB2	1:D:426:TYR:CZ	2.50	0.46
1:E:89:GLU:OE1	1:F:461:MET:HG3	2.16	0.46
1:E:229:TYR:CD1	1:E:423:GLU:HG2	2.51	0.46
1:C:226:ARG:CZ	1:C:230:LYS:HG3	2.45	0.45
1:A:173:MET:SD	1:A:428:THR:HG22	2.56	0.45
1:B:371:ALA:HB2	1:B:415:LEU:HD21	1.99	0.45
1:A:465:GLU:OE1	1:B:55:ARG:NH2	2.48	0.45
1:B:75:MET:HG2	1:B:81:ARG:O	2.16	0.45
1:B:41:LEU:HB3	1:B:207:TYR:OH	2.16	0.45
1:E:417:ASN:OD1	1:E:422:THR:HG23	2.15	0.45
1:F:139:LYS:HD2	1:F:139:LYS:H	1.81	0.45
1:F:270:SER:O	1:F:435:ARG:HD3	2.16	0.45
1:A:343:LEU:HD21	1:A:349:ILE:HG12	1.98	0.45
1:C:75:MET:HG2	1:C:81:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:TRP:CE3	1:C:319:ILE:HD12	2.51	0.45
1:D:129:TRP:CG	1:D:137:PRO:HB3	2.51	0.45
1:D:319:ILE:HD13	1:D:384:VAL:HG22	1.99	0.45
1:C:189:PHE:HD1	1:C:205:PRO:HG2	1.81	0.45
1:A:77:ILE:HD12	1:B:87:LEU:HD22	1.98	0.44
1:B:225:TYR:HB2	1:B:426:TYR:CZ	2.52	0.44
1:C:371:ALA:HB2	1:C:415:LEU:HD21	1.99	0.44
1:B:189:PHE:HD1	1:B:205:PRO:HG2	1.81	0.44
1:A:315:VAL:HG11	1:A:410:ALA:HA	1.98	0.44
1:A:371:ALA:HB2	1:A:415:LEU:HD21	2.00	0.44
1:B:156:PRO:HG2	1:B:159:VAL:HG23	1.99	0.44
1:D:392:PRO:HA	1:D:404:PRO:HB2	2.00	0.44
1:E:392:PRO:HA	1:E:404:PRO:HB2	1.99	0.44
1:F:225:TYR:HB2	1:F:426:TYR:CZ	2.52	0.44
1:C:228:MET:O	1:F:340:TRP:HZ2	2.00	0.44
1:D:129:TRP:CD1	1:D:137:PRO:HB3	2.53	0.44
1:A:83:MET:HG2	1:B:71:ILE:HD11	2.00	0.44
1:D:88:TRP:CE3	1:D:442:GLN:HG2	2.53	0.44
1:A:342:THR:O	1:A:347:LYS:HB2	2.18	0.43
1:B:210:CYS:HB3	1:B:440:CYS:HB3	2.00	0.43
1:A:463:TRP:HZ3	1:B:68:LEU:HD22	1.83	0.43
1:E:364:TYR:CD1	1:E:411:HIS:HB2	2.53	0.43
1:B:132:LEU:HD21	1:B:444:ILE:HD12	2.00	0.43
1:B:391:VAL:HG22	1:B:392:PRO:HD3	2.01	0.43
1:C:132:LEU:HD21	1:C:444:ILE:HD12	2.00	0.43
1:F:112:VAL:HG22	1:F:136:VAL:HG21	2.00	0.43
1:F:41:LEU:HD21	1:F:132:LEU:HD12	2.00	0.43
1:C:39:LEU:H	1:C:141:GLN:HE21	1.65	0.43
1:D:421:LEU:HA	1:D:421:LEU:HD12	1.85	0.43
1:E:375:LEU:HD13	1:E:418:HIS:CG	2.54	0.43
1:B:257:LYS:HA	1:B:257:LYS:HD3	1.85	0.43
1:A:342:THR:CG2	1:A:347:LYS:HZ2	2.32	0.43
1:A:124:PRO:HD2	3:A:605:HOH:O	2.18	0.43
1:F:364:TYR:CD2	1:F:411:HIS:HB2	2.53	0.43
1:D:257:LYS:HD2	1:D:374:HIS:CD2	2.53	0.43
1:F:152:ARG:NH1	1:F:212:ASN:OD1	2.39	0.43
