



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:42 PM UTC

PDB ID : 3A6F / pdb_00003a6f
Title : W174F mutant creatininase, Type II
Authors : Nakajima, Y.; Yamashita, K.; Ito, K.; Yoshimoto, T.
Deposited on : 2009-08-31
Resolution : 1.78 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

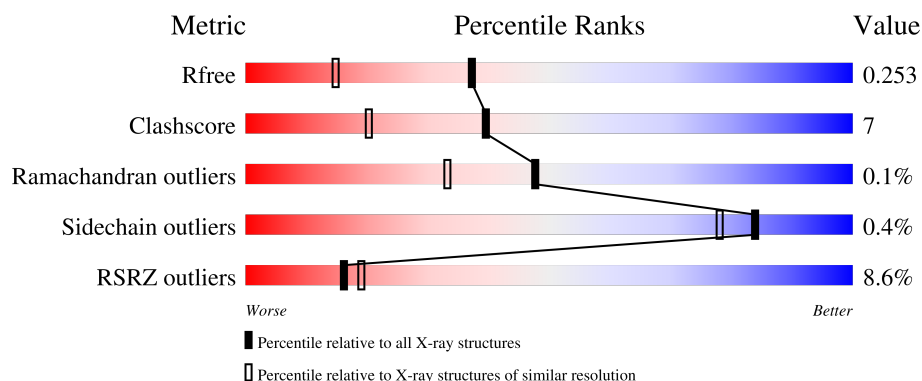
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	260	11% 80% 18% ..
1	B	260	9% 82% 16% ..
1	C	260	9% 82% 16% ..
1	D	260	8% 82% 16% .
1	E	260	7% 85% 13% ..

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Mol	Chain	Length	Quality of chain
1	F	260	7% 82% 15% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12656 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 Creatinine amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1984	1271	337	365	11			
1	B	257	Total	C	N	O	S	0	0	0
			1981	1269	336	365	11			
1	C	257	Total	C	N	O	S	0	0	0
			1977	1267	335	364	11			
1	D	257	Total	C	N	O	S	0	0	0
			1977	1266	335	365	11			
1	E	257	Total	C	N	O	S	0	0	0
			1970	1263	334	362	11			
1	F	256	Total	C	N	O	S	0	0	0
			1961	1257	332	361	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	PHE	TRP	engineered mutation	UNP P83772
B	174	PHE	TRP	engineered mutation	UNP P83772
C	174	PHE	TRP	engineered mutation	UNP P83772
D	174	PHE	TRP	engineered mutation	UNP P83772
E	174	PHE	TRP	engineered mutation	UNP P83772
F	174	PHE	TRP	engineered mutation	UNP P83772

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

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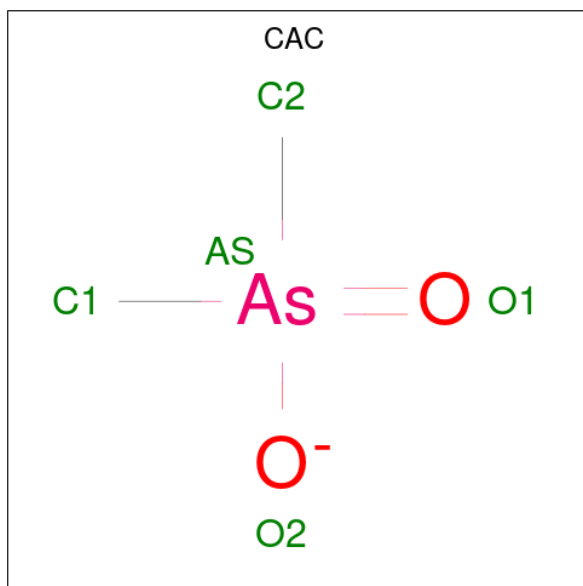
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Mn 1	0	0
2	E	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	C	1	Total	As	C	O	0	0
			5	1	2	2		
4	D	1	Total	As	C	O	0	0
			5	1	2	2		
4	E	1	Total	As	C	O	0	0
			5	1	2	2		
4	F	1	Total	As	C	O	0	0
			5	1	2	2		

