



Full wwPDB X-ray Structure Validation Report i

Sep 12, 2023 – 09:15 AM EDT

PDB ID : 4OFC
Title : 2.0 Angstroms X-ray crystal structure of human 2-amino-3-carboxymuconate -6-semialdehyde decarboxylase
Authors : Huo, L.; Liu, F.; Iwaki, H.; Chen, L.; Hasegawa, Y.; Liu, A.
Deposited on : 2014-01-14
Resolution : 1.99 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

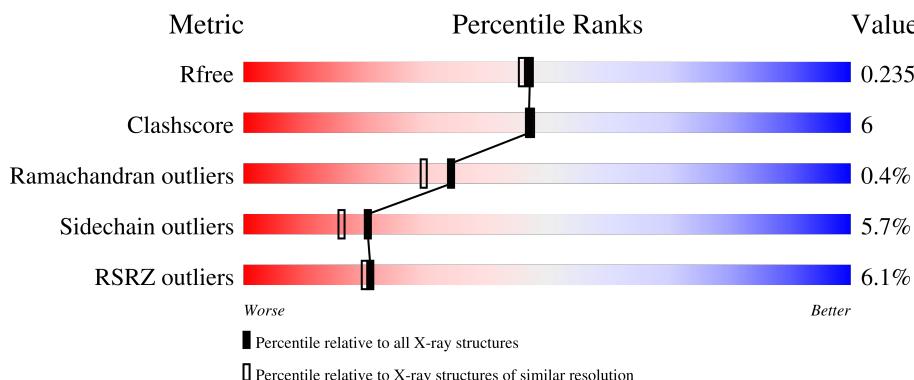
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

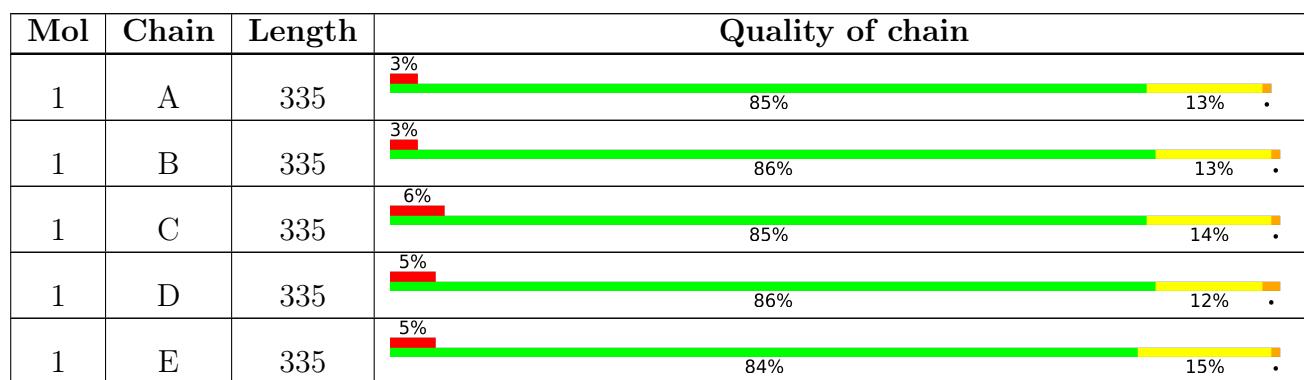
The reported resolution of this entry is 1.99 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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



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Mol	Chain	Length	Quality of chain		
1	F	335	14%	77%	20% •

2 Entry composition [\(i\)](#)

There are 3 unique types of molecules in this entry. The entry contains 16984 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 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2664	1723	448	472	21			
1	B	335	Total	C	N	O	S	0	0	0
			2664	1723	448	472	21			
1	C	335	Total	C	N	O	S	0	0	0
			2664	1723	448	472	21			
1	D	335	Total	C	N	O	S	0	0	0
			2664	1723	448	472	21			
1	E	335	Total	C	N	O	S	0	0	0
			2664	1723	448	472	21			
1	F	335	Total	C	N	O	S	0	0	0
			2664	1723	448	472	21			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