1:B:102:ARG:HG3	1:B:130:LEU:O	2.18	0.43
1:E:322:VAL:HG22	1:E:338:TYR:HE2	1.84	0.43
1:A:96:GLU:HB2	1:A:358:ARG:HH21	1.84	0.42
1:E:64:GLY:O	1:F:72:THR:OG1	2.36	0.42
1:E:285:VAL:HG13	1:F:302:GLY:HA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:VAL:HG22	1:F:383:LEU:HD13	2.01	0.42
1:A:88:TRP:CE3	1:A:442:GLN:HG2	2.53	0.42
1:B:184:GLN:HG3	1:B:294:LEU:HG	2.01	0.42
1:B:65:LYS:HD3	1:B:65:LYS:HA	1.76	0.42
1:E:163:ILE:HD11	1:E:220:VAL:HG13	2.01	0.42
1:E:253:PHE:CB	1:E:258:VAL:HG11	2.49	0.42
1:D:381:PHE:O	1:D:385:SER:OG	2.36	0.42
1:B:139:LYS:H	1:B:139:LYS:HD2	1.84	0.42
1:A:465:GLU:CD	1:B:55:ARG:HH21	2.22	0.42
1:C:102:ARG:HG3	1:C:130:LEU:O	2.20	0.42
1:D:340:TRP:CZ3	1:D:398:LEU:HD21	2.55	0.42
1:C:253:PHE:CB	1:C:258:VAL:HG11	2.50	0.42
1:D:139:LYS:HE2	1:D:139:LYS:HB3	1.90	0.42
1:A:461:MET:HG3	1:B:89:GLU:OE1	2.20	0.42
1:C:364:TYR:CD2	1:C:411:HIS:HB2	2.54	0.42
1:C:417:ASN:OD1	1:C:422:THR:HG23	2.20	0.42
1:D:135:LYS:HB2	1:D:135:LYS:HE2	1.84	0.42
1:F:125:GLU:OE2	1:F:146:SER:OG	2.37	0.42
1:B:392:PRO:HB2	1:B:393:PRO:HD3	2.02	0.42
1:A:337:GLU:HG3	1:A:341:LYS:HE2	2.01	0.41
1:A:229:TYR:CD1	1:A:423:GLU:HG2	2.54	0.41
1:F:311:ALA:O	1:F:315:VAL:HG13	2.20	0.41
1:A:152:ARG:NH1	1:A:212:ASN:OD1	2.44	0.41
1:A:372:LEU:O	1:A:376:PRO:HG3	2.20	0.41
1:D:44:GLN:O	1:D:48:LEU:HD23	2.20	0.41
1:A:71:ILE:HD11	1:B:83:MET:HG3	2.02	0.41
1:D:58:LYS:HD3	1:D:58:LYS:HA	1.82	0.41
1:D:257:LYS:HA	1:D:257:LYS:HD3	1.81	0.41
1:A:257:LYS:HA	1:A:257:LYS:HD3	1.85	0.41
1:D:157:ASP:HA	1:D:160:TYR:HD2	1.85	0.41
1:B:229:TYR:CE1	1:B:423:GLU:HG2	2.55	0.41
1:D:315:VAL:HG11	1:D:410:ALA:HA	2.01	0.41
1:E:319:ILE:HD13	1:E:384:VAL:HG22	2.01	0.41
1:F:106:ILE:HB	1:F:362:PRO:HB2	2.02	0.41
1:E:176:PHE:HZ	1:E:217:VAL:HG13	1.86	0.41
1:E:303:LEU:HA	1:E:308:HIS:CD2	2.56	0.41
1:A:445:TRP:HA	1:A:448:ALA:HB3	2.02	0.41
1:F:315:VAL:HG21	1:F:410:ALA:HA	2.03	0.41
1:A:315:VAL:HG21	1:A:410:ALA:HA	2.03	0.40
1:B:226:ARG:NH1	1:B:230:LYS:HE2	2.36	0.40
1:D:70:ASN:HA	1:D:70:ASN:HD22	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ILE:O	1:E:434:SER:OG	2.37	0.40
1:A:395:LEU:HB3	1:A:401:VAL:HG21	2.03	0.40
1:B:56:LEU:HD22	1:B:449:LEU:HB3	2.02	0.40
