W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:18 PM GMT

PDB ID	:	4OFC
Title	:	2.0 Angstroms X-ray crystal structure of human 2-amino-3-carboxymuconate -6-semialdehye 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

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

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

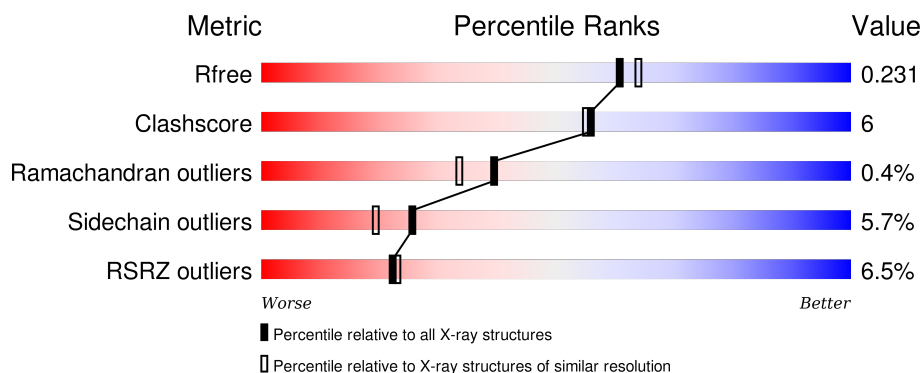|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	Percentile Ranks	Value
Rfree		0.231
Clashscore		6
Ramachandran outliers		0.4%
Sidechain outliers		5.7%
RSRZ outliers		6.5%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	335	4% 85% 13% •
1	B	335	3% 86% 13% •
1	C	335	7% 85% 14% •
1	D	335	6% 86% 12% •
1	E	335	5% 84% 15% •

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Mol	Chain	Length	Quality of chain
1	F	335	15% ▬▬▬▬ 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	D	1	Total	Zn	0	0
			1	1		
2	E	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	A	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 169	O 169	0	0
3	B	233	Total 233	O 233	0	0
3	C	171	Total 171	O 171	0	0
3	D	174	Total 174	O 174	0	0
3	E	140	Total 140	O 140	0	0
3	F	107	Total 107	O 107	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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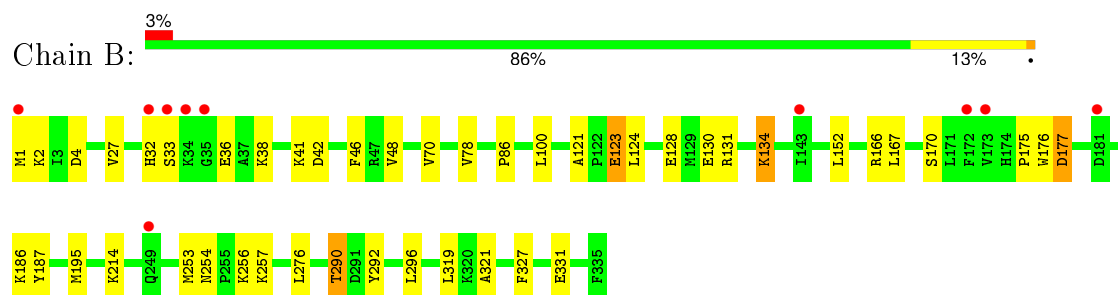 geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
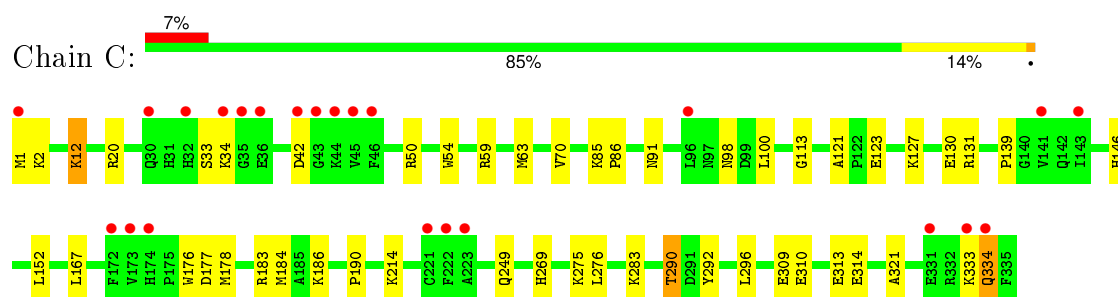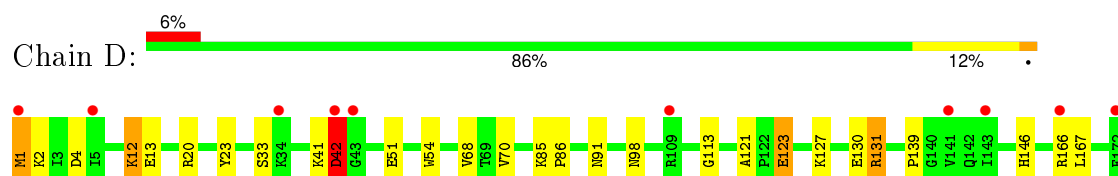
- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase

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V173 H174 P175 W176 D177 D181 M184 P190 M195 C221 F222 A223 R235 Q249 N254 K257 T290 D291 Y292 L296 L299 E300 P301 E310 E314 A321 K333 Q334 F335

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

Chain E:

5%

84%   15%   •

M1 K2 K12 E13 W14 P15 K19 R20 Q30 H31 H32 S33 K34 D42 G43 K44 V45 F46 E51 W54 R59 I60 M63 K66 V70 L73 P77 P86 E87 N91 N98 D99 L100 A101 S102 V105 A121 E130 R131 E135

G140 E149 L152 L167 K168 C169 H174 P175 W176 D177 M178 M195 T199 I203 Q249 G260 H269 K285 T290 D291 Y292 P293 F294 P295 L296 E300 E309 E314 A321 E331 R332 K333 Q334 F335

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

Chain F:

15%

77%   20%   •

M1 K2 I3 D4 I9 K12 E13 W14 P15 D16 L17 K18 K19 R20 F21 G22 Y23 G24 G25 W26 V27 Q28 L29 Q30 H31 H32 S33 K34 G35 E36 A37 K38 L39 L40 K41 D42 G43 K44 V45 F46 R47 V48 V49 R50 E51 W54 V58 R61 E62 M63 D64 Q65 T69 V70

K85 P86 E87 D88 T89 L90 N91 N98 D99 L100 R110 F111 P118 M119 Q120 A121 L124 A125 V126 K127 E128 M129 E130 R131 K134 Q142 I143 N148 E149 W150 D151 L152 R166 L167 S170 V173 W176 D177 M178 Q179 M180 D181 G182 R183 M184 A185 K186

L189 M195 A202 F222 A223 R235 M242 Q249 D250 N251 P252 M253 N254 P255 K256 K257 L276 I281 K285 T290 P295 L296 L299 E300 P301 E309 E313 A321 F327 E331 R332 K333 Q334 F335

