Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2023 – 09:45 AM EDT

PDB ID	:	2QFW
Title	:	Crystal structure of Saccharomyces cerevesiae mitochondrial NADP(+)-dependent isocitrate dehydrogenase in complex with isocitrate
Authors	:	Peng, Y.J.; Ding, J.P.
Deposited on	:	2007-06-28
Resolution	:	2.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

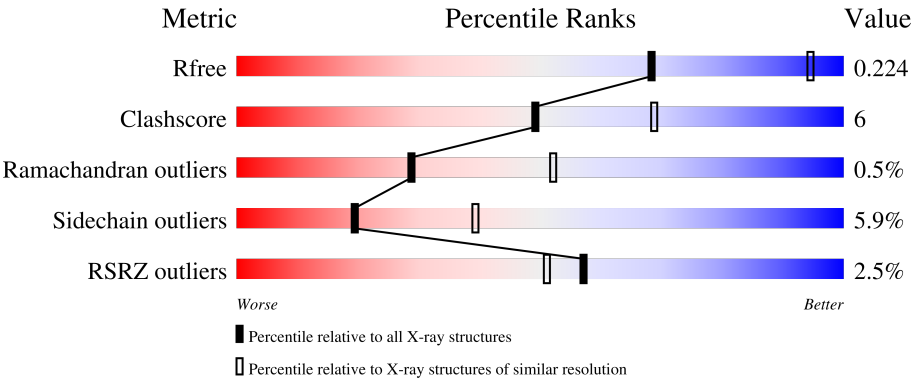
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	427	79% 15% • 5%
1	B	427	79% 15% • •
1	C	427	3% 75% 20% • •
1	D	427	3% 77% 17% • •
1	E	427	4% 77% 17% • •

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Mol	Chain	Length	Quality of chain
1	F	427	3% 78% 17%

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	ICT	D	2104	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20688 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 Isocitrate dehydrogenase [NADP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3222	2052	546	612	12			
1	B	408	Total	C	N	O	S	0	0	0
			3231	2058	548	613	12			
1	C	410	Total	C	N	O	S	0	0	0
			3245	2067	550	616	12			
1	D	412	Total	C	N	O	S	0	0	0
			3261	2079	552	618	12			
1	E	409	Total	C	N	O	S	0	0	0
			3237	2061	549	615	12			
1	F	411	Total	C	N	O	S	0	0	0
			3256	2076	551	617	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP P21954
A	-12	HIS	-	expression tag	UNP P21954
A	-11	HIS	-	expression tag	UNP P21954
A	-10	HIS	-	expression tag	UNP P21954
A	-9	HIS	-	expression tag	UNP P21954
A	-8	HIS	-	expression tag	UNP P21954
A	-7	HIS	-	expression tag	UNP P21954
A	-6	ALA	-	expression tag	UNP P21954
A	-5	MET	-	expression tag	UNP P21954
A	-4	GLY	-	expression tag	UNP P21954
A	-3	ILE	-	expression tag	UNP P21954
A	-2	PRO	-	expression tag	UNP P21954
A	-1	GLY	-	expression tag	UNP P21954
A	0	HIS	-	expression tag	UNP P21954
B	-13	MET	-	expression tag	UNP P21954
B	-12	HIS	-	expression tag	UNP P21954
B	-11	HIS	-	expression tag	UNP P21954

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP P21954
B	-9	HIS	-	expression tag	UNP P21954
B	-8	HIS	-	expression tag	UNP P21954
B	-7	HIS	-	expression tag	UNP P21954
B	-6	ALA	-	expression tag	UNP P21954
B	-5	MET	-	expression tag	UNP P21954
B	-4	GLY	-	expression tag	UNP P21954
B	-3	ILE	-	expression tag	UNP P21954
B	-2	PRO	-	expression tag	UNP P21954
B	-1	GLY	-	expression tag	UNP P21954
B	0	HIS	-	expression tag	UNP P21954
C	-13	MET	-	expression tag	UNP P21954
C	-12	HIS	-	expression tag	UNP P21954
C	-11	HIS	-	expression tag	UNP P21954
C	-10	HIS	-	expression tag	UNP P21954
C	-9	HIS	-	expression tag	UNP P21954
C	-8	HIS	-	expression tag	UNP P21954
C	-7	HIS	-	expression tag	UNP P21954
C	-6	ALA	-	expression tag	UNP P21954
C	-5	MET	-	expression tag	UNP P21954
C	-4	GLY	-	expression tag	UNP P21954
C	-3	ILE	-	expression tag	UNP P21954
C	-2	PRO	-	expression tag	UNP P21954
C	-1	GLY	-	expression tag	UNP P21954
C	0	HIS	-	expression tag	UNP P21954
D	-13	MET	-	expression tag	UNP P21954
D	-12	HIS	-	expression tag	UNP P21954
D	-11	HIS	-	expression tag	UNP P21954
D	-10	HIS	-	expression tag	UNP P21954
D	-9	HIS	-	expression tag	UNP P21954
D	-8	HIS	-	expression tag	UNP P21954
D	-7	HIS	-	expression tag	UNP P21954
D	-6	ALA	-	expression tag	UNP P21954
D	-5	MET	-	expression tag	UNP P21954
D	-4	GLY	-	expression tag	UNP P21954
D	-3	ILE	-	expression tag	UNP P21954
D	-2	PRO	-	expression tag	UNP P21954
D	-1	GLY	-	expression tag	UNP P21954
D	0	HIS	-	expression tag	UNP P21954
E	-13	MET	-	expression tag	UNP P21954
E	-12	HIS	-	expression tag	UNP P21954
E	-11	HIS	-	expression tag	UNP P21954