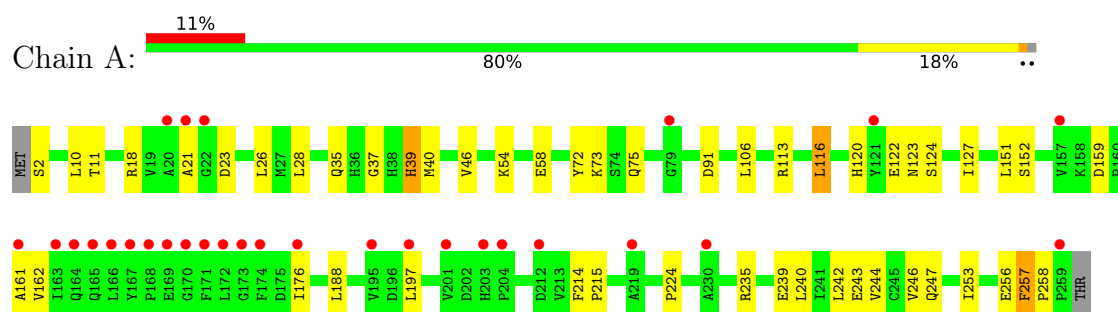
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total	O	0	0
			111	111		
5	B	124	Total	O	0	0
			124	124		
5	C	126	Total	O	0	0
			126	126		
5	D	128	Total	O	0	0
			128	128		
5	E	125	Total	O	0	0
			125	125		
5	F	150	Total	O	0	0
			150	150		

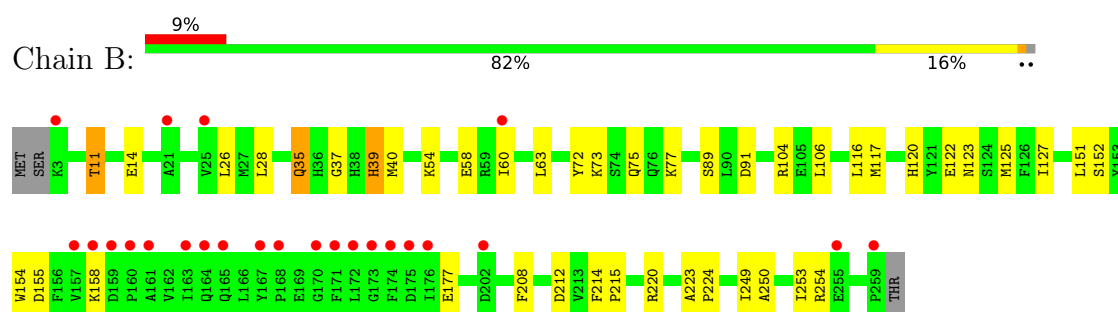
3 Residue-property plots

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.

