



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:45 PM UTC

PDB ID : 4OFC / pdb_00004ofc
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 ⓘ 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

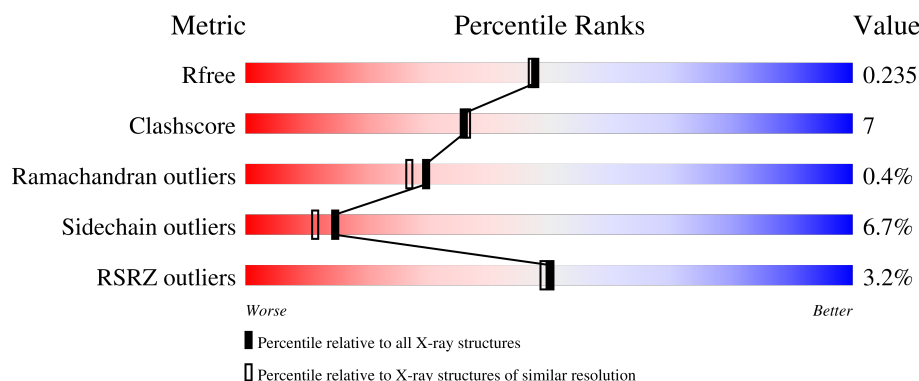
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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.

Mol	Chain	Length	Quality of chain
1	A	335	83% 15% .
1	B	335	86% 13% .
1	C	335	81% 17% .
1	D	335	83% 15% .
1	E	335	82% 16% .

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Mol	Chain	Length	Quality of chain
1	F	335	8% 73% 22%

2 Entry composition

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 (CCD ID: 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		

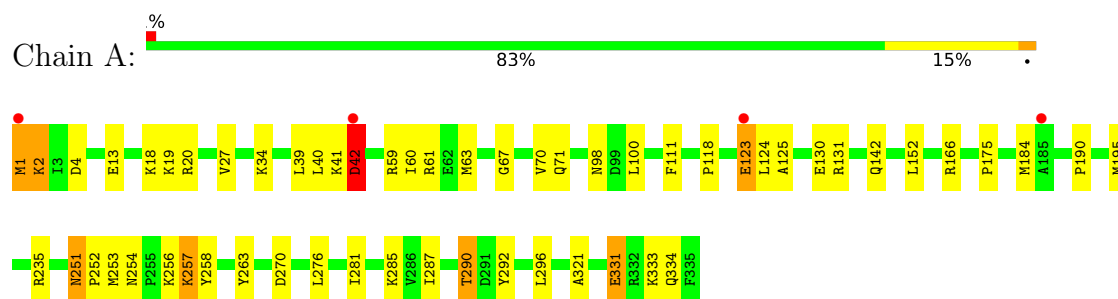
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total 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

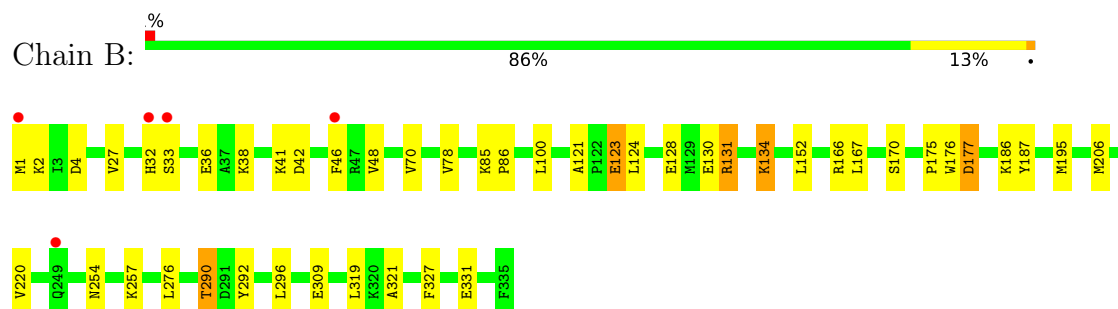
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