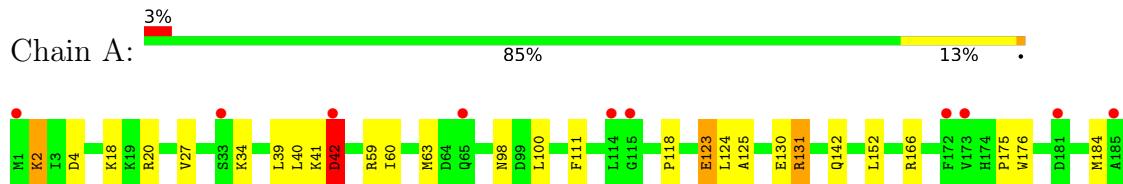
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	169	Total O 169 169	0	0
3	B	233	Total O 233 233	0	0
3	C	171	Total O 171 171	0	0
3	D	174	Total O 174 174	0	0
3	E	140	Total O 140 140	0	0
3	F	107	Total O 107 107	0	0

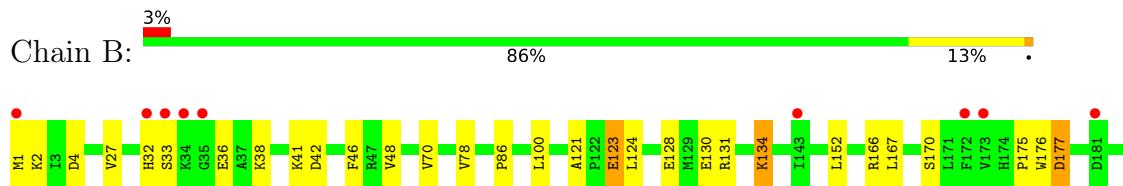
3 Residue-property plots

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.

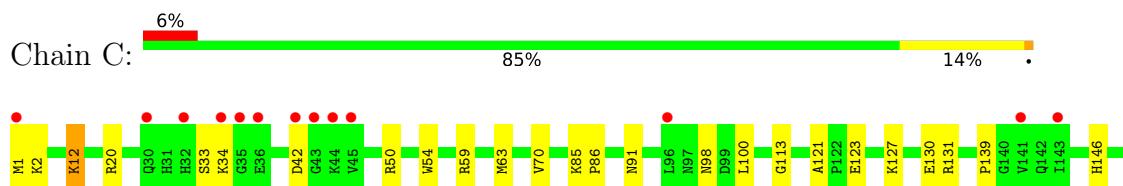
- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase



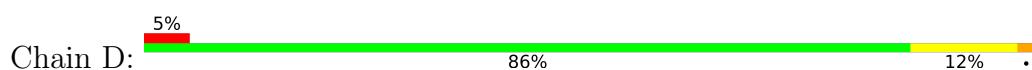
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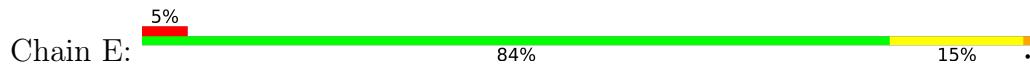


- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase

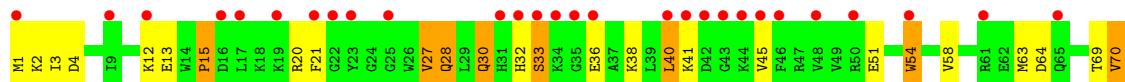
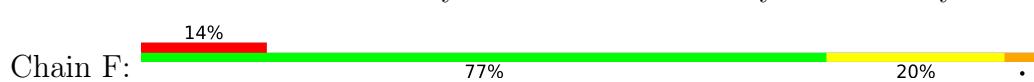




- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase



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4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.70 Å 101.08 Å 232.82 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.11 – 1.99 27.11 – 1.96	Depositor EDS
% Data completeness (in resolution range)	86.4 (27.11-1.99) 82.4 (27.11-1.96)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	2.26 (at 1.96 Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R , R_{free}	0.197 , 0.241 0.193 , 0.235	Depositor DCC
R_{free} test set	6563 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.7	EDS
L-test for twinning ²	$< L > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16984	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

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

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	0.43	0/2736	0.57	1/3701 (0.0%)
1	B	0.45	0/2736	0.57	0/3701
1	C	0.42	0/2736	0.55	0/3701
1	D	0.42	0/2736	0.56	0/3701
1	E	0.40	0/2736	0.54	0/3701
1	F	0.37	0/2736	0.54	0/3701
All	All	0.42	0/16416	0.55	1/22206 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	131	ARG	NE-CZ-NH2	-5.52	117.54	120.30