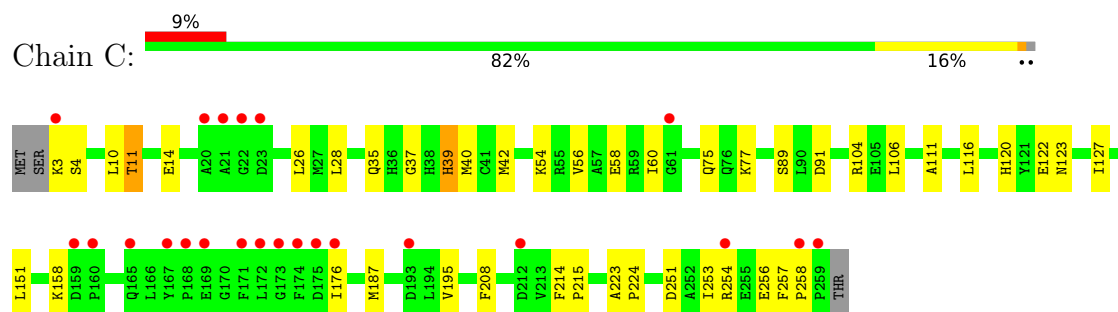
- Molecule 1: Creatinine amidohydrolase



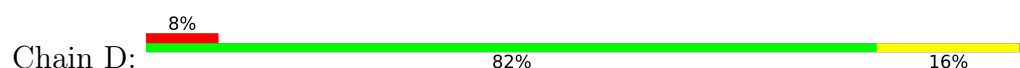
- Molecule 1: Creatinine amidohydrolase

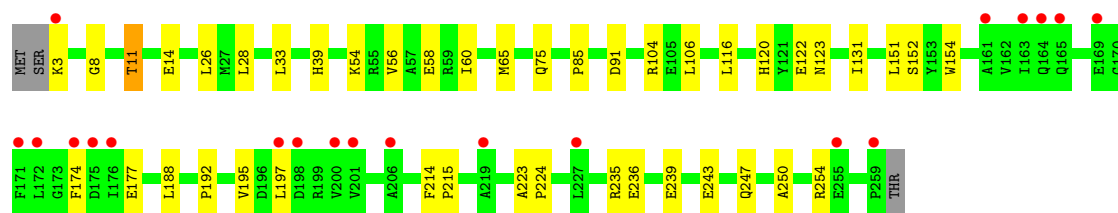


- Molecule 1: Creatinine amidohydrolase

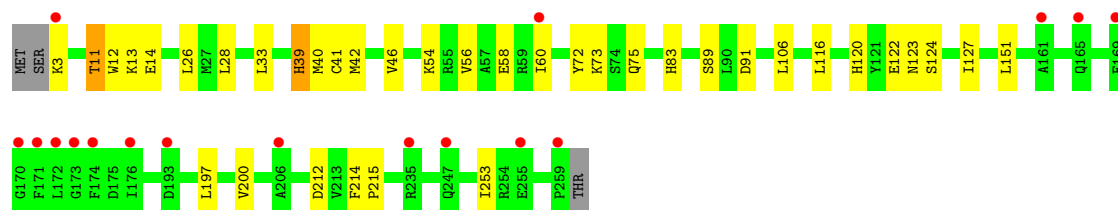
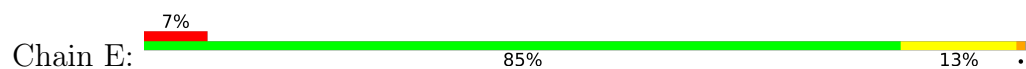


- Molecule 1: Creatinine amidohydrolase

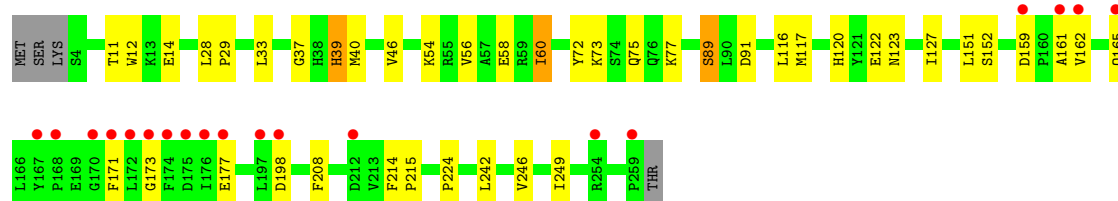
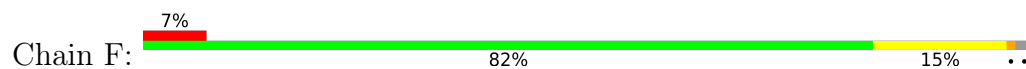