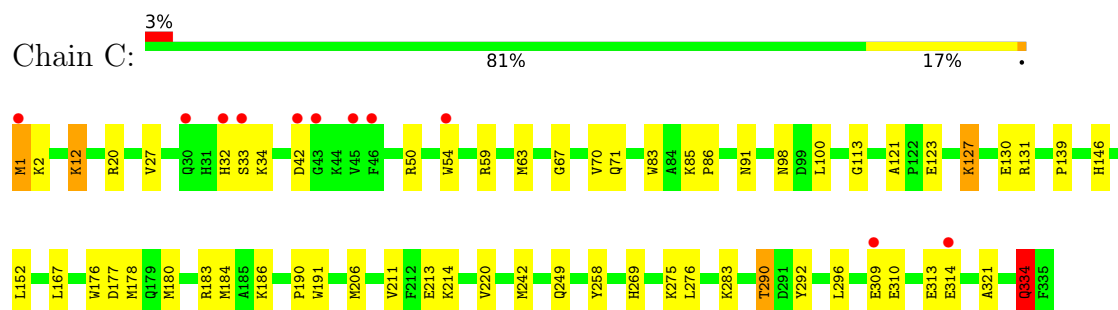
- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase



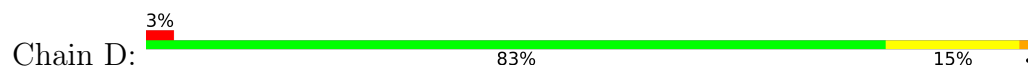
- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase

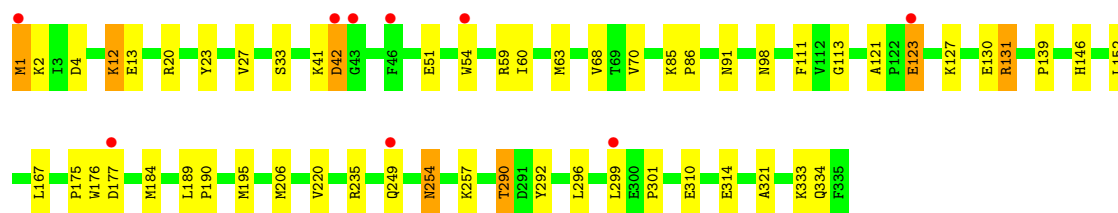


- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase

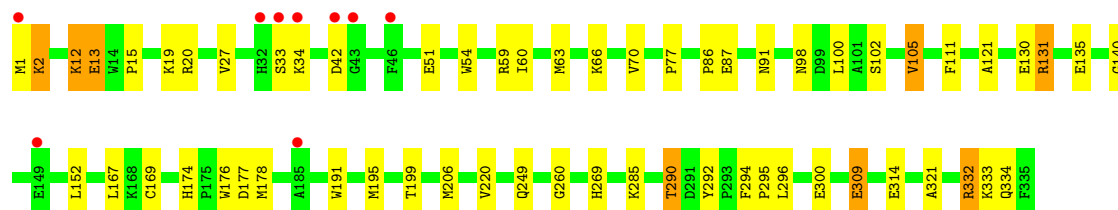
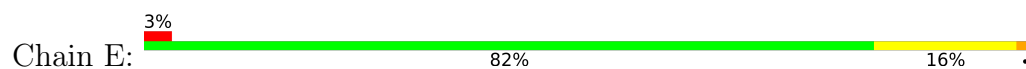


- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase

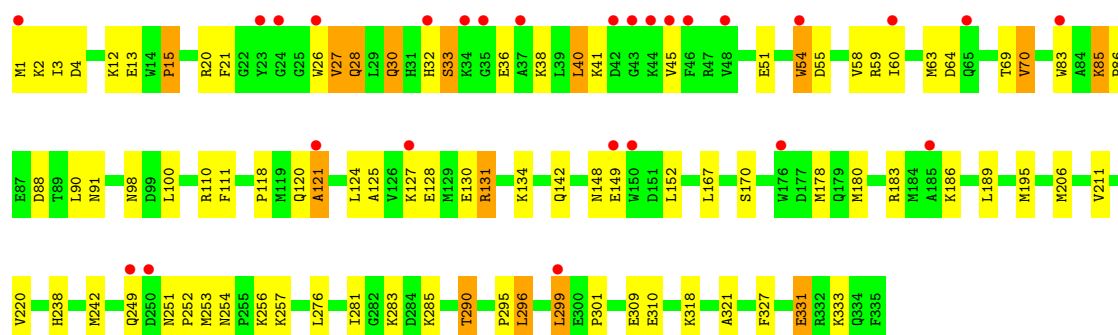
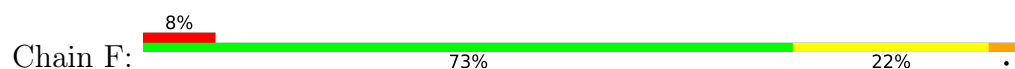




- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase



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4 Data and refinement statistics

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 – 1.99	Depositor EDS
% Data completeness (in resolution range)	86.4 (27.11-1.99) 83.4 (27.11-1.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.96Å)	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 (4.36%)	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 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.51	0/2736	0.79	2/3701 (0.1%)
1	B	0.54	0/2736	0.81	2/3701 (0.1%)
1	C	0.50	0/2736	0.84	1/3701 (0.0%)
1	D	0.49	0/2736	0.81	4/3701 (0.1%)
1	E	0.47	0/2736	0.80	0/3701
1	F	0.45	0/2736	0.84	6/3701 (0.2%)
All	All	0.50	0/16416	0.82	15/22206 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	GLN	N-CA-C	-6.47	104.65	112.54
1	F	85	LYS	CA-C-N	5.90	126.04	119.32
1	F	85	LYS	C-N-CA	5.90	126.04	119.32
1	A	251	ASN	CA-C-N	5.70	125.39	119.64
1	A	251	ASN	C-N-CA	5.70	125.39	119.64
1	F	121	ALA	CA-C-N	5.23	125.03	119.28
1	F	121	ALA	C-N-CA	5.23	125.03	119.28
1	D	254	ASN	CA-C-N	5.21	125.51	119.47
1	D	254	ASN	C-N-CA	5.21	125.51	119.47
1	D	189	LEU	CA-C-N	-5.21	113.56	119.28
1	D	189	LEU	C-N-CA	-5.21	113.56	119.28
1	F	55	ASP	CA-C-N	5.14	124.76	119.05
1	F	55	ASP	C-N-CA	5.14	124.76	119.05
1	B	85	LYS	CA-C-N	5.12	124.57	119.24
1	B	85	LYS	C-N-CA	5.12	124.57	119.24

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	2664	0	2673	40	0
1	B	2664	0	2673	35	0
1	C	2664	0	2673	41	0
1	D	2664	0	2673	37	0
1	E	2664	0	2673	36	0
1	F	2664	0	2673	51	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	235	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 7.