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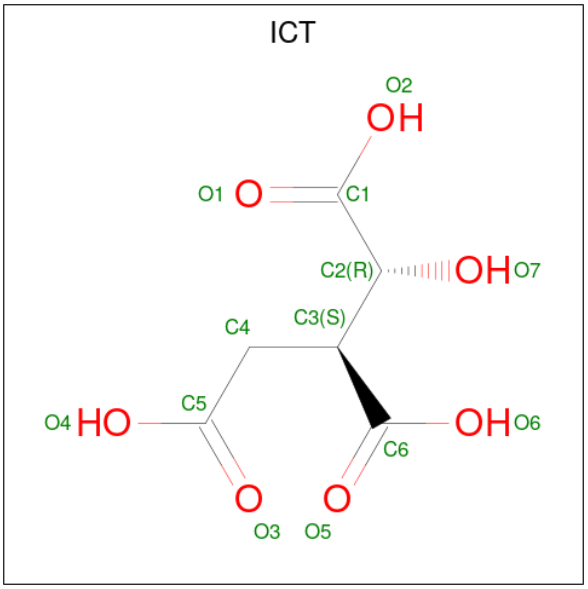
Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP P21954
E	-9	HIS	-	expression tag	UNP P21954
E	-8	HIS	-	expression tag	UNP P21954
E	-7	HIS	-	expression tag	UNP P21954
E	-6	ALA	-	expression tag	UNP P21954
E	-5	MET	-	expression tag	UNP P21954
E	-4	GLY	-	expression tag	UNP P21954
E	-3	ILE	-	expression tag	UNP P21954
E	-2	PRO	-	expression tag	UNP P21954
E	-1	GLY	-	expression tag	UNP P21954
E	0	HIS	-	expression tag	UNP P21954
F	-13	MET	-	expression tag	UNP P21954
F	-12	HIS	-	expression tag	UNP P21954
F	-11	HIS	-	expression tag	UNP P21954
F	-10	HIS	-	expression tag	UNP P21954
F	-9	HIS	-	expression tag	UNP P21954
F	-8	HIS	-	expression tag	UNP P21954
F	-7	HIS	-	expression tag	UNP P21954
F	-6	ALA	-	expression tag	UNP P21954
F	-5	MET	-	expression tag	UNP P21954
F	-4	GLY	-	expression tag	UNP P21954
F	-3	ILE	-	expression tag	UNP P21954
F	-2	PRO	-	expression tag	UNP P21954
F	-1	GLY	-	expression tag	UNP P21954
F	0	HIS	-	expression tag	UNP P21954

- Molecule 2 is ISOCITRIC ACID (three-letter code: ICT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

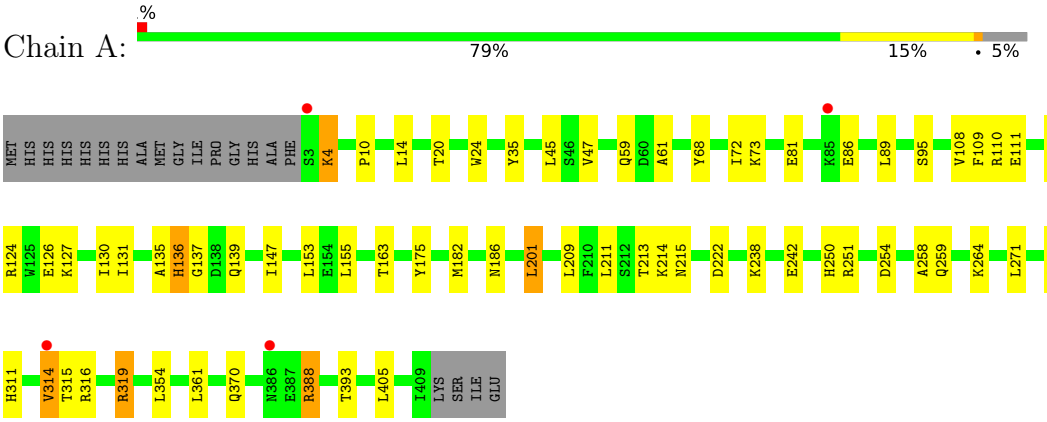
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	217	Total O 217 217	0	0
3	B	252	Total O 252 252	0	0
3	C	161	Total O 161 161	0	0
3	D	185	Total O 185 185	0	0
3	E	163	Total O 163 163	0	0
3	F	180	Total O 180 180	0	0

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.

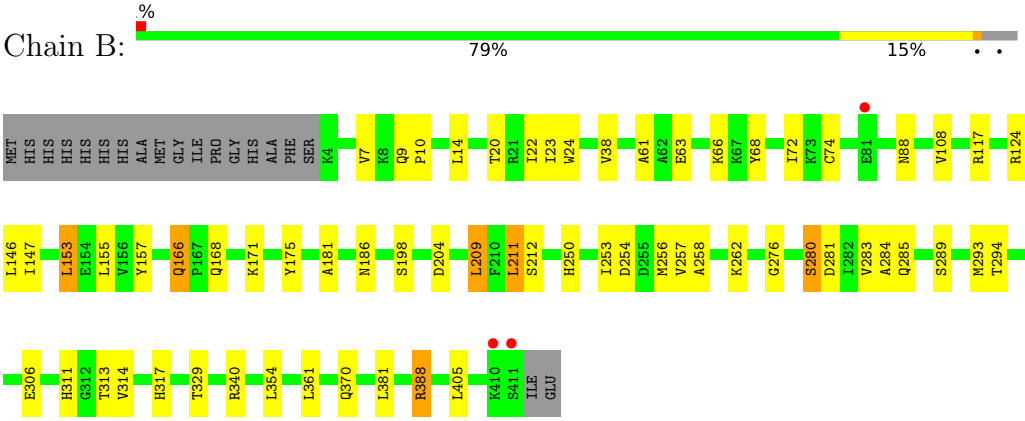
• Molecule 1: Isocitrate dehydrogenase [NADP]

Chain A:



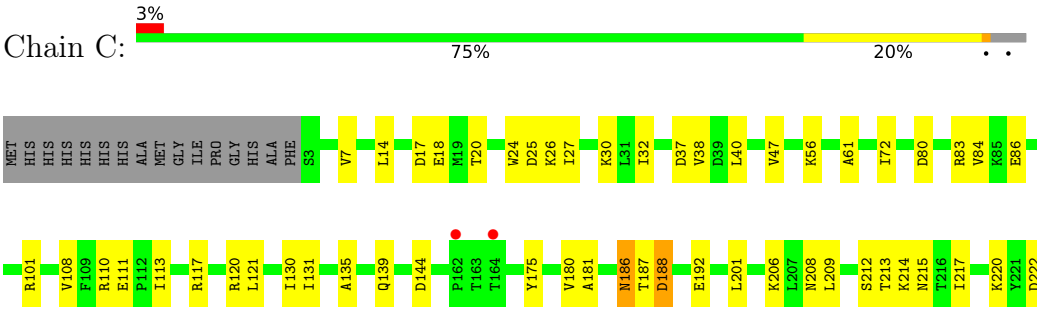
• Molecule 1: Isocitrate dehydrogenase [NADP]

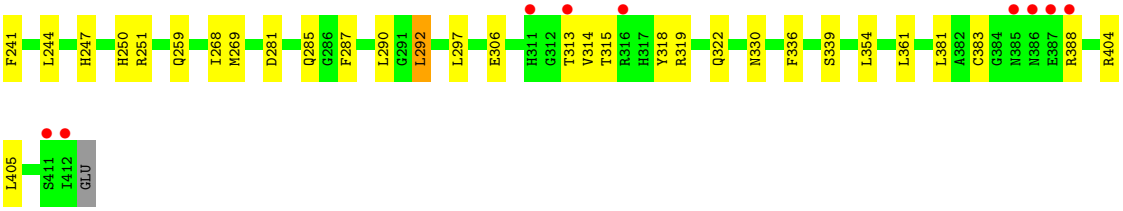
Chain B:



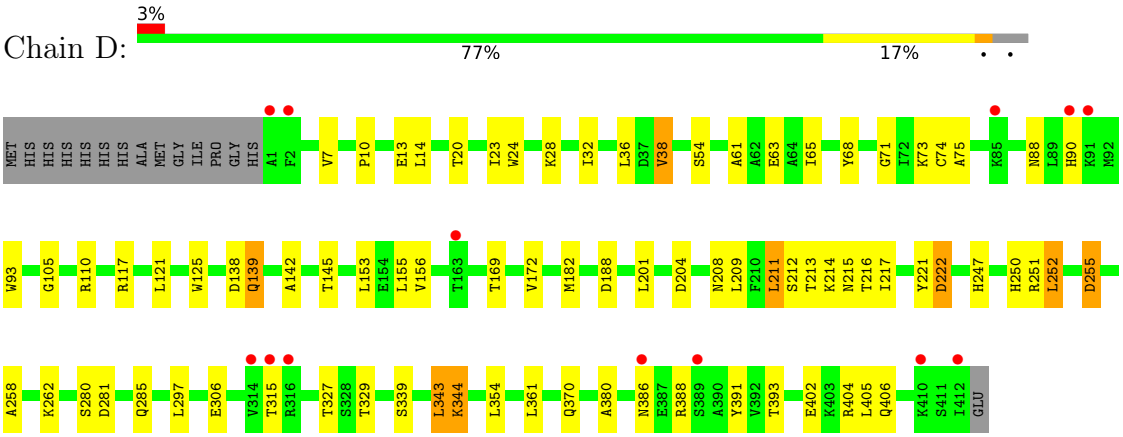
• Molecule 1: Isocitrate dehydrogenase [NADP]

Chain C:

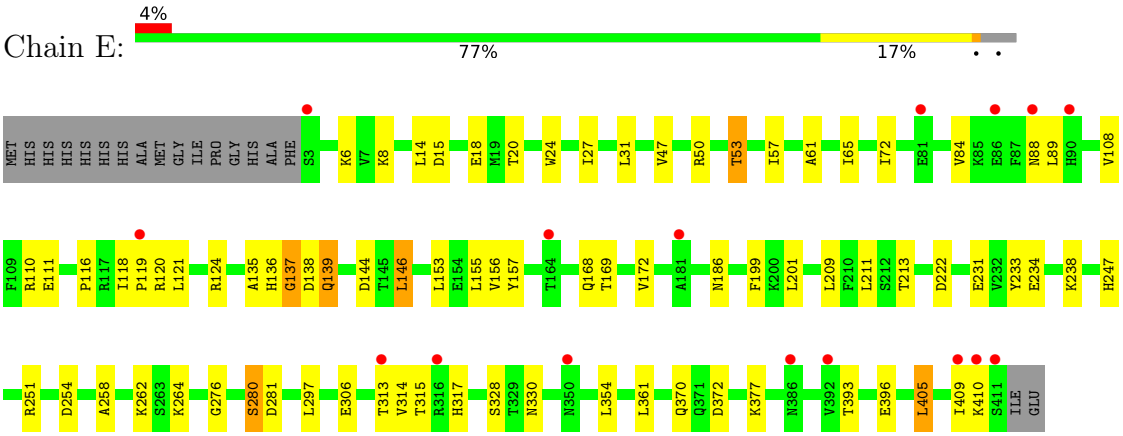




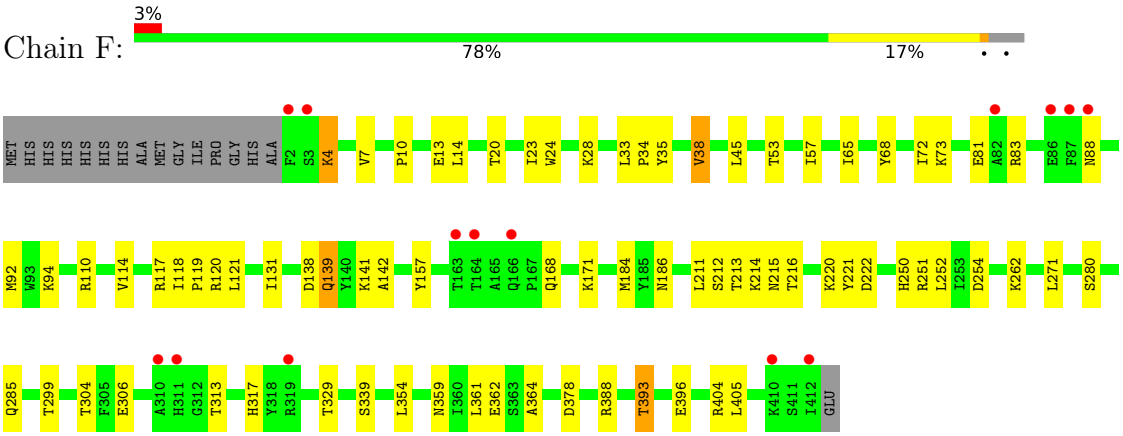
• Molecule 1: Isocitrate dehydrogenase [NADP]



• Molecule 1: Isocitrate dehydrogenase [NADP]



• Molecule 1: Isocitrate dehydrogenase [NADP]



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.70Å 97.89Å 190.65Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-2.60) 98.4 (19.79-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.59Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.232 , 0.292 0.224 , 0.224	Depositor DCC
R_{free} test set	4114 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20688	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: ICT

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	0.29	0/3284	0.64	0/4431
1	B	0.29	0/3293	0.63	1/4442 (0.0%)
1	C	0.29	0/3307	0.64	2/4461 (0.0%)
1	D	0.29	0/3324	0.64	3/4484 (0.1%)
1	E	0.29	0/3299	0.64	1/4450 (0.0%)
1	F	0.29	0/3319	0.64	0/4477
All	All	0.29	0/19826	0.64	7/26745 (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	D	188	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	37	ASP	CB-CG-OD2	5.51	123.25	118.30
1	D	281	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	188	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	222	ASP	CB-CG-OD2	5.23	123.01	118.30
1	E	281	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	281	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3222	0	3264	33	0
1	B	3231	0	3277	34	0
1	C	3245	0	3293	49	0
1	D	3261	0	3310	50	0
1	E	3237	0	3282	39	0
1	F	3256	0	3302	44	0
2	A	13	0	5	1	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	0	0
3	A	217	0	0	1	0
3	B	252	0	0	1	0
3	C	161	0	0	1	0
3	D	185	0	0	2	0
3	E	163	0	0	4	0
3	F	180	0	0	2	0
All	All	20688	0	19758	233	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 6.