● Molecule 1: Creatinine amidohydrolase



● Molecule 1: Creatinine amidohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.30Å 164.30Å 163.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.78 20.00 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.78) 99.7 (20.00-1.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.257 0.233 , 0.253	Depositor DCC
R_{free} test set	12157 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12656	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: MN, CAC, 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	0.39	0/2032	0.90	9/2764 (0.3%)
1	B	0.39	0/2029	0.88	6/2760 (0.2%)
1	C	0.39	0/2025	0.89	5/2755 (0.2%)
1	D	0.39	0/2025	0.89	4/2756 (0.1%)
1	E	0.41	0/2018	0.90	7/2747 (0.3%)
1	F	0.40	0/2009	0.91	9/2736 (0.3%)
All	All	0.39	0/12138	0.89	40/16518 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	THR	N-CA-C	-7.90	100.33	110.53
1	E	11	THR	N-CA-C	-6.08	101.53	110.52
1	B	11	THR	N-CA-C	-6.03	102.41	110.55
1	C	91	ASP	N-CA-C	-5.98	102.64	110.53
1	B	39	HIS	N-CA-C	5.97	120.72	113.38
1	C	11	THR	N-CA-C	-5.77	101.98	110.52
1	E	33	LEU	N-CA-C	-5.72	97.86	107.99
1	E	127	ILE	N-CA-C	-5.70	104.96	110.72
1	F	33	LEU	N-CA-C	-5.70	98.05	108.02
1	E	91	ASP	N-CA-C	-5.68	103.04	110.53
1	F	127	ILE	N-CA-C	-5.66	105.00	110.72
1	C	39	HIS	N-CA-C	5.65	120.33	113.38
1	F	152	SER	N-CA-C	-5.56	99.35	108.41
1	E	39	HIS	N-CA-C	5.54	120.20	113.38
1	F	177	GLU	N-CA-C	5.54	117.94	109.62
1	C	127	ILE	N-CA-C	-5.54	105.13	110.72
1	A	91	ASP	N-CA-C	-5.50	103.27	110.53
1	D	91	ASP	N-CA-C	-5.48	103.16	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	89	SER	N-CA-C	5.43	118.59	109.95
1	D	39	HIS	N-CA-C	5.42	120.04	113.38
1	B	177	GLU	N-CA-C	5.40	117.97	109.39
1	F	91	ASP	N-CA-C	-5.38	103.29	110.55
1	F	39	HIS	N-CA-C	5.34	119.90	113.17
1	A	46	VAL	N-CA-C	-5.32	106.61	111.67
1	C	89	SER	N-CA-C	5.28	118.34	109.95
1	F	60	ILE	N-CA-C	5.23	117.14	112.17
1	A	152	SER	N-CA-C	-5.20	100.05	108.52
1	A	124	SER	N-CA-C	5.19	121.86	110.80
1	E	42	MET	N-CA-C	5.18	119.60	113.28
1	A	257	PHE	CA-C-N	5.16	123.38	119.66
1	A	257	PHE	C-N-CA	5.16	123.38	119.66
1	A	127	ILE	N-CA-C	-5.11	105.56	110.72
1	A	39	HIS	N-CA-C	5.11	119.66	113.38
1	F	46	VAL	N-CA-C	-5.10	106.83	111.67
1	E	46	VAL	N-CA-C	-5.10	106.83	111.67
1	D	33	LEU	N-CA-C	-5.08	98.99	107.99
1	B	89	SER	N-CA-C	5.08	118.03	109.95
1	D	11	THR	N-CA-C	-5.06	103.03	110.52
1	B	91	ASP	N-CA-C	-5.06	103.85	110.53
1	B	127	ILE	N-CA-C	-5.03	105.64	110.72