1:F:266:ILE:HD13	1:F:434:SER:HB2	2.04	0.40
1:A:73:VAL:O	1:A:77:ILE:HG12	2.21	0.40
1:D:364:TYR:CD2	1:D:411:HIS:HB2	2.56	0.40
1:E:380:LEU:O	1:E:384:VAL:HG23	2.22	0.40
1:C:94:ASP:HB2	1:C:100:ARG:HD2	2.04	0.40
1:E:70:ASN:HD22	1:E:70:ASN:HA	1.66	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:GLU:OE2	1:F:169:THR:OG1[1_545]	2.02	0.18

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	431/458 (94%)	423 (98%)	8 (2%)	0	100	100
1	B	428/458 (93%)	421 (98%)	7 (2%)	0	100	100
1	C	431/458 (94%)	424 (98%)	7 (2%)	0	100	100
1	D	428/458 (93%)	421 (98%)	7 (2%)	0	100	100
1	E	428/458 (93%)	422 (99%)	6 (1%)	0	100	100
1	F	430/458 (94%)	424 (99%)	6 (1%)	0	100	100
All	All	2576/2748 (94%)	2535 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	370/392 (94%)	359 (97%)	11 (3%)	41	70
1	B	367/392 (94%)	359 (98%)	8 (2%)	52	79
1	C	370/392 (94%)	359 (97%)	11 (3%)	41	70
1	D	367/392 (94%)	345 (94%)	22 (6%)	19	42
1	E	367/392 (94%)	355 (97%)	12 (3%)	38	67
1	F	369/392 (94%)	354 (96%)	15 (4%)	30	59
All	All	2210/2352 (94%)	2131 (96%)	79 (4%)	35	64

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	157	ASP
1	A	169	THR
1	A	217	VAL
1	A	323	VAL
1	A	347	LYS
1	A	375	LEU
1	A	377	ASP
1	A	401	VAL
1	A	421	LEU
1	A	431	PHE
1	B	217	VAL
1	B	227	ARG
1	B	329	ASP
1	B	375	LEU
1	B	377	ASP
1	B	383	LEU
1	B	431	PHE
1	B	460	THR
1	C	76	VAL
1	C	169	THR
1	C	217	VAL

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Mol	Chain	Res	Type
1	C	308	HIS
1	C	319	ILE
1	C	356	VAL
1	C	375	LEU
1	C	377	ASP
1	C	431	PHE
1	C	443	LEU
1	C	470	LYS
1	D	39	LEU
1	D	51	GLU
1	D	59	LEU
1	D	76	VAL
1	D	93	LEU
1	D	188	GLU
1	D	217	VAL
1	D	239	LYS
1	D	331	SER
1	D	357	LEU
1	D	358	ARG
1	D	375	LEU
1	D	377	ASP
1	D	385	SER
1	D	387	LEU
1	D	390	VAL
1	D	396	THR
1	D	400	LYS
1	D	401	VAL
1	D	402	LYS
1	D	431	PHE
1	D	462	ASP
1	E	115	THR
1	E	217	VAL
1	E	317	LEU
1	E	330	ILE
1	E	375	LEU
1	E	377	ASP
1	E	383	LEU
1	E	400	LYS
1	E	411	HIS
1	E	421	LEU
1	E	431	PHE
1	E	460	THR

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Mol	Chain	Res	Type
1	F	40	ASP
1	F	72	THR
1	F	76	VAL
1	F	136	VAL
1	F	139	LYS
1	F	146	SER
1	F	168	SER
1	F	169	THR
1	F	211	LEU
1	F	319	ILE
1	F	375	LEU