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.70Å 101.08Å 232.82Å 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]	3.01 (at 1.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.197 , 0.241 0.187 , 0.231	Depositor DCC
R_{free} test set	5997 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	1 of 130266 reflections (0.001%)	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 7.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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:H	1:E:332:ARG:HE	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:D:146:HIS:CE1	1:D:177:ASP:HB3	2.45	0.52
1:B:254:ASN:H	1:B:257:LYS:NZ	2.07	0.52
1:D:12:LYS:H	1:D:12:LYS:HD3	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:E:15:PRO:HG2	1:E:20:ARG:NH2	2.24	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: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:N	1:E:332:ARG:HE	2.08	0.49
1:F:32:HIS:CD2	1:F:38:LYS:HG3	2.48	0.49
1:A:123:GLU:HG3	1:A:124:LEU:N	2.26	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:CE	1:C:12:LYS:H	2.27	0.46
1:A:254:ASN:O	1:A:257:LYS:HD3	2.16	0.46
1:E:12:LYS:H	1:E:12:LYS:HD3	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:D:42:ASP:CB	3:D:632:HOH:O	2.58	0.44
1:A:252:PRO:HG2	1:A:253:MET:SD	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:F:186:LYS:O	1:F:189:LEU:HG	2.18	0.44
1:A:20:ARG:NH2	3:A:663:HOH:O	2.48	0.44
1:F:170:SER:HB3	1:F:327:PHE:CZ	2.52	0.43
1:E:332:ARG:H	1:E:332:ARG:NE	2.06	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: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: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:A:270:ASP:OD2	1:F:256:LYS:NZ	2.47	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:F:38:LYS:HD3	1:F:45:VAL:HG21	2.01	0.42
1:E:59:ARG:HB3	1:E:63:MET:CE	2.50	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:F:85:LYS:HA	1:F:86:PRO:HD3	1.84	0.42
1:B:134:LYS:HD2	1:B:134:LYS:HA	1.81	0.42
1:A:142:GLN:HB3	3:A:530:HOH:O	2.19	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:HA	1:A:39:LEU:HD23	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:D:235:ARG:NH2	1:E:195:MET:HE3	2.34	0.41
1:B:186:LYS:HD2	1:B:187:TYR:CE1	2.55	0.41
1:E:178:MET:SD	1:E:195:MET:HG2	2.60	0.41
1:A:118:PRO:HD2	1:A:125:ALA:HA	2.01	0.41
1:F:296:LEU:HA	1:F:296:LEU:HD23	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:F:178:MET:SD	1:F:195:MET:HG3	2.60	0.41
1:F:32:HIS:HD2	1:F:38:LYS:HG3	1.85	0.41
1:D:51:GLU:HA	1:D:54:TRP:CE2	2.55	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:F:63:MET:HE1	1:F:111:PHE:CE1	2.56	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:77:PRO:HG2	1:E:174:HIS:CE1	2.57	0.40
1:E:51:GLU:HA	1:E:54:TRP:CE2	2.56	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	333/335 (99%)	324 (97%)	8 (2%)	1 (0%)	46	41
1	B	333/335 (99%)	324 (97%)	9 (3%)	0	100	100
1	C	333/335 (99%)	321 (96%)	11 (3%)	1 (0%)	46	41
1	D	333/335 (99%)	324 (97%)	7 (2%)	2 (1%)	30	22
1	E	333/335 (99%)	320 (96%)	12 (4%)	1 (0%)	46	41
1	F	333/335 (99%)	317 (95%)	13 (4%)	3 (1%)	21	13
All	All	1998/2010 (99%)	1930 (97%)	60 (3%)	8 (0%)	39	33

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%)	31	25
1	B	288/288 (100%)	271 (94%)	17 (6%)	24	18
1	C	288/288 (100%)	274 (95%)	14 (5%)	31	25
1	D	288/288 (100%)	271 (94%)	17 (6%)	24	18
1	E	288/288 (100%)	272 (94%)	16 (6%)	26	20
1	F	288/288 (100%)	267 (93%)	21 (7%)	17	11
All	All	1728/1728 (100%)	1629 (94%)	99 (6%)	25	19

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

Some 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 carbohydrates 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 ⓘ