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	2664	0	2673	35	0
1	B	2664	0	2673	31	0
1	C	2664	0	2673	32	0
1	D	2664	0	2673	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2664	0	2673	31	0
1	F	2664	0	2673	45	0
2	A	1	0	0	0	0
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	169	0	0	5	0
3	B	233	0	0	5	0
3	C	171	0	0	12	0
3	D	174	0	0	6	0
3	E	140	0	0	3	0
3	F	107	0	0	4	0
All	All	16984	0	16038	198	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 (198) 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:85:LYS:NZ	3:C:640:HOH:O	2.04	0.90
1:F:98:ASN:OD1	1:F:131:ARG:NH2	2.10	0.85
1:E:98:ASN:OD1	1:E:131:ARG:NH2	2.11	0.82
1:F:20:ARG:NH1	1:F:91:ASN:OD1	2.13	0.82
1:C:98:ASN:OD1	1:C:131:ARG:NH2	2.12	0.82
1:C:334:GLN:OE1	3:C:623:HOH:O	1.98	0.79
1:D:12:LYS:HE2	1:D:13:GLU:H	1.48	0.77
1:B:195:MET:SD	3:B:567:HOH:O	2.42	0.76
1:C:2:LYS:HB3	1:C:321:ALA:HB2	1.68	0.75
1:C:290:THR:HG23	3:C:576:HOH:O	1.86	0.75
1:E:15:PRO:HG2	1:E:20:ARG:HH21	1.52	0.74
1:A:98:ASN:OD1	1:A:131:ARG:NH2	2.18	0.74
1:F:30:GLN:HB2	1:F:40:LEU:HD11	1.70	0.74
1:E:332:ARG:HE	1:E:332:ARG:H	1.34	0.73
1:D:98:ASN:OD1	1:D:131:ARG:NH2	2.15	0.72
1:F:64:ASP:O	3:F:557:HOH:O	2.09	0.71
1:C:314:GLU:OE2	3:C:533:HOH:O	2.09	0.71
1:B:128:GLU:OE2	1:B:131:ARG:NH1	2.24	0.70
1:D:175:PRO:HG2	1:D:195:MET:HE3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ASP:HB2	3:D:632:HOH:O	1.92	0.68
1:D:42:ASP:N	3:D:632:HOH:O	2.27	0.67
1:E:12:LYS:HE2	1:E:13:GLU:H	1.59	0.66
1:B:175:PRO:HG2	1:B:195:MET:CE	2.26	0.66
1:A:290:THR:HG22	1:A:292:TYR:H	1.58	0.66
1:F:2:LYS:HB3	1:F:321:ALA:HB2	1.77	0.65
1:A:254:ASN:H	1:A:257:LYS:NZ	1.95	0.65
1:C:290:THR:HG22	1:C:292:TYR:H	1.61	0.65
1:B:32:HIS:HE1	1:B:36:GLU:HG2	1.62	0.65
1:F:253:MET:HG3	1:F:257:LYS:HD2	1.78	0.65
1:C:59:ARG:HB3	1:C:63:MET:CE	2.27	0.64
1:F:33:SER:HB3	1:F:36:GLU:HB2	1.79	0.64
1:B:175:PRO:HG2	1:B:195:MET:HE2	1.80	0.64
1:F:15:PRO:O	1:F:28:GLN:NE2	2.29	0.64
1:B:290:THR:HG23	3:B:683:HOH:O	1.98	0.64
1:D:1:MET:O	1:D:68:VAL:HA	1.98	0.63
1:F:178:MET:HB2	1:F:180:MET:HE1	1.81	0.63
1:D:254:ASN:H	1:D:257:LYS:HZ3	1.47	0.63
1:F:128:GLU:OE2	1:F:131:ARG:NH1	2.33	0.62
1:B:2:LYS:NZ	3:B:621:HOH:O	2.33	0.61
1:D:257:LYS:NZ	3:D:613:HOH:O	2.33	0.60
1:D:1:MET:SD	1:D:1:MET:N	2.74	0.60
1:B:290:THR:HG22	1:B:292:TYR:H	1.67	0.60
1:E:12:LYS:HE2	1:E:13:GLU:N	2.16	0.60
1:F:183:ARG:O	1:F:186:LYS:NZ	2.31	0.59
1:C:2:LYS:NZ	3:C:551:HOH:O	2.36	0.59
1:B:33:SER:HB3	1:B:36:GLU:HB3	1.83	0.59
1:B:38:LYS:HG2	1:B:48:VAL:HG22	1.85	0.58
1:B:130:GLU:HG3	1:B:167:LEU:HD11	1.86	0.58
1:D:254:ASN:H	1:D:257:LYS:NZ	2.02	0.58
1:F:90:LEU:HD22	1:F:124:LEU:HD22	1.85	0.58
1:C:283:LYS:NZ	3:C:626:HOH:O	2.37	0.57
1:E:66:LYS:NZ	1:E:300:GLU:OE2	2.24	0.57
1:D:290:THR:HG22	1:D:292:TYR:H	1.70	0.57
1:F:27:VAL:HA	1:F:40:LEU:O	2.04	0.57
1:A:253:MET:HG3	1:A:257:LYS:HE2	1.87	0.56
1:F:118:PRO:HD2	1:F:125:ALA:HA	1.87	0.56
1:C:2:LYS:CB	1:C:321:ALA:HB2	2.35	0.56
1:B:32:HIS:CE1	1:B:36:GLU:HG2	2.41	0.55
1:A:175:PRO:HG2	1:A:195:MET:HE3	1.88	0.55
1:D:1:MET:HB3	1:D:301:PRO:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:ASP:OD2	1:F:290:THR:HB	2.07	0.55
1:A:59:ARG:HB3	1:A:63:MET:CE	2.38	0.54