All (233) 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:18:GLU:HB2	1:C:313:THR:HG21	1.19	1.15
1:C:238:LYS:HD2	1:C:239:SER:H	1.31	0.92
1:C:180:VAL:HG21	1:D:221:TYR:HA	1.59	0.85
1:A:117:ARG:H	1:A:370:GLN:HE22	1.25	0.84
1:D:214:LYS:HE3	1:D:217:ILE:HD13	1.60	0.83
1:D:117:ARG:H	1:D:370:GLN:HE22	1.25	0.83
1:C:18:GLU:HB2	1:C:313:THR:CG2	2.08	0.81
1:C:186:ASN:HD22	1:C:187:THR:H	1.27	0.80
1:E:276:GLY:O	1:E:280:SER:HB2	1.80	0.80
1:E:110:ARG:HD3	1:E:280:SER:OG	1.86	0.76
1:F:213:THR:HG23	1:F:222:ASP:HB3	1.69	0.75
1:D:213:THR:CG2	1:D:222:ASP:HB3	2.16	0.75
1:F:393:THR:HG22	1:F:396:GLU:H	1.51	0.75
1:F:138:ASP:HB3	1:F:139:GLN:OE1	1.87	0.74
1:D:213:THR:HG23	1:D:222:ASP:HB3	1.68	0.74
1:B:117:ARG:H	1:B:370:GLN:HE22	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLN:HE21	1:B:166:GLN:HA	1.54	0.72
1:D:65:ILE:HD12	1:D:71:GLY:HA3	1.72	0.71
1:E:24:TRP:HH2	1:E:72:ILE:HG22	1.55	0.70
1:E:124:ARG:HH21	1:E:264:LYS:HE3	1.57	0.69
1:C:121:LEU:HD13	1:D:262:LYS:HA	1.75	0.67
1:A:213:THR:HG23	1:A:222:ASP:HB3	1.76	0.67
1:C:319:ARG:HA	1:C:322:GLN:HE21	1.60	0.66
1:F:213:THR:CG2	1:F:222:ASP:HB3	2.26	0.66
1:F:184:MET:HE1	3:F:2136:HOH:O	1.95	0.65
1:A:213:THR:CG2	1:A:222:ASP:HB3	2.27	0.65
1:C:213:THR:HG23	1:C:215:ASN:H	1.60	0.65
1:C:238:LYS:HD2	1:C:239:SER:N	2.08	0.65
1:B:276:GLY:O	1:B:280:SER:HB2	1.97	0.64
1:F:364:ALA:HB1	1:F:404:ARG:HB3	1.79	0.63
1:B:117:ARG:N	1:B:370:GLN:HE22	1.98	0.62
1:A:108:VAL:HG23	1:A:135:ALA:HB2	1.82	0.62
1:D:213:THR:HB	1:D:250:HIS:NE2	2.15	0.61
1:E:53:THR:HG21	1:E:57:ILE:H	1.66	0.61
1:C:180:VAL:CG2	1:D:221:TYR:HA	2.30	0.61
1:D:208:ASN:ND2	1:D:247:HIS:H	1.99	0.60
1:E:297:LEU:HB3	1:E:306:GLU:HB3	1.84	0.60
1:E:24:TRP:CH2	1:E:72:ILE:HG22	2.36	0.59
1:C:24:TRP:HH2	1:C:72:ILE:HG22	1.67	0.59
1:D:110:ARG:HD3	1:D:280:SER:OG	2.03	0.59
1:D:7:VAL:HG21	1:D:38:VAL:HG13	1.86	0.58
1:C:290:LEU:HB2	1:C:292:LEU:HD23	1.86	0.57
1:A:251:ARG:HH22	1:A:259:GLN:HE22	1.53	0.57
1:C:213:THR:HG22	1:C:250:HIS:NE2	2.20	0.57
1:E:14:LEU:HD22	1:E:61:ALA:HB1	1.86	0.57
1:A:238:LYS:O	1:A:242:GLU:HG3	2.05	0.56
1:F:24:TRP:HH2	1:F:72:ILE:HG22	1.69	0.56
1:B:108:VAL:HG23	1:B:135:ALA:HB2	1.87	0.56
1:E:108:VAL:HG23	1:E:135:ALA:HB2	1.88	0.56
1:F:213:THR:HB	1:F:250:HIS:NE2	2.20	0.56
1:E:199:PHE:CZ	1:E:233:TYR:HB2	2.39	0.56
1:D:252:LEU:HB2	1:D:255:ASP:OD2	2.05	0.55
1:D:138:ASP:HB3	1:D:139:GLN:OE1	2.07	0.55
1:C:24:TRP:CH2	1:C:72:ILE:HG22	2.41	0.55
1:B:24:TRP:HH2	1:B:72:ILE:HG22	1.72	0.54
1:C:281:ASP:HB3	1:D:258:ALA:HB2	1.89	0.54
1:E:53:THR:CG2	1:E:57:ILE:H	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:VAL:HG12	1:E:169:THR:HG23	1.90	0.53
1:D:213:THR:HG22	1:D:215:ASN:N	2.24	0.53
1:B:153:LEU:HD11	1:B:181:ALA:HB1	1.91	0.53
1:C:213:THR:OG1	1:C:222:ASP:HB3	2.09	0.53
1:D:402:GLU:O	1:D:406:GLN:HG3	2.09	0.53
1:D:20:THR:HG21	1:D:75:ALA:HB3	1.90	0.53
1:E:328:SER:HB3	1:E:377:LYS:HB2	1.89	0.53
1:E:258:ALA:O	1:F:285:GLN:HG2	2.09	0.52
1:F:24:TRP:CH2	1:F:72:ILE:HG22	2.44	0.52
1:F:81:GLU:HG3	1:F:92:MET:HE1	1.91	0.52
1:A:126:GLU:HG3	1:A:127:LYS:HG3	1.91	0.52
1:E:313:THR:HB	3:E:2107:HOH:O	2.08	0.52
1:E:27:ILE:HG23	1:E:31:LEU:HD12	1.90	0.52
1:A:111:GLU:HB3	1:A:130:ILE:HG12	1.92	0.51
1:B:294:THR:HG21	1:B:340:ARG:HE	1.74	0.51
1:E:405:LEU:O	1:E:409:ILE:HG13	2.10	0.51
1:D:61:ALA:O	1:D:65:ILE:HG12	2.09	0.51
1:D:213:THR:HG22	1:D:215:ASN:H	1.75	0.51
1:C:84:VAL:HG13	1:C:89:LEU:HB2	1.93	0.51
1:B:24:TRP:CH2	1:B:72:ILE:HG22	2.46	0.51
1:F:7:VAL:HG21	1:F:38:VAL:HG13	1.93	0.51
1:A:14:LEU:HB2	1:A:73:LYS:HG3	1.92	0.51