All (235) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:178:MET:HE2	1:F:180:MET:HE1	1.69	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	1.75	0.69
1:A:254:ASN:H	1:A:257:LYS:HZ3	1.39	0.69
1:C:59:ARG:C	1:C:63:MET:HE3	2.19	0.68
1:D:42:ASP:HB2	3:D:632:HOH:O	1.92	0.68
1:B:175:PRO:HG2	1:B:195:MET:HE2	1.76	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:A:1:MET:HE3	1:A:67:GLY:HA3	1.78	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:F:63:MET:HE1	1:F:111:PHE:CZ	2.32	0.65
1:B:32:HIS:HE1	1:B:36:GLU:HG2	1.62	0.65
1:F:238:HIS:CE1	1:F:242:MET:HE3	2.32	0.65
1:F:253:MET:HG3	1:F:257:LYS:HD2	1.78	0.65
1:C:206:MET:HE1	1:C:220:VAL:HG21	1.79	0.64
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: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:D:254:ASN:H	1:D:257:LYS:HZ3	1.47	0.63
1:C:214:LYS:NZ	3:C:621:HOH:O	2.30	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:ARG:C	1:F:63:MET:HE3	2.28	0.58
1:A:235:ARG:NH2	1:F:195:MET:HE2	2.19	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:D:235:ARG:NH2	1:E:195:MET:HE3	2.20	0.57
1:C:1:MET:HE3	1:C:67:GLY:HA3	1.86	0.57
1:A:59:ARG:C	1:A:63:MET:HE3	2.30	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:A:41:LYS:O	1:A:42:ASP:C	2.49	0.55
1:B:32:HIS:CE1	1:B:36:GLU:HG2	2.41	0.55
1:B:254:ASN:H	1:B:257:LYS:HZ3	1.54	0.55
1:D:1:MET:HB3	1:D:301:PRO:O	2.07	0.55
1:F:4:ASP:OD2	1:F:290:THR:HB	2.07	0.55
1:A:175:PRO:HG2	1:A:195:MET:HE3	1.87	0.54
1:D:63:MET:HE1	1:D:111:PHE:CZ	2.42	0.54
1:E:59:ARG:C	1:E:63:MET:HE3	2.32	0.54
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:F:206:MET:HE1	1:F:220:VAL:HG21	1.88	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:C:180:MET:HE1	1:C:191:TRP:CZ3	2.44	0.53
1:E:66:LYS:NZ	1:E:300:GLU:OE2	2.24	0.53
1:D:12:LYS:HE2	1:D:13:GLU:N	2.20	0.53
1:E:63:MET:HE1	1:E:111:PHE:CZ	2.44	0.53
1:B:166:ARG:NH2	3:B:700:HOH:O	2.32	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:D:59:ARG:C	1:D:63:MET:HE3	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:MET:HE1	1:A:111:PHE:CE1	2.44	0.52
1:D:206:MET:HE1	1:D:220:VAL:HG21	1.90	0.52
1:C:33:SER:OG	1:C:34:LYS:N	2.43	0.52
1:C:206:MET:HE3	1:C:211:VAL:HG11	1.92	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: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:206:MET:HE1	1:E:220:VAL:HG21	1.92	0.51
1:E:290:THR:HG22	1:E:292:TYR:H	1.75	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:A:63:MET:HE2	1:A:71:GLN:CD	2.35	0.51
1:C:59:ARG:O	1:C:63:MET:HE3	2.11	0.51
1:C:249:GLN:HG2	3:C:529:HOH:O	2.10	0.51
1:B:2:LYS:HB2	1:B:321:ALA:HB2	1.93	0.50
1:F:83:TRP:CD1	1:F:83:TRP:H	2.29	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:F:63:MET:HE1	1:F:111:PHE:CE1	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ARG:NH1	1:C:91:ASN:OD1	2.47	0.47
1:B:176:TRP:CG	1:B:177:ASP:N	2.83	0.47
1:A:270:ASP:OD2	1:F:256:LYS:NZ	2.47	0.47
1:F:206:MET:HE3	1:F:211:VAL:HG11	1.95	0.47
1:B:176:TRP:CG	1:B:177:ASP:H	2.33	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:98:ASN:CG	1:A:131:ARG:HH22	2.18	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:C:275:LYS:NZ	1:C:310:GLU:OE2	2.48	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:C:213:GLU:OE1	1:C:258:TYR:OH	2.27	0.46
1:D:63:MET:HE1	1:D:111:PHE:CE1	2.50	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:C:83:TRP:CD1	1:C:83:TRP:H	2.32	0.46
1:B:290:THR:CG2	1:B:292:TYR:HB2	2.46	0.45
1:B:206:MET:HE1	1:B:220:VAL:HG21	1.98	0.45
1:B:86:PRO:HB3	1:B:121:ALA:HB2	1.98	0.45
1:C:63:MET:HE2	1:C:71:GLN:CD	2.41	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:175:PRO:HG2	1:B:195:MET:HE3	1.99	0.43
1:E:1:MET:HE2	1:E:1:MET:HB3	1.93	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: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:A:63:MET:HE1	1:A:111:PHE:HE1	1.85	0.42
1:C:242:MET:HE2	1:C:242:MET:HA	2.01	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:B:4:ASP:CG	1:B:290:THR:HB	2.45	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:A:1:MET:HE2	1:A:1:MET:HB3	1.86	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:A:59:ARG:O	1:A:63:MET:HE3	2.20	0.41
1:B:186:LYS:HD2	1:B:187:TYR:CE1	2.55	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:D:176:TRP:CG	1:D:177:ASP:H	2.39	0.41
1:F:296:LEU:HD23	1:F:296:LEU:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:26:TRP:H	1:F:26:TRP:CD1	2.37	0.41
1:F:69:THR:HA	1:F:110:ARG:HH12	1.84	0.41
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:D:60:ILE:HA	1:D:63:MET:HE3	2.02	0.41
1:E:191:TRP:CD1	1:E:195:MET:HE2	2.56	0.41
1:F:32:HIS:HD2	1:F:38:LYS:HG3	1.85	0.41
1:F:178:MET:SD	1:F:195:MET:HG3	2.60	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:D:4:ASP:CG	1:D:290:THR:HB	2.46	0.40
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%)	36	35
1	B	333/335 (99%)	324 (97%)	9 (3%)	0	100	100
1	C	333/335 (99%)	321 (96%)	11 (3%)	1 (0%)	36	35
1	D	333/335 (99%)	324 (97%)	7 (2%)	2 (1%)	21	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	333/335 (99%)	320 (96%)	12 (4%)	1 (0%)	36	35
1	F	333/335 (99%)	317 (95%)	13 (4%)	3 (1%)	14	9
All	All	1998/2010 (99%)	1930 (97%)	60 (3%)	8 (0%)	30	27