1:A:281:ILE:HG22	1:A:285:LYS:HB2	1.89	0.54
1:C:334:GLN:NE2	3:C:619:HOH:O	2.28	0.54
1:D:20:ARG:NH1	1:D:91:ASN:OD1	2.38	0.54
1:A:18:LYS:NZ	3:A:536:HOH:O	2.40	0.54
1:C:12:LYS:HE3	1:C:12:LYS:H	1.73	0.53
1:D:12:LYS:HE2	1:D:13:GLU:N	2.20	0.53
1:B:166:ARG:NH2	3:B:700:HOH:O	2.32	0.53
1:C:214:LYS:NZ	3:C:621:HOH:O	2.30	0.53
1:D:123:GLU:HB3	3:D:638:HOH:O	2.09	0.53
1:E:260:GLY:O	1:E:285:LYS:NZ	2.42	0.52
1:C:33:SER:OG	1:C:34:LYS:N	2.43	0.52
1:B:254:ASN:H	1:B:257:LYS:NZ	2.07	0.52
1:D:146:HIS:CE1	1:D:177:ASP:HB3	2.45	0.52
1:D:12:LYS:HD3	1:D:12:LYS:H	1.75	0.52
1:B:2:LYS:CB	1:B:321:ALA:HB2	2.40	0.51
1:E:290:THR:HG22	1:E:292:TYR:H	1.75	0.51
1:C:59:ARG:HB3	1:C:63:MET:HE3	1.92	0.51
1:E:130:GLU:HG2	1:E:167:LEU:HD11	1.92	0.51
1:B:46:PHE:HZ	1:B:78:VAL:HG11	1.75	0.51
1:C:249:GLN:HG2	3:C:529:HOH:O	2.10	0.51
1:A:41:LYS:O	1:A:42:ASP:C	2.49	0.51
1:B:2:LYS:HB2	1:B:321:ALA:HB2	1.93	0.50
1:F:130:GLU:HG3	1:F:167:LEU:HD11	1.92	0.50
1:E:290:THR:HG22	1:E:292:TYR:N	2.25	0.50
1:A:331:GLU:O	1:A:334:GLN:HG2	2.12	0.50
1:C:86:PRO:HB3	1:C:121:ALA:HB2	1.94	0.50
1:E:15:PRO:HG2	1:E:20:ARG:NH2	2.24	0.50
1:A:290:THR:HG22	1:A:292:TYR:N	2.26	0.50
1:C:269:HIS:HD2	3:C:614:HOH:O	1.94	0.50
1:D:290:THR:HG22	1:D:292:TYR:N	2.27	0.50
1:D:4:ASP:OD2	1:D:290:THR:HB	2.11	0.49
1:E:332:ARG:HE	1:E:332:ARG:N	2.08	0.49
1:A:123:GLU:HG3	1:A:124:LEU:N	2.26	0.49
1:F:32:HIS:CD2	1:F:38:LYS:HG3	2.48	0.49
1:A:334:GLN:OE1	3:A:648:HOH:O	2.19	0.49
1:F:120:GLN:OE1	1:F:120:GLN:N	2.41	0.49
1:C:146:HIS:CE1	1:C:177:ASP:HB3	2.48	0.49
1:D:86:PRO:HB3	1:D:121:ALA:HB2	1.93	0.49
1:A:254:ASN:H	1:A:257:LYS:HZ3	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASN:ND2	1:A:258:TYR:OH	2.39	0.48
1:E:309:GLU:HG3	3:E:534:HOH:O	2.13	0.48
1:B:166:ARG:NE	3:B:700:HOH:O	2.33	0.48
1:D:176:TRP:CG	1:D:177:ASP:N	2.82	0.48
1:B:46:PHE:CZ	1:B:78:VAL:HG11	2.48	0.48
1:F:51:GLU:HG2	1:F:58:VAL:HG21	1.96	0.48
1:A:2:LYS:HB3	1:A:321:ALA:HB2	1.96	0.48
1:C:20:ARG:NH1	1:C:91:ASN:OD1	2.47	0.47
1:A:299:LEU:HD11	1:F:242:MET:HE3	1.95	0.47
1:B:176:TRP:CG	1:B:177:ASP:N	2.83	0.47
1:C:184:MET:O	1:C:190:PRO:HD3	2.14	0.47
1:E:86:PRO:HB3	1:E:121:ALA:HB2	1.95	0.47
1:D:127:LYS:HB3	3:D:532:HOH:O	2.15	0.47
1:A:195:MET:HE2	1:F:235:ARG:NH2	2.29	0.47
1:E:2:LYS:HB2	1:E:321:ALA:HB2	1.98	0.46
1:F:86:PRO:HB3	1:F:121:ALA:HB2	1.97	0.46
1:B:175:PRO:HG2	1:B:195:MET:HE3	1.95	0.46
1:F:254:ASN:H	1:F:257:LYS:NZ	2.13	0.46
1:C:50:ARG:HD3	3:C:652:HOH:O	2.15	0.46
1:C:12:LYS:H	1:C:12:LYS:CE	2.27	0.46
1:A:254:ASN:O	1:A:257:LYS:HD3	2.16	0.46
1:E:12:LYS:HD3	1:E:12:LYS:H	1.81	0.46
1:E:102:SER:O	1:E:105:VAL:HG12	2.16	0.46
1:B:290:THR:CG2	1:B:292:TYR:HB2	2.46	0.45
1:B:86:PRO:HB3	1:B:121:ALA:HB2	1.98	0.45
1:B:276:LEU:HD22	1:C:276:LEU:HD22	1.99	0.45
1:B:290:THR:HG22	1:B:292:TYR:N	2.31	0.45
1:E:269:HIS:HA	3:E:631:HOH:O	2.17	0.45
1:C:275:LYS:NZ	1:C:310:GLU:OE2	2.48	0.45
1:A:42:ASP:N	3:A:506:HOH:O	2.28	0.45
1:A:276:LEU:HD22	1:F:276:LEU:HD22	1.99	0.45
1:D:130:GLU:HG3	1:D:167:LEU:HD11	1.99	0.44
1:B:170:SER:HB3	1:B:327:PHE:CZ	2.52	0.44
1:A:4:ASP:OD2	1:A:290:THR:HB	2.16	0.44
1:F:299:LEU:O	1:F:301:PRO:HD3	2.16	0.44
1:A:63:MET:HE1	1:A:111:PHE:HE1	1.81	0.44