1:E:146:LEU:HD13	1:F:220:LYS:HB3	1.91	0.51
1:B:284:ALA:HB2	1:B:293:MET:SD	2.52	0.50
1:C:80:ASP:O	1:C:84:VAL:HG23	2.10	0.50
1:D:156:VAL:HG22	1:D:169:THR:HG23	1.92	0.50
1:B:253:ILE:O	1:B:257:VAL:HG22	2.11	0.50
1:A:258:ALA:O	1:B:285:GLN:HG2	2.12	0.50
1:B:7:VAL:HG21	1:B:38:VAL:HB	1.94	0.50
1:A:47:VAL:HG12	1:A:89:LEU:HD21	1.93	0.50
1:C:208:ASN:ND2	1:C:247:HIS:H	2.10	0.49
1:D:344:LYS:HE3	1:D:344:LYS:HA	1.93	0.49
1:A:213:THR:HG22	1:A:215:ASN:N	2.26	0.49
1:F:20:THR:OG1	1:F:313:THR:HB	2.12	0.49
1:D:13:GLU:OE2	1:D:28:LYS:HE2	2.11	0.49
1:F:339:SER:OG	1:F:362:GLU:HG3	2.12	0.49
1:A:315:THR:HG21	1:A:319:ARG:HH21	1.78	0.49
1:A:213:THR:HB	1:A:250:HIS:NE2	2.28	0.48
1:D:14:LEU:HD22	1:D:61:ALA:HB1	1.95	0.48
1:D:297:LEU:HB3	1:D:306:GLU:HB3	1.96	0.48
1:F:359:ASN:HA	3:F:2185:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ARG:HB2	3:B:2104:HOH:O	2.12	0.48
1:A:285:GLN:HG2	1:B:258:ALA:O	2.12	0.48
1:C:251:ARG:NH1	1:C:259:GLN:OE1	2.46	0.48
1:C:318:TYR:O	1:C:322:GLN:HG3	2.13	0.48
1:E:116:PRO:HG2	1:E:370:GLN:NE2	2.28	0.48
1:F:299:THR:OG1	1:F:304:THR:HB	2.14	0.48
1:B:212:SER:OG	1:B:256:MET:HG2	2.13	0.48
1:C:7:VAL:HG21	1:C:38:VAL:HG22	1.94	0.48
1:E:153:LEU:HD12	1:E:172:VAL:HB	1.95	0.47
1:B:297:LEU:HB3	1:B:306:GLU:HB3	1.95	0.47
1:E:144:ASP:HB2	1:F:221:TYR:HB2	1.95	0.47
1:A:136:HIS:CG	1:A:137:GLY:N	2.82	0.47
1:C:25:ASP:HB2	3:C:2106:HOH:O	2.14	0.47
1:C:117:ARG:HD3	1:C:383:CYS:SG	2.55	0.47
1:F:13:GLU:OE2	1:F:28:LYS:HE2	2.15	0.47
1:A:124:ARG:HH21	1:A:264:LYS:HE3	1.80	0.47
1:D:153:LEU:HD12	1:D:172:VAL:HB	1.97	0.47
1:F:14:LEU:HD12	1:F:73:LYS:HD2	1.96	0.47
1:C:108:VAL:HG23	1:C:135:ALA:HB2	1.96	0.46
1:B:314:VAL:HB	1:B:317:HIS:HD2	1.80	0.46
1:E:111:GLU:HG3	3:E:2125:HOH:O	2.14	0.46
1:F:23:ILE:HD11	1:F:329:THR:HB	1.97	0.46
1:F:53:THR:HG21	1:F:57:ILE:HG22	1.97	0.46
1:F:213:THR:CG2	1:F:214:LYS:N	2.78	0.46
1:A:147:ILE:HG13	1:A:175:TYR:CZ	2.51	0.46
1:C:285:GLN:NE2	1:D:262:LYS:HD3	2.30	0.46
1:C:130:ILE:HB	1:C:268:ILE:HG12	1.98	0.46
1:D:139:GLN:HA	1:D:142:ALA:HB2	1.98	0.46
1:C:220:LYS:HD3	1:D:145:THR:HA	1.97	0.45
1:B:198:SER:HB3	1:B:209:LEU:HD11	1.99	0.45
1:B:388:ARG:O	1:B:388:ARG:HD3	2.17	0.45
1:D:212:SER:HA	1:D:251:ARG:O	2.17	0.45
1:D:216:THR:HG23	1:D:252:LEU:HD11	1.98	0.45
1:F:114:VAL:HG13	1:F:120:ARG:HH21	1.82	0.45
1:F:213:THR:HG22	1:F:214:LYS:N	2.32	0.45
1:C:297:LEU:HB3	1:C:306:GLU:HB3	1.99	0.45
1:C:212:SER:HA	1:C:251:ARG:O	2.17	0.45
1:E:14:LEU:HD11	1:E:65:ILE:HD11	1.98	0.45
1:E:234:GLU:HA	1:E:238:LYS:HB2	1.99	0.45
1:A:121:LEU:HD13	1:B:262:LYS:HA	1.99	0.45
1:C:26:LYS:O	1:C:30:LYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LYS:HE3	1:C:217:ILE:HD13	1.99	0.45
1:D:339:SER:O	1:D:343:LEU:HB2	2.17	0.45
1:F:139:GLN:HA	1:F:142:ALA:HB2	1.99	0.45
1:C:213:THR:CG2	1:C:250:HIS:NE2	2.80	0.44
1:D:24:TRP:CD2	1:D:74:CYS:HB2	2.51	0.44
1:A:109:PHE:CE1	1:A:201:LEU:HD12	2.52	0.44
1:A:213:THR:CG2	1:A:214:LYS:N	2.80	0.44
1:E:262:LYS:HA	1:F:121:LEU:CD2	2.47	0.44
1:E:314:VAL:HG11	1:E:317:HIS:HD2	1.82	0.44
1:B:117:ARG:H	1:B:370:GLN:NE2	2.07	0.44
1:A:4:LYS:HA	1:A:35:TYR:O	2.18	0.44
1:A:110:ARG:HH22	2:A:2101:ICT:C1	2.30	0.44
1:E:50:ARG:HD2	3:E:2127:HOH:O	2.18	0.44
1:E:116:PRO:HA	3:E:2263:HOH:O	2.18	0.44
1:C:120:ARG:HG2	1:C:287:PHE:O	2.18	0.44
1:F:213:THR:HG23	1:F:222:ASP:CB	2.44	0.44
1:C:111:GLU:HG3	1:C:130:ILE:HG12	2.00	0.44
1:A:213:THR:HG22	1:A:215:ASN:H	1.83	0.43
1:C:131:ILE:HD13	1:C:269:MET:HB2	2.00	0.43
1:C:285:GLN:HG2	1:D:258:ALA:O	2.18	0.43
1:F:10:PRO:HG2	1:F:68:TYR:CD2	2.53	0.43
1:A:213:THR:HG22	1:A:214:LYS:N	2.32	0.43