1	F	377	ASP
1	F	401	VAL
1	F	402	LYS
1	F	431	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	C	67	GLN
1	D	67	GLN
1	D	70	ASN
1	E	70	ASN
1	F	67	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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(Å ²)	Q<0.9
1	A	433/458 (94%)	0.34	23 (5%)	26 25	30, 55, 85, 100	0
1	B	430/458 (93%)	0.06	4 (0%)	84 85	30, 48, 70, 85	0
1	C	433/458 (94%)	0.09	4 (0%)	84 85	33, 54, 79, 105	0
1	D	430/458 (93%)	0.17	9 (2%)	63 65	34, 57, 94, 107	0
1	E	430/458 (93%)	0.04	8 (1%)	66 69	35, 48, 74, 96	0
1	F	432/458 (94%)	0.27	15 (3%)	44 44	34, 60, 87, 100	0
All	All	2588/2748 (94%)	0.16	63 (2%)	59 60	30, 53, 84, 107	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	118	SER	4.8
1	A	340	TRP	4.5
1	F	401	VAL	4.0
1	F	140	GLU	3.7
1	A	396	THR	3.6
1	A	467	HIS	3.6
1	E	401	VAL	3.6
1	E	117	GLN	3.6
1	E	400	LYS	3.6
1	A	397	GLU	3.5
1	E	402	LYS	3.2
1	A	354	HIS	3.2
1	A	322	VAL	3.2
1	B	202	PHE	3.1
1	A	326	CYS	3.1
1	A	343	LEU	3.0
1	F	197	ILE	3.0
1	F	402	LYS	2.9
1	A	39	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	358	ARG	2.9
1	F	334	GLN	2.9
1	D	388	TYR	2.9
1	E	39	LEU	2.8
1	A	414	VAL	2.8
1	C	427	TYR	2.8
1	B	59	LEU	2.8
1	D	109	CYS	2.7
1	F	354	HIS	2.7
1	F	39	LEU	2.6
1	D	377	ASP	2.6
1	A	400	LYS	2.6
1	F	404	PRO	2.6
1	C	317	LEU	2.6
1	D	68	LEU	2.6
1	E	356	VAL	2.5
1	A	402	LYS	2.5
1	A	319	ILE	2.5
1	B	39	LEU	2.5
1	A	64	GLY	2.5
1	A	65	LYS	2.5
1	C	468	CYS	2.5
1	E	299	ALA	2.4
1	F	54	ASP	2.4
1	F	151	ASN	2.4
1	D	104	LEU	2.4
1	A	395	LEU	2.4
1	C	51	GLU	2.3
1	F	347	LYS	2.3
1	A	311	ALA	2.3
1	A	427	TYR	2.2
1	F	255	ASP	2.2
1	D	157	ASP	2.2
1	B	65	LYS	2.1
1	A	358	ARG	2.1
1	D	400	LYS	2.1
1	A	346	GLY	2.1
1	A	349	ILE	2.1
1	E	463	TRP	2.1
1	A	333	GLU	2.1
1	F	295	SER	2.1
1	A	380	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	117	GLN	2.0
1	D	57	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	CL	B	501	1/1	0.97	0.27	44,44,44,44	0
2	CL	D	501	1/1	0.97	0.34	49,49,49,49	0
2	CL	E	501	1/1	0.97	0.24	54,54,54,54	0
2	CL	F	501	1/1	0.97	0.22	56,56,56,56	0
2	CL	C	501	1/1	0.98	0.24	44,44,44,44	0
2	CL	A	501	1/1	0.98	0.39	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.