1:C:130:GLU:HG3	1:C:167:LEU:HD11	1.99	0.44
1:A:252:PRO:HG2	1:A:253:MET:SD	2.58	0.44
1:D:42:ASP:CB	3:D:632:HOH:O	2.58	0.44
1:E:140:GLY:HA2	1:E:169:CYS:SG	2.58	0.44
1:A:254:ASN:HB3	1:A:257:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:NH2	3:A:663:HOH:O	2.48	0.44
1:F:186:LYS:O	1:F:189:LEU:HG	2.18	0.44
1:F:170:SER:HB3	1:F:327:PHE:CZ	2.52	0.43
1:C:113:GLY:O	1:C:139:PRO:HD2	2.18	0.43
1:D:113:GLY:O	1:D:139:PRO:HD2	2.18	0.43
1:E:332:ARG:H	1:E:332:ARG:NE	2.06	0.43
1:A:184:MET:O	1:A:190:PRO:HD3	2.18	0.43
1:D:184:MET:O	1:D:190:PRO:HD3	2.18	0.43
1:E:176:TRP:CG	1:E:177:ASP:N	2.87	0.43
1:F:251:ASN:HA	1:F:252:PRO:HD3	1.80	0.43
1:A:60:ILE:HD13	1:A:60:ILE:HA	1.88	0.43
1:A:270:ASP:OD2	1:F:256:LYS:NZ	2.47	0.42
1:B:123:GLU:HG3	1:B:124:LEU:N	2.32	0.42
1:E:33:SER:OG	1:E:34:LYS:N	2.51	0.42
1:F:295:PRO:HG2	3:F:572:HOH:O	2.19	0.42
1:F:3:ILE:HG12	1:F:70:VAL:HG13	2.01	0.42
1:F:331:GLU:HG2	3:F:587:HOH:O	2.18	0.42
1:E:59:ARG:HB3	1:E:63:MET:CE	2.50	0.42
1:F:38:LYS:HD3	1:F:45:VAL:HG21	2.01	0.42
1:B:4:ASP:OD2	1:B:290:THR:HB	2.18	0.42
1:C:127:LYS:HE3	1:C:127:LYS:HB3	1.82	0.42
1:A:142:GLN:HB3	3:A:530:HOH:O	2.19	0.42
1:B:134:LYS:HA	1:B:134:LYS:HD2	1.81	0.42
1:F:85:LYS:HA	1:F:86:PRO:HD3	1.84	0.42
1:F:142:GLN:HB3	3:F:502:HOH:O	2.20	0.42
1:C:183:ARG:O	1:C:186:LYS:NZ	2.48	0.42
1:E:131:ARG:O	1:E:135:GLU:HB2	2.20	0.42
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.93	0.41
1:D:2:LYS:CB	1:D:321:ALA:HB2	2.50	0.41
1:C:334:GLN:HG2	3:C:619:HOH:O	2.19	0.41
1:E:199:THR:HG23	3:E:612:HOH:O	2.20	0.41
1:E:294:PHE:HA	1:E:295:PRO:HD3	1.92	0.41
1:B:186:LYS:HD2	1:B:187:TYR:CE1	2.55	0.41
1:D:235:ARG:NH2	1:E:195:MET:HE3	2.34	0.41
1:A:118:PRO:HD2	1:A:125:ALA:HA	2.01	0.41
1:E:178:MET:SD	1:E:195:MET:HG2	2.60	0.41
1:F:296:LEU:HD23	1:F:296:LEU:HA	1.96	0.41
1:F:28:GLN:O	1:F:40:LEU:HD12	2.21	0.41
1:F:281:ILE:HG22	1:F:285:LYS:HB2	2.02	0.41
1:C:176:TRP:CG	1:C:177:ASP:N	2.88	0.41
1:F:69:THR:HA	1:F:110:ARG:HH12	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:THR:HG22	1:B:292:TYR:HB2	2.02	0.41
1:A:263:TYR:CD1	1:A:287:ILE:HD11	2.56	0.41
1:D:23:TYR:CE2	1:D:85:LYS:HE2	2.56	0.41
1:D:51:GLU:HA	1:D:54:TRP:CE2	2.55	0.41
1:F:32:HIS:HD2	1:F:38:LYS:HG3	1.85	0.41
1:F:63:MET:HE1	1:F:111:PHE:CE1	2.56	0.41
1:F:178:MET:SD	1:F:195:MET:HG3	2.60	0.41
1:A:98:ASN:CG	1:A:131:ARG:HH22	2.18	0.41
1:A:253:MET:SD	1:A:253:MET:N	2.94	0.41
1:F:51:GLU:HA	1:F:54:TRP:CH2	2.56	0.41
1:E:20:ARG:NH1	1:E:91:ASN:OD1	2.52	0.40
1:F:2:LYS:CB	1:F:321:ALA:HB2	2.49	0.40
1:F:21:PHE:HB3	1:F:88:ASP:OD2	2.20	0.40
1:E:51:GLU:HA	1:E:54:TRP:CE2	2.56	0.40
1:E:77:PRO:HG2	1:E:174:HIS:CE1	2.57	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	333/335 (99%)	324 (97%)	8 (2%)	1 (0%)	41 37
1	B	333/335 (99%)	324 (97%)	9 (3%)	0	100 100
1	C	333/335 (99%)	321 (96%)	11 (3%)	1 (0%)	41 37
1	D	333/335 (99%)	324 (97%)	7 (2%)	2 (1%)	25 19
1	E	333/335 (99%)	320 (96%)	12 (4%)	1 (0%)	41 37
1	F	333/335 (99%)	317 (95%)	13 (4%)	3 (1%)	17 11
All	All	1998/2010 (99%)	1930 (97%)	60 (3%)	8 (0%)	34 30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	334	GLN
1	E	334	GLN
1	D	42	ASP
1	F	33	SER
1	C	42	ASP
1	F	15	PRO
1	F	148	ASN
1	A	42	ASP