1:B:388:ARG:HD3	1:B:388:ARG:C	2.39	0.43
1:D:23:ILE:HD11	1:D:329:THR:HB	1.99	0.43
1:E:136:HIS:CG	1:E:137:GLY:N	2.86	0.43
1:A:131:ILE:HG23	1:A:271:LEU:HD12	2.01	0.43
1:A:314:VAL:HG12	1:A:316:ARG:HG2	2.00	0.43
1:D:208:ASN:HD22	1:D:247:HIS:H	1.63	0.43
1:E:393:THR:HG22	1:E:396:GLU:HB2	2.00	0.43
1:B:9:GLN:HE21	1:B:10:PRO:HD2	1.84	0.43
1:C:14:LEU:HD22	1:C:61:ALA:HB1	2.00	0.43
1:C:217:ILE:HD11	3:D:2254:HOH:O	2.19	0.43
1:E:53:THR:HG21	1:E:57:ILE:HB	2.00	0.43
1:E:110:ARG:HD3	1:E:280:SER:HG	1.81	0.43
1:F:141:LYS:HD2	1:F:141:LYS:HA	1.83	0.43
1:D:10:PRO:HG2	1:D:68:TYR:CD2	2.54	0.43
1:A:24:TRP:CH2	1:A:72:ILE:HG22	2.54	0.43
1:D:213:THR:CG2	1:D:215:ASN:HB3	2.49	0.43
1:F:118:ILE:HA	1:F:119:PRO:HD3	1.90	0.43
1:D:213:THR:HG22	1:D:214:LYS:N	2.34	0.42
1:D:14:LEU:HB2	1:D:73:LYS:HG3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:THR:HG23	1:D:222:ASP:CB	2.42	0.42
1:D:32:ILE:HG23	1:D:36:LEU:HD12	2.01	0.42
1:E:84:VAL:HG13	1:E:89:LEU:HB2	2.01	0.42
1:E:157:TYR:HB3	1:E:168:GLN:HB2	2.01	0.42
1:F:65:ILE:HD13	1:F:306:GLU:HG3	2.01	0.42
1:F:131:ILE:HD12	1:F:280:SER:HA	2.02	0.42
1:C:336:PHE:HA	1:C:339:SER:OG	2.20	0.42
1:D:121:LEU:HD12	1:D:285:GLN:O	2.20	0.42
1:E:118:ILE:HA	1:E:119:PRO:HD3	1.88	0.42
1:F:213:THR:HG22	1:F:215:ASN:H	1.83	0.42
1:A:14:LEU:CD2	1:A:61:ALA:HB1	2.50	0.42
1:B:211:LEU:HD13	1:B:250:HIS:HD2	1.85	0.42
1:C:83:ARG:HA	1:C:86:GLU:HG2	2.00	0.42
1:A:10:PRO:HG2	1:A:68:TYR:CD2	2.54	0.42
1:A:259:GLN:HG2	3:A:2310:HOH:O	2.20	0.42
1:C:144:ASP:HB2	1:D:221:TYR:HB2	2.00	0.42
1:E:213:THR:HB	1:E:222:ASP:HB3	2.00	0.42
1:A:251:ARG:HH12	1:A:259:GLN:NE2	2.17	0.42
1:D:213:THR:CG2	1:D:214:LYS:N	2.83	0.42
1:F:33:LEU:N	1:F:34:PRO:CD	2.83	0.42
1:B:24:TRP:CD2	1:B:74:CYS:HB2	2.54	0.42
1:D:380:ALA:HB2	1:D:391:TYR:HB3	2.00	0.42
1:D:315:THR:HG21	3:D:2267:HOH:O	2.20	0.41
1:C:206:LYS:HG2	1:C:244:LEU:HD13	2.02	0.41
1:F:212:SER:HB2	1:F:271:LEU:HD23	2.01	0.41
1:B:14:LEU:HD22	1:B:61:ALA:HB1	2.02	0.41
1:F:213:THR:HG22	1:F:215:ASN:N	2.36	0.41
1:B:10:PRO:HG2	1:B:68:TYR:CD2	2.55	0.41
1:B:23:ILE:HD11	1:B:329:THR:HB	2.02	0.41
1:B:157:TYR:HB3	1:B:168:GLN:HB2	2.01	0.41
1:B:301:ASP:OD1	1:B:303:LYS:HG2	2.20	0.41
1:C:27:ILE:HG22	1:C:32:ILE:HD13	2.02	0.41
1:F:4:LYS:HA	1:F:35:TYR:O	2.19	0.41
1:B:20:THR:OG1	1:B:313:THR:HB	2.21	0.41
1:B:147:ILE:HG13	1:B:175:TYR:CZ	2.55	0.41
1:E:138:ASP:HB3	1:E:139:GLN:OE1	2.20	0.41
1:B:131:ILE:HD11	1:B:283:VAL:HG21	2.02	0.41
1:C:101:ARG:HG2	1:C:297:LEU:HD12	2.02	0.41
1:C:188:ASP:O	1:C:192:GLU:HG3	2.21	0.41
1:D:211:LEU:HD13	1:D:250:HIS:HD2	1.86	0.41
1:E:121:LEU:HD13	1:F:262:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ARG:HH22	1:A:393:THR:HG22	1.86	0.40
1:C:113:ILE:HB	1:C:292:LEU:HB3	2.03	0.40
1:E:18:GLU:OE2	1:E:315:THR:HG23	2.21	0.40
1:F:110:ARG:HD2	1:F:280:SER:OG	2.21	0.40
1:C:17:ASP:OD1	1:C:47:VAL:HG23	2.21	0.40
1:D:54:SER:HA	1:D:93:TRP:CH2	2.56	0.40
1:F:212:SER:HA	1:F:251:ARG:O	2.21	0.40
1:F:254:ASP:OD1	1:F:254:ASP:N	2.52	0.40
1:F:216:THR:HG23	1:F:252:LEU:HD21	2.02	0.40
1:C:175:TYR:OH	1:C:181:ALA:HB2	2.21	0.40
1:D:105:GLY:O	1:D:297:LEU:HD11	2.20	0.40
1:F:157:TYR:HB3	1:F:168:GLN:HB2	2.03	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	405/427 (95%)	388 (96%)	14 (4%)	3 (1%)	22	43
1	B	406/427 (95%)	390 (96%)	15 (4%)	1 (0%)	47	71
1	C	408/427 (96%)	385 (94%)	21 (5%)	2 (0%)	29	52
1	D	410/427 (96%)	393 (96%)	15 (4%)	2 (0%)	29	52
1	E	407/427 (95%)	379 (93%)	25 (6%)	3 (1%)	22	43
1	F	409/427 (96%)	390 (95%)	17 (4%)	2 (0%)	29	52
All	All	2445/2562 (95%)	2325 (95%)	107 (4%)	13 (0%)	29	52