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 ⓘ

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%)	267 (93%)	21 (7%)	13	9
1	B	288/288 (100%)	272 (94%)	16 (6%)	19	16
1	C	288/288 (100%)	272 (94%)	16 (6%)	19	16
1	D	288/288 (100%)	272 (94%)	16 (6%)	19	16
1	E	288/288 (100%)	268 (93%)	20 (7%)	14	11
1	F	288/288 (100%)	261 (91%)	27 (9%)	8	5
All	All	1728/1728 (100%)	1612 (93%)	116 (7%)	15	11

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS

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Mol	Chain	Res	Type
1	A	13	GLU
1	A	19	LYS
1	A	27	VAL
1	A	34	LYS
1	A	40	LEU
1	A	42	ASP
1	A	61	ARG
1	A	70	VAL
1	A	100	LEU
1	A	123	GLU
1	A	130	GLU
1	A	152	LEU
1	A	166	ARG
1	A	256	LYS
1	A	257	LYS
1	A	290	THR
1	A	296	LEU
1	A	331	GLU
1	A	333	LYS
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	131	ARG
1	B	134	LYS
1	B	152	LEU
1	B	177	ASP
1	B	290	THR
1	B	296	LEU
1	B	309	GLU
1	B	319	LEU
1	B	331	GLU
1	C	1	MET
1	C	12	LYS
1	C	27	VAL
1	C	32	HIS
1	C	54	TRP
1	C	70	VAL
1	C	100	LEU

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Mol	Chain	Res	Type
1	C	123	GLU
1	C	127	LYS
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	334	GLN
1	D	1	MET
1	D	12	LYS
1	D	27	VAL
1	D	33	SER
1	D	41	LYS
1	D	70	VAL
1	D	123	GLU
1	D	131	ARG
1	D	152	LEU
1	D	249	GLN
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	2	LYS
1	E	12	LYS
1	E	13	GLU
1	E	19	LYS
1	E	27	VAL
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	290	THR
1	E	296	LEU
1	E	309	GLU