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	288/288 (100%)	274 (95%)	14 (5%)	25 21
1	B	288/288 (100%)	271 (94%)	17 (6%)	19 15
1	C	288/288 (100%)	274 (95%)	14 (5%)	25 21
1	D	288/288 (100%)	271 (94%)	17 (6%)	19 15
1	E	288/288 (100%)	272 (94%)	16 (6%)	21 17
1	F	288/288 (100%)	267 (93%)	21 (7%)	14 9
All	All	1728/1728 (100%)	1629 (94%)	99 (6%)	20 16

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	27	VAL
1	A	34	LYS
1	A	40	LEU
1	A	42	ASP
1	A	100	LEU
1	A	123	GLU
1	A	130	GLU
1	A	152	LEU
1	A	166	ARG
1	A	176	TRP

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Mol	Chain	Res	Type
1	A	257	LYS
1	A	290	THR
1	A	296	LEU
1	B	1	MET
1	B	27	VAL
1	B	41	LYS
1	B	42	ASP
1	B	70	VAL
1	B	100	LEU
1	B	123	GLU
1	B	134	LYS
1	B	152	LEU
1	B	177	ASP
1	B	214	LYS
1	B	253	MET
1	B	256	LYS
1	B	290	THR
1	B	296	LEU
1	B	319	LEU
1	B	331	GLU
1	C	1	MET
1	C	12	LYS
1	C	54	TRP
1	C	70	VAL
1	C	100	LEU
1	C	123	GLU
1	C	152	LEU
1	C	178	MET
1	C	290	THR
1	C	296	LEU
1	C	309	GLU
1	C	313	GLU
1	C	333	LYS
1	C	334	GLN
1	D	1	MET
1	D	12	LYS
1	D	33	SER
1	D	41	LYS
1	D	42	ASP
1	D	70	VAL
1	D	123	GLU
1	D	131	ARG