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	1984	0	1967	29	0
1	B	1981	0	1964	28	0
1	C	1977	0	1958	28	0
1	D	1977	0	1953	31	0
1	E	1970	0	1945	23	0
1	F	1961	0	1932	22	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
4	F	5	0	0	0	0
5	A	111	0	0	1	0
5	B	124	0	0	3	0
5	C	126	0	0	3	0
5	D	128	0	0	4	0
5	E	125	0	0	2	0
5	F	150	0	0	1	0
All	All	12656	0	11719	159	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 (159) 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:E:120:HIS:HB3	1:E:123:ASN:ND2	1.94	0.81
1:A:120:HIS:HB3	1:A:123:ASN:ND2	2.00	0.76
1:C:28:LEU:HD23	1:C:116:LEU:HD21	1.69	0.75
1:A:54:LYS:O	1:A:58:GLU:HG3	1.90	0.72
1:D:188:LEU:O	1:D:192:PRO:HG3	1.91	0.70
1:E:28:LEU:HD23	1:E:116:LEU:HD21	1.75	0.68
1:B:72:TYR:H	1:B:123:ASN:ND2	1.93	0.66
1:F:198:ASP:HB2	5:F:1336:HOH:O	1.96	0.65
1:C:54:LYS:O	1:C:58:GLU:HG3	1.97	0.65
1:C:120:HIS:HB3	1:C:123:ASN:ND2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:LEU:HD23	1:F:116:LEU:HD21	1.78	0.65
1:D:120:HIS:HB3	1:D:123:ASN:ND2	2.13	0.64
1:E:3:LYS:HE2	5:E:1666:HOH:O	1.99	0.63
1:D:188:LEU:HD21	1:D:197:LEU:HD11	1.81	0.62
1:C:4:SER:HB2	5:C:1586:HOH:O	1.98	0.62
1:A:23:ASP:HB2	1:A:113:ARG:NH2	2.16	0.60
1:F:72:TYR:O	1:F:120:HIS:HE1	1.84	0.60
1:F:120:HIS:HB3	1:F:123:ASN:ND2	2.16	0.60
1:B:28:LEU:HD23	1:B:116:LEU:HD21	1.84	0.60
1:F:54:LYS:O	1:F:58:GLU:HG3	2.03	0.59
1:E:120:HIS:HA	4:E:303:CAC:O1	2.03	0.58
1:B:54:LYS:O	1:B:58:GLU:HG3	2.04	0.58
1:A:243:GLU:O	1:A:247:GLN:HG3	2.03	0.58
1:A:28:LEU:HD23	1:A:116:LEU:HD21	1.85	0.58
1:D:235:ARG:O	1:D:239:GLU:HG3	2.04	0.58
1:F:28:LEU:HD23	1:F:116:LEU:CD2	2.33	0.57
1:C:120:HIS:HA	4:C:303:CAC:O1	2.04	0.57
1:D:243:GLU:HG3	1:D:247:GLN:HE21	1.70	0.57
1:E:214:PHE:HA	1:E:215:PRO:C	2.30	0.56
1:F:151:LEU:C	1:F:151:LEU:HD12	2.30	0.56
1:C:104:ARG:HD2	5:C:1454:HOH:O	2.05	0.56
1:B:11:THR:OG1	1:B:14:GLU:HG3	2.06	0.55
1:D:195:VAL:HG12	1:D:197:LEU:HD12	1.89	0.55
1:C:256:GLU:C	1:C:258:PRO:HD3	2.32	0.55
1:B:220:ARG:HD3	5:B:1610:HOH:O	2.07	0.54
1:D:214:PHE:HA	1:D:215:PRO:C	2.32	0.54
1:F:161:ALA:O	1:F:165:GLN:HG2	2.07	0.54
1:C:214:PHE:HA	1:C:215:PRO:C	2.33	0.54
1:F:56:VAL:O	1:F:60:ILE:HG13	2.07	0.54
1:B:214:PHE:HA	1:B:215:PRO:C	2.32	0.53
1:A:214:PHE:HA	1:A:215:PRO:C	2.33	0.53
1:A:256:GLU:C	1:A:258:PRO:HD3	2.33	0.53
1:C:26:LEU:HD13	1:C:106:LEU:HD22	1.91	0.53
1:F:214:PHE:HA	1:F:215:PRO:C	2.33	0.53
1:C:56:VAL:O	1:C:60:ILE:HG12	2.08	0.52
1:D:11:THR:OG1	1:D:14:GLU:HG3	2.09	0.52
1:B:72:TYR:H	1:B:123:ASN:HD21	1.57	0.52
1:E:54:LYS:O	1:E:58:GLU:HG3	2.10	0.52
1:E:12:TRP:CZ2	1:E:13:LYS:HD3	2.46	0.51
1:E:151:LEU:C	1:E:151:LEU:HD12	2.34	0.51
1:C:26:LEU:CD1	1:C:106:LEU:HD22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ALA:N	1:B:224:PRO:HD2	2.26	0.51
1:E:56:VAL:O	1:E:60:ILE:HG12	2.11	0.51
1:D:3:LYS:N	5:D:1238:HOH:O	2.44	0.50
1:D:223:ALA:HB3	1:D:224:PRO:HD3	1.92	0.50
1:E:60:ILE:HD12	1:E:253:ILE:HG21	1.93	0.50
1:B:250:ALA:O	1:B:254:ARG:HG3	2.11	0.50
1:F:11:THR:OG1	1:F:14:GLU:HG3	2.11	0.50
1:D:54:LYS:O	1:D:58:GLU:HG3	2.12	0.50
1:D:116:LEU:HD12	1:D:131:ILE:HD11	1.94	0.50
1:D:188:LEU:HD21	1:D:197:LEU:CD1	2.42	0.49
1:B:75:GLN:HG2	1:B:122:GLU:HG2	1.92	0.49
1:D:75:GLN:HG2	1:D:122:GLU:HG2	1.94	0.49
1:F:159:ASP:OD2	1:F:162:VAL:HG23	2.13	0.49
1:F:117:MET:HE2	1:F:249:ILE:HD13	1.94	0.49
1:E:28:LEU:HD23	1:E:116:LEU:CD2	2.42	0.49
1:A:120:HIS:HA	4:A:303:CAC:O2	2.13	0.49
1:F:39:HIS:CD2	1:F:40:MET:HG3	2.47	0.49
1:A:240:LEU:O	1:A:244:VAL:HG23	2.12	0.48
1:D:104:ARG:HD2	5:D:1681:HOH:O	2.13	0.48
1:D:26:LEU:HD13	1:D:106:LEU:HD22	1.95	0.48
1:C:176:ILE:HD12	1:C:176:ILE:C	2.37	0.48
1:F:75:GLN:HG2	1:F:122:GLU:HG2	1.95	0.48
1:B:35:GLN:NE2	1:B:37:GLY:H	2.11	0.48
1:A:39:HIS:CD2	1:A:40:MET:HG3	2.48	0.48
1:B:117:MET:HE2	1:B:249:ILE:HD13	1.96	0.47
1:E:39:HIS:CD2	1:E:40:MET:HG3	2.49	0.47
1:C:251:ASP:HA	1:C:254:ARG:HH11	1.79	0.47
1:B:120:HIS:HA	4:B:303:CAC:O2	2.15	0.47
1:B:26:LEU:HD23	1:B:63:LEU:HB2	1.96	0.47
1:D:151:LEU:HD12	1:D:151:LEU:C	2.40	0.47
1:C:60:ILE:HD12	1:C:253:ILE:HG21	1.97	0.47
1:B:26:LEU:HD13	1:B:106:LEU:HD22	1.96	0.46
1:B:39:HIS:CD2	1:B:40:MET:HG3	2.49	0.46
1:D:28:LEU:HD23	1:D:116:LEU:HD21	1.96	0.46
1:A:159:ASP:HB3	1:A:162:VAL:HG23	1.98	0.46
1:B:120:HIS:HB3	1:B:123:ASN:OD1	2.16	0.46
1:E:120:HIS:HB3	1:E:123:ASN:HD21	1.77	0.46
1:B:60:ILE:HD12	1:B:253:ILE:HG21	1.98	0.45
1:E:11:THR:OG1	1:E:14:GLU:HG3	2.17	0.45
1:E:197:LEU:HA	1:E:200:VAL:HG23	1.99	0.45
1:A:26:LEU:CD1	1:A:106:LEU:HD22	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ARG:HB3	5:D:1681:HOH:O	2.17	0.45
1:E:83:HIS:H	1:E:83:HIS:CD2	2.35	0.45
1:B:120:HIS:HD2	1:B:123:ASN:ND2	2.15	0.45
1:A:2:SER:O	1:A:10:LEU:HD23	2.17	0.44
1:A:37:GLY:HA2	1:A:224:PRO:O	2.17	0.44
1:A:235:ARG:NH2	1:A:239:GLU:OE2	2.49	0.44
1:B:104:ARG:HD2	5:B:1365:HOH:O	2.17	0.44
1:D:85:PRO:HD3	5:D:1600:HOH:O	2.16	0.44
1:A:159:ASP:OD2	1:A:162:VAL:HG23	2.17	0.44
1:C:77:LYS:HE2	1:C:208:PHE:HB3	1.99	0.44
1:F:73:LYS:HA	1:F:89:SER:CB	2.47	0.44
1:C:111:ALA:HB1	5:C:1488:HOH:O	2.18	0.44
1:D:174:PHE:HD1	1:D:177:GLU:HG3	1.83	0.44
1:A:72:TYR:CG	1:A:73:LYS:N	2.86	0.44
1:D:236:GLU:OE1	1:D:236:GLU:N	2.48	0.44
1:B:72:TYR:CG	1:B:73:LYS:N	2.85	0.44
1:A:28:LEU:HD23	1:A:116:LEU:CD2	2.48	0.44
1:C:75:GLN:HG2	1:C:122:GLU:HG2	2.00	0.43
1:C:223:ALA:HB3	1:C:224:PRO:HD3	1.99	0.43
1:A:18:ARG:O	1:A:21:ALA:HB3	2.18	0.43
1:B:104:ARG:HB3	5:B:1365:HOH:O	2.18	0.43
1:B:155:ASP:O	1:B:158:LYS:HE3	2.18	0.43
1:A:242:LEU:O	1:A:246:VAL:HG23	2.18	0.43
1:E:83:HIS:HE1	5:E:1109:HOH:O	2.00	0.43
1:C:151:LEU:HD12	1:C:151:LEU:C	2.43	0.43
1:A:253:ILE:HG23	1:A:257:PHE:HD2	1.83	0.43
1:E:73:LYS:HA	1:E:89:SER:CB	2.49	0.43
1:A:235:ARG:HG2	1:A:239:GLU:OE2	2.18	0.43
1:C:60:ILE:CD1	1:C:253:ILE:HG21	2.49	0.43
1:B:152:SER:HB3	1:B:154:TRP:CE2	2.53	0.43
1:A:159:ASP:HB3	1:A:162:VAL:CG2	2.49	0.42
1:A:35:GLN:HB2	1:F:12:TRP:CD1	2.54	0.42
1:D:56:VAL:O	1:D:60:ILE:HG12	2.19	0.42
1:D:152:SER:HB3	1:D:154:TRP:CE2	2.54	0.42
1:E:60:ILE:CD1	1:E:253:ILE:HG21	2.49	0.42
1:A:159:ASP:OD2	1:A:161:ALA:HB3	2.19	0.42
1:B:77:LYS:HE2	1:B:208:PHE:CB	2.49	0.42
1:C:35:GLN:HA	1:C:42:MET:HG2	2.02	0.42
1:C:3:LYS:HG3	1:C:10:LEU:HD22	2.02	0.42
1:D:26:LEU:CD1	1:D:106:LEU:HD22	2.49	0.42
1:A:151:LEU:C	1:A:151:LEU:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:LEU:HD23	1:D:116:LEU:CD2	2.49	0.42
1:F:242:LEU:O	1:F:246:VAL:HG23	2.20	0.41
1:C:11:THR:OG1	1:C:14:GLU:HG3	2.21	0.41
1:A:75:GLN:HG2	1:A:122:GLU:HG2	2.03	0.41
1:B:28:LEU:HD23	1:B:116:LEU:CD2	2.48	0.41
1:B:151:LEU:C	1:B:151:LEU:HD12	2.46	0.41
1:C:39:HIS:CD2	1:C:40:MET:HG3	2.55	0.41
1:E:26:LEU:CD1	1:E:106:LEU:HD22	2.50	0.41
1:E:72:TYR:CG	1:E:73:LYS:N	2.89	0.41
1:C:187:MET:HB3	1:C:195:VAL:CG2	2.51	0.41
1:D:243:GLU:CG	1:D:247:GLN:HE21	2.34	0.41
1:D:65:MET:HE2	1:D:106:LEU:HD21	2.01	0.40
1:F:77:LYS:HE2	1:F:208:PHE:HB3	2.02	0.40
1:A:176:ILE:C	1:A:176:ILE:HD12	2.47	0.40
1:C:28:LEU:HD23	1:C:116:LEU:CD2	2.47	0.40
1:C:37:GLY:HA2	1:C:224:PRO:O	2.21	0.40
1:D:8:GLY:O	1:E:41:CYS:HB2	2.21	0.40
1:D:188:LEU:HD11	1:D:197:LEU:HD11	2.02	0.40
1:D:250:ALA:O	1:D:254:ARG:HG3	2.20	0.40
5:A:1120:HOH:O	1:B:125:MET:HG3	2.20	0.40
1:F:28:LEU:HA	1:F