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Mol	Chain	Res	Type
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	60	ILE
1	F	70	VAL
1	F	100	LEU
1	F	127	LYS
1	F	131	ARG
1	F	134	LYS
1	F	149	GLU
1	F	152	LEU
1	F	249	GLN
1	F	283	LYS
1	F	290	THR
1	F	296	LEU
1	F	299	LEU
1	F	309	GLU
1	F	310	GLU
1	F	318	LYS
1	F	331	GLU
1	F	333	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	B	251	ASN
1	C	148	ASN
1	C	269	HIS
1	D	148	ASN
1	D	251	ASN
1	D	269	HIS
1	E	148	ASN

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Mol	Chain	Res	Type
1	E	238	HIS
1	E	251	ASN
1	E	269	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/335 (100%)	0.06	4 (1%) 76 76	14, 26, 43, 54	0
1	B	335/335 (100%)	-0.17	5 (1%) 72 71	13, 22, 37, 60	0
1	C	335/335 (100%)	0.02	11 (3%) 49 48	17, 26, 45, 69	0
1	D	335/335 (100%)	0.01	9 (2%) 56 55	17, 26, 42, 53	0
1	E	335/335 (100%)	0.18	9 (2%) 56 55	19, 29, 48, 63	0
1	F	335/335 (100%)	0.63	27 (8%) 18 17	20, 34, 67, 81	0
All	All	2010/2010 (100%)	0.12	65 (3%) 50 49	13, 27, 49, 81	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1	MET	7.6
1	B	1	MET	7.0
1	E	1	MET	5.9
1	D	1	MET	5.6
1	C	1	MET	5.4
1	A	1	MET	4.6
1	F	176	TRP	4.2
1	F	43	GLY	3.9
1	F	32	HIS	3.9
1	B	32	HIS	3.7
1	F	54	TRP	3.5
1	D	42	ASP	3.5
1	F	46	PHE	3.3
1	A	42	ASP	3.2
1	F	45	VAL	3.1
1	B	46	PHE	3.1
1	F	35	GLY	3.1
1	F	34	LYS	3.0
1	E	46	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	149	GLU	3.0
1	F	48	VAL	2.9
1	F	249	GLN	2.9
1	F	42	ASP	2.9
1	C	32	HIS	2.8
1	D	177	ASP	2.8
1	C	54	TRP	2.8
1	F	299	LEU	2.8
1	F	185	ALA	2.8
1	E	149	GLU	2.7
1	C	43	GLY	2.7
1	F	26	TRP	2.7
1	D	249	GLN	2.5
1	F	65	GLN	2.5
1	C	42	ASP	2.5
1	E	185	ALA	2.5
1	C	46	PHE	2.5
1	D	43	GLY	2.5
1	F	24	GLY	2.5
1	F	150	TRP	2.4
1	A	123	GLU	2.4
1	E	32	HIS	2.4
1	E	43	GLY	2.4
1	F	83	TRP	2.4
1	F	250	ASP	2.3
1	F	23	TYR	2.3
1	E	42	ASP	2.3
1	B	249	GLN	2.3
1	D	299	LEU	2.3
1	D	46	PHE	2.2
1	E	33	SER	2.2
1	F	127	LYS	2.2
1	B	33	SER	2.2
1	E	34	LYS	2.2
1	C	309	GLU	2.2
1	F	44	LYS	2.2
1	D	123	GLU	2.1
1	C	30	GLN	2.1
1	D	54	TRP	2.1
1	C	314	GLU	2.1
1	F	37	ALA	2.1
1	A	185	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	45	VAL	2.0
1	F	121	ALA	2.0
1	C	33	SER	2.0
1	F	60	ILE	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	ZN	F	401	1/1	0.97	0.04	33,33,33,33	0
2	ZN	C	401	1/1	0.98	0.03	25,25,25,25	0
2	ZN	D	401	1/1	0.99	0.01	26,26,26,26	0
2	ZN	B	401	1/1	0.99	0.01	20,20,20,20	0
2	ZN	E	401	1/1	1.00	0.01	29,29,29,29	0
2	ZN	A	401	1/1	1.00	0.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.