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Mol	Chain	Res	Type
1	D	166	ARG
1	D	249	GLN
1	D	257	LYS
1	D	290	THR
1	D	296	LEU
1	D	299	LEU
1	D	310	GLU
1	D	314	GLU
1	D	333	LYS
1	E	12	LYS
1	E	19	LYS
1	E	42	ASP
1	E	60	ILE
1	E	70	VAL
1	E	87	GLU
1	E	100	LEU
1	E	105	VAL
1	E	131	ARG
1	E	152	LEU
1	E	249	GLN
1	E	296	LEU
1	E	309	GLU
1	E	314	GLU
1	E	332	ARG
1	E	333	LYS
1	F	1	MET
1	F	12	LYS
1	F	13	GLU
1	F	27	VAL
1	F	28	GLN
1	F	30	GLN
1	F	40	LEU
1	F	41	LYS
1	F	54	TRP
1	F	70	VAL
1	F	100	LEU
1	F	131	ARG
1	F	134	LYS
1	F	149	GLU
1	F	152	LEU
1	F	249	GLN
1	F	296	LEU

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Mol	Chain	Res	Type
1	F	299	LEU
1	F	309	GLU
1	F	313	GLU
1	F	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	HIS
1	C	269	HIS
1	D	30	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

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 [\(i\)](#)