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS

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Mol	Chain	Res	Type
1	A	314	VAL
1	A	136	HIS
1	C	292	LEU
1	D	90	HIS
1	D	125	TRP
1	E	137	GLY
1	F	88	ASN
1	B	88	ASN
1	C	315	THR
1	E	88	ASN
1	E	8	LYS
1	F	4	LYS

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	351/367 (96%)	328 (93%)	23 (7%)	16	33
1	B	352/367 (96%)	331 (94%)	21 (6%)	19	39
1	C	354/367 (96%)	335 (95%)	19 (5%)	22	44
1	D	355/367 (97%)	333 (94%)	22 (6%)	18	37
1	E	353/367 (96%)	329 (93%)	24 (7%)	16	32
1	F	355/367 (97%)	339 (96%)	16 (4%)	27	52
All	All	2120/2202 (96%)	1995 (94%)	125 (6%)	19	39

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	45	LEU
1	A	59	GLN
1	A	81	GLU
1	A	86	GLU
1	A	95	SER

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Mol	Chain	Res	Type
1	A	139	GLN
1	A	153	LEU
1	A	155	LEU
1	A	163	THR
1	A	182	MET
1	A	186	ASN
1	A	201	LEU
1	A	209	LEU
1	A	211	LEU
1	A	254	ASP
1	A	297	LEU
1	A	311	HIS
1	A	319	ARG
1	A	354	LEU
1	A	361	LEU
1	A	388	ARG
1	A	405	LEU
1	B	22	ILE
1	B	63	GLU
1	B	66	LYS
1	B	146	LEU
1	B	153	LEU
1	B	155	LEU
1	B	166	GLN
1	B	171	LYS
1	B	186	ASN
1	B	204	ASP
1	B	209	LEU
1	B	211	LEU
1	B	254	ASP
1	B	280	SER
1	B	289	SER
1	B	311	HIS
1	B	354	LEU
1	B	361	LEU
1	B	381	LEU
1	B	388	ARG
1	B	405	LEU
1	C	20	THR
1	C	40	LEU
1	C	56	LYS
1	C	95	SER

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Mol	Chain	Res	Type
1	C	110	ARG
1	C	139	GLN
1	C	186	ASN
1	C	201	LEU
1	C	209	LEU
1	C	238	LYS
1	C	241	PHE
1	C	314	VAL
1	C	330	ASN
1	C	354	LEU
1	C	361	LEU
1	C	381	LEU
1	C	388	ARG
1	C	404	ARG
1	C	405	LEU
1	D	38	VAL
1	D	63	GLU
1	D	88	ASN
1	D	139	GLN
1	D	155	LEU
1	D	182	MET
1	D	201	LEU
1	D	204	ASP
1	D	209	LEU
1	D	211	LEU
1	D	252	LEU
1	D	255	ASP
1	D	327	THR
1	D	343	LEU
1	D	344	LYS
1	D	354	LEU
1	D	361	LEU
1	D	386	ASN
1	D	388	ARG
1	D	393	THR
1	D	404	ARG
1	D	405	LEU
1	E	6	LYS
1	E	15	ASP
1	E	20	THR
1	E	47	VAL
1	E	53	THR

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Mol	Chain	Res	Type
1	E	120	ARG
1	E	139	GLN
1	E	146	LEU
1	E	155	LEU
1	E	186	ASN
1	E	201	LEU
1	E	209	LEU
1	E	211	LEU
1	E	231	GLU
1	E	247	HIS
1	E	251	ARG
1	E	254	ASP
1	E	280	SER
1	E	330	ASN
1	E	354	LEU
1	E	361	LEU
1	E	372	ASP
1	E	405	LEU
1	E	410	LYS
1	F	38	VAL
1	F	45	LEU
1	F	83	ARG
1	F	94	LYS
1	F	117	ARG
1	F	139	GLN
1	F	171	LYS
1	F	186	ASN
1	F	211	LEU
1	F	317	HIS
1	F	354	LEU
1	F	361	LEU
1	F	378	ASP
1	F	388	ARG
1	F	393	THR
1	F	405	LEU

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

Mol	Chain	Res	Type
1	A	9	GLN
1	A	243	GLN
1	A	259	GLN

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Mol	Chain	Res	Type
1	A	370	GLN
1	B	9	GLN
1	B	90	HIS
1	B	166	GLN
1	B	247	HIS
1	B	317	HIS
1	B	370	GLN
1	B	371	GLN
1	C	186	ASN
1	C	208	ASN
1	C	285	GLN
1	C	317	HIS
1	C	322	GLN
1	C	330	ASN
1	D	208	ASN
1	D	236	GLN
1	D	370	GLN
1	E	166	GLN
1	E	230	GLN
1	E	317	HIS
1	E	322	GLN
1	E	330	ASN
1	E	370	GLN
1	F	9	GLN
1	F	259	GLN
1	F	317	HIS
1	F	370	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 (i)

6 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	ICT	D	2104	-	12,12,12	2.40	3 (25%)	13,16,16	1.47	3 (23%)
2	ICT	C	2103	-	12,12,12	2.42	3 (25%)	13,16,16	1.43	3 (23%)
2	ICT	A	2101	-	12,12,12	2.40	3 (25%)	13,16,16	1.49	4 (30%)
2	ICT	B	2102	-	12,12,12	2.43	3 (25%)	13,16,16	1.57	4 (30%)
2	ICT	F	2106	-	12,12,12	2.43	3 (25%)	13,16,16	1.52	5 (38%)
2	ICT	E	2105	-	12,12,12	2.40	3 (25%)	13,16,16	1.46	3 (23%)

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	ICT	D	2104	-	-	4/16/16/16	-
2	ICT	C	2103	-	-	4/16/16/16	-
2	ICT	A	2101	-	-	3/16/16/16	-
2	ICT	B	2102	-	-	10/16/16/16	-
2	ICT	F	2106	-	-	7/16/16/16	-
2	ICT	E	2105	-	-	0/16/16/16	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2102	ICT	O1-C1	5.82	1.39	1.22
2	F	2106	ICT	O1-C1	5.72	1.39	1.22
2	D	2104	ICT	O1-C1	5.70	1.39	1.22
2	A	2101	ICT	O1-C1	5.65	1.39	1.22
2	E	2105	ICT	O1-C1	5.63	1.39	1.22
2	C	2103	ICT	O1-C1	5.62	1.39	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2106	ICT	O3-C5	5.27	1.39	1.22
2	C	2103	ICT	O3-C5	5.22	1.39	1.22
2	E	2105	ICT	O3-C5	5.20	1.39	1.22
2	D	2104	ICT	O3-C5	5.20	1.39	1.22
2	B	2102	ICT	O3-C5	5.17	1.39	1.22
2	A	2101	ICT	O3-C5	5.08	1.39	1.22
2	F	2106	ICT	O5-C6	2.92	1.31	1.22
2	E	2105	ICT	O5-C6	2.88	1.30	1.22
2	C	2103	ICT	O5-C6	2.87	1.30	1.22
2	A	2101	ICT	O5-C6	2.85	1.30	1.22
2	B	2102	ICT	O5-C6	2.82	1.30	1.22
2	D	2104	ICT	O5-C6	2.81	1.30	1.22