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 (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%)	0.30	12 (3%)	46	48	14, 26, 43, 54	0
1	B	335/335 (100%)	0.13	10 (2%)	54	55	13, 22, 37, 60	0
1	C	335/335 (100%)	0.37	23 (6%)	20	21	17, 26, 45, 69	0
1	D	335/335 (100%)	0.35	20 (5%)	25	27	17, 26, 42, 53	0
1	E	335/335 (100%)	0.36	16 (4%)	34	36	19, 29, 48, 63	0
1	F	335/335 (100%)	0.93	49 (14%)	3	4	20, 34, 67, 81	0
All	All	2010/2010 (100%)	0.41	130 (6%)	22	23	13, 27, 49, 81	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	9.9
1	F	43	GLY	9.8
1	F	1	MET	9.6
1	E	1	MET	8.0
1	C	43	GLY	7.6
1	C	1	MET	7.4
1	A	1	MET	7.0
1	B	1	MET	6.7
1	F	32	HIS	6.4
1	F	46	PHE	5.8
1	F	34	LYS	5.6
1	C	32	HIS	5.0
1	F	42	ASP	4.7
1	F	33	SER	4.5
1	F	44	LYS	4.4
1	B	32	HIS	4.3
1	F	249	GLN	4.3
1	F	45	VAL	4.3
1	E	32	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	185	ALA	4.0
1	F	25	GLY	4.0
1	F	176	TRP	3.9
1	C	143	ILE	3.9
1	C	34	LYS	3.9
1	F	21	PHE	3.7
1	F	17	LEU	3.5
1	F	50	ARG	3.4
1	C	45	VAL	3.4
1	B	173	VAL	3.4
1	C	223	ALA	3.3
1	E	332	ARG	3.3
1	F	54	TRP	3.3
1	F	87	GLU	3.2
1	F	149	GLU	3.2
1	F	150	TRP	3.2
1	A	185	ALA	3.2
1	E	33	SER	3.2
1	F	35	GLY	3.2
1	D	223	ALA	3.1
1	E	43	GLY	3.1
1	E	333	LYS	3.1
1	D	109	ARG	3.1
1	F	65	GLN	3.1
1	F	41	LYS	3.0
1	D	249	GLN	3.0
1	D	173	VAL	3.0
1	C	35	GLY	3.0
1	C	173	VAL	2.9
1	F	19	LYS	2.9
1	C	30	GLN	2.9
1	F	36	GLU	2.9
1	F	127	LYS	2.9
1	F	23	TYR	2.9
1	D	334	GLN	2.9
1	F	299	LEU	2.9
1	E	44	LYS	2.9
1	A	172	PHE	2.8
1	E	149	GLU	2.8
1	B	33	SER	2.8
1	F	40	LEU	2.8
1	F	143	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	333	LYS	2.8
1	A	223	ALA	2.7
1	D	5	ILE	2.7
1	D	333	LYS	2.7
1	F	31	HIS	2.7
1	F	180	MET	2.7
1	F	181	ASP	2.6
1	F	309	GLU	2.6
1	C	222	PHE	2.6
1	D	42	ASP	2.6
1	E	334	GLN	2.6
1	F	202	ALA	2.6
1	C	221	CYS	2.5
1	B	143	ILE	2.5
1	C	333	LYS	2.5
1	E	203	ILE	2.5
1	E	73	LEU	2.5
1	E	34	LYS	2.5
1	F	173	VAL	2.5
1	F	334	GLN	2.5
1	A	181	ASP	2.4
1	B	249	GLN	2.4
1	F	16	ASP	2.4
1	C	331	GLU	2.4
1	D	34	LYS	2.4
1	F	61	ARG	2.4
1	A	173	VAL	2.4
1	D	172	PHE	2.4
1	C	36	GLU	2.3
1	C	334	GLN	2.3
1	E	30	GLN	2.3
1	F	9	ILE	2.3
1	F	250	ASP	2.3
1	A	33	SER	2.3
1	C	44	LYS	2.3
1	D	299	LEU	2.3
1	F	22	GLY	2.3
1	F	48	VAL	2.3
1	A	65	GLN	2.3
1	F	12	LYS	2.3
1	C	42	ASP	2.2
1	B	34	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	43	GLY	2.2
1	B	172	PHE	2.2
1	C	141	VAL	2.2
1	D	181	ASP	2.2
1	E	46	PHE	2.2
1	B	181	ASP	2.2
1	D	166	ARG	2.2
1	F	223	ALA	2.1
1	E	331	GLU	2.1
1	C	172	PHE	2.1
1	D	143	ILE	2.1
1	A	42	ASP	2.1
1	B	35	GLY	2.1
1	E	249	GLN	2.1
1	A	114	LEU	2.1
1	C	96	LEU	2.1
1	C	46	PHE	2.1
1	D	222	PHE	2.1
1	F	222	PHE	2.1
1	D	221	CYS	2.1
1	D	141	VAL	2.1
1	A	115	GLY	2.1
1	D	177	ASP	2.1
1	F	166	ARG	2.0
1	A	5	ILE	2.0
1	F	26	TRP	2.0
1	C	174	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	401	1/1	1.00	0.10	-0.91	23,23,23,23	0
2	ZN	C	401	1/1	0.99	0.09	-1.50	25,25,25,25	0
2	ZN	B	401	1/1	0.99	0.08	-2.63	20,20,20,20	0
2	ZN	F	401	1/1	0.98	0.09	-3.09	33,33,33,33	0
2	ZN	E	401	1/1	1.00	0.09	-4.45	29,29,29,29	0
2	ZN	D	401	1/1	0.99	0.07	-5.02	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.