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 i

6.1 Protein, DNA and RNA chains i

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	335/335 (100%)	0.26	11 (3%)	46	45	14, 26, 43, 54	0
1	B	335/335 (100%)	0.10	10 (2%)	50	49	13, 22, 37, 60	0
1	C	335/335 (100%)	0.33	21 (6%)	20	19	17, 26, 45, 69	0
1	D	335/335 (100%)	0.31	18 (5%)	25	24	17, 26, 42, 53	0
1	E	335/335 (100%)	0.32	16 (4%)	30	29	19, 29, 48, 63	0
1	F	335/335 (100%)	0.88	46 (13%)	3	2	20, 34, 67, 81	0
All	All	2010/2010 (100%)	0.37	122 (6%)	21	20	13, 27, 49, 81	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	9.9
1	F	43	GLY	9.6
1	F	1	MET	9.6
1	E	1	MET	7.8
1	C	43	GLY	7.5
1	C	1	MET	7.3
1	A	1	MET	6.9
1	B	1	MET	6.7
1	F	32	HIS	6.4
1	F	46	PHE	5.7
1	F	34	LYS	5.6
1	C	32	HIS	4.9
1	F	42	ASP	4.7
1	F	33	SER	4.6
1	F	44	LYS	4.4
1	F	249	GLN	4.3
1	B	32	HIS	4.2
1	E	32	HIS	4.2
1	F	45	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	25	GLY	3.9
1	F	176	TRP	3.8
1	F	185	ALA	3.8
1	C	143	ILE	3.8
1	C	34	LYS	3.7
1	F	21	PHE	3.7
1	F	17	LEU	3.5
1	F	50	ARG	3.4
1	F	87	GLU	3.2
1	C	45	VAL	3.2
1	F	150	TRP	3.2
1	F	54	TRP	3.2
1	F	149	GLU	3.2
1	E	332	ARG	3.2
1	F	35	GLY	3.2
1	C	223	ALA	3.2
1	B	173	VAL	3.2
1	E	33	SER	3.1
1	E	43	GLY	3.1
1	F	41	LYS	3.0
1	D	109	ARG	3.0
1	D	223	ALA	3.0
1	E	333	LYS	3.0
1	A	185	ALA	3.0
1	F	65	GLN	3.0
1	F	36	GLU	3.0
1	D	249	GLN	3.0
1	F	19	LYS	2.9
1	C	30	GLN	2.9
1	C	35	GLY	2.9
1	E	44	LYS	2.9
1	D	173	VAL	2.9
1	F	23	TYR	2.8
1	D	334	GLN	2.8
1	C	173	VAL	2.8
1	F	299	LEU	2.8
1	E	149	GLU	2.8
1	F	127	LYS	2.8
1	F	333	LYS	2.8
1	A	172	PHE	2.7
1	F	40	LEU	2.7
1	B	33	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	180	MET	2.7
1	F	143	ILE	2.6
1	F	31	HIS	2.6
1	D	333	LYS	2.6
1	F	309	GLU	2.6
1	D	5	ILE	2.6
1	A	223	ALA	2.6
1	F	181	ASP	2.6
1	C	221	CYS	2.5
1	C	222	PHE	2.5
1	E	34	LYS	2.5
1	E	334	GLN	2.5
1	D	42	ASP	2.5
1	F	202	ALA	2.5
1	C	333	LYS	2.5
1	F	334	GLN	2.4
1	B	249	GLN	2.4
1	B	143	ILE	2.4
1	E	203	ILE	2.4
1	F	173	VAL	2.4
1	E	73	LEU	2.4
1	A	181	ASP	2.4
1	F	61	ARG	2.4
1	D	34	LYS	2.3
1	C	331	GLU	2.3
1	C	36	GLU	2.3
1	F	250	ASP	2.3
1	F	16	ASP	2.3
1	D	299	LEU	2.3
1	E	30	GLN	2.3
1	D	172	PHE	2.3
1	F	48	VAL	2.3
1	C	44	LYS	2.3
1	F	22	GLY	2.2
1	C	334	GLN	2.2
1	D	43	GLY	2.2
1	A	173	VAL	2.2
1	F	9	ILE	2.2
1	A	65	GLN	2.2
1	A	33	SER	2.2
1	C	42	ASP	2.2
1	B	34	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	12	LYS	2.2
1	D	181	ASP	2.2
1	B	181	ASP	2.1
1	D	166	ARG	2.1
1	A	115	GLY	2.1
1	B	172	PHE	2.1
1	C	141	VAL	2.1
1	A	114	LEU	2.1
1	E	249	GLN	2.1
1	E	331	GLU	2.1
1	C	172	PHE	2.1
1	D	141	VAL	2.1
1	A	42	ASP	2.1
1	D	143	ILE	2.1
1	C	96	LEU	2.1
1	E	46	PHE	2.0
1	F	223	ALA	2.0
1	D	221	CYS	2.0
1	B	35	GLY	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(Å ²)	Q<0.9
2	ZN	F	401	1/1	0.98	0.09	33,33,33,33	0
2	ZN	C	401	1/1	0.99	0.09	25,25,25,25	0
2	ZN	D	401	1/1	0.99	0.07	26,26,26,26	0
2	ZN	B	401	1/1	0.99	0.08	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	E	401	1/1	1.00	0.08	29,29,29,29	0
2	ZN	A	401	1/1	1.00	0.10	23,23,23,23	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.