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2102	ICT	O2-C1-C2	2.62	120.36	113.27
2	E	2105	ICT	O2-C1-C2	2.57	120.22	113.27
2	A	2101	ICT	O2-C1-C2	2.56	120.20	113.27
2	D	2104	ICT	O2-C1-C2	2.52	120.09	113.27
2	F	2106	ICT	O2-C1-C2	2.40	119.76	113.27
2	B	2102	ICT	O6-C6-C3	2.37	120.56	114.03
2	F	2106	ICT	O6-C6-O5	-2.37	118.72	124.09
2	A	2101	ICT	O6-C6-O5	-2.32	118.82	124.09
2	C	2103	ICT	O6-C6-O5	-2.26	118.95	124.09
2	F	2106	ICT	O6-C6-C3	2.23	120.18	114.03
2	C	2103	ICT	O2-C1-C2	2.21	119.23	113.27
2	B	2102	ICT	O4-C5-C4	2.17	121.02	114.07
2	D	2104	ICT	O6-C6-O5	-2.15	119.21	124.09
2	A	2101	ICT	O4-C5-C4	2.14	120.92	114.07
2	E	2105	ICT	O4-C5-C4	2.11	120.82	114.07
2	E	2105	ICT	O6-C6-O5	-2.10	119.33	124.09
2	B	2102	ICT	O6-C6-O5	-2.09	119.35	124.09
2	A	2101	ICT	O6-C6-C3	2.07	119.72	114.03
2	D	2104	ICT	O4-C5-C4	2.06	120.69	114.07
2	C	2103	ICT	O4-C5-C4	2.06	120.67	114.07
2	F	2106	ICT	O2-C1-O1	-2.03	119.47	124.09
2	F	2106	ICT	O4-C5-C4	2.02	120.55	114.07

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2102	ICT	O7-C2-C3-C4
2	B	2102	ICT	O2-C1-C2-C3
2	B	2102	ICT	O1-C1-C2-C3
2	B	2102	ICT	O1-C1-C2-O7
2	B	2102	ICT	O2-C1-C2-O7
2	F	2106	ICT	O1-C1-C2-C3
2	F	2106	ICT	O2-C1-C2-C3
2	D	2104	ICT	O1-C1-C2-C3
2	B	2102	ICT	C4-C3-C6-O5
2	B	2102	ICT	C4-C3-C6-O6
2	D	2104	ICT	O2-C1-C2-C3
2	D	2104	ICT	C4-C3-C6-O5
2	D	2104	ICT	C4-C3-C6-O6
2	A	2101	ICT	O7-C2-C3-C4
2	F	2106	ICT	O7-C2-C3-C4
2	C	2103	ICT	O1-C1-C2-C3
2	B	2102	ICT	C1-C2-C3-C4
2	B	2102	ICT	C1-C2-C3-C6
2	F	2106	ICT	C1-C2-C3-C6
2	F	2106	ICT	O1-C1-C2-O7
2	C	2103	ICT	O1-C1-C2-O7
2	C	2103	ICT	O2-C1-C2-C3
2	A	2101	ICT	C1-C2-C3-C6
2	C	2103	ICT	O2-C1-C2-O7
2	F	2106	ICT	O2-C1-C2-O7
2	A	2101	ICT	C1-C2-C3-C4
2	F	2106	ICT	C1-C2-C3-C4
2	B	2102	ICT	C3-C4-C5-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2101	ICT	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	407/427 (95%)	-0.09	4 (0%)	82	80	34, 43, 72, 81	0
1	B	408/427 (95%)	-0.15	3 (0%)	87	86	29, 42, 70, 90	0
1	C	410/427 (96%)	0.12	12 (2%)	51	45	36, 50, 80, 116	0
1	D	412/427 (96%)	0.12	13 (3%)	47	40	34, 50, 83, 97	0
1	E	409/427 (95%)	0.22	16 (3%)	39	32	39, 52, 86, 116	0
1	F	411/427 (96%)	0.06	14 (3%)	45	38	33, 48, 79, 101	0
All	All	2457/2562 (95%)	0.05	62 (2%)	57	51	29, 47, 80, 116	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	6.6
1	D	2	PHE	4.5
1	E	3	SER	4.4
1	F	2	PHE	4.4
1	A	314	VAL	4.3
1	C	388	ARG	4.1
1	E	316	ARG	4.0
1	D	315	THR	3.9
1	F	164	THR	3.9
1	E	350	ASN	3.8
1	E	410	LYS	3.8
1	C	412	ILE	3.8
1	E	411	SER	3.6
1	C	387	GLU	3.5
1	E	86	GLU	3.5
1	F	166	GLN	3.5
1	A	3	SER	3.5
1	C	164	THR	3.4
1	C	385	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	311	HIS	3.3
1	F	87	PHE	3.3
1	C	386	ASN	3.2
1	F	311	HIS	3.2
1	D	91	LYS	3.1
1	D	85	LYS	3.1
1	C	162	PRO	3.0
1	D	412	ILE	3.0
1	C	316	ARG	3.0
1	E	386	ASN	3.0
1	C	90	HIS	2.9
1	E	409	ILE	2.9
1	D	314	VAL	2.9
1	B	410	LYS	2.8
1	E	313	THR	2.8
1	F	86	GLU	2.8
1	D	316	ARG	2.7
1	F	82	ALA	2.7
1	E	88	ASN	2.7
1	C	313	THR	2.7
1	B	411	SER	2.7
1	F	3	SER	2.6
1	F	163	THR	2.6
1	D	90	HIS	2.6
1	E	90	HIS	2.6
1	F	319	ARG	2.5
1	F	410	LYS	2.5
1	F	310	ALA	2.5
1	A	386	ASN	2.5
1	F	412	ILE	2.4
1	D	389	SER	2.4
1	A	85	LYS	2.3
1	E	81	GLU	2.3
1	E	164	THR	2.3
1	D	163	THR	2.2
1	B	81	GLU	2.2
1	C	411	SER	2.2
1	D	386	ASN	2.1
1	E	392	VAL	2.1
1	D	410	LYS	2.1
1	F	88	ASN	2.1
1	E	181	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	119	PRO	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, 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	ICT	D	2104	13/13	0.50	0.47	96,100,101,101	0
2	ICT	F	2106	13/13	0.69	0.26	81,82,84,84	0
2	ICT	B	2102	13/13	0.76	0.28	76,80,81,81	0
2	ICT	E	2105	13/13	0.82	0.26	75,76,77,77	0
2	ICT	C	2103	13/13	0.88	0.20	54,55,56,58	0
2	ICT	A	2101	13/13	0.90	0.18	43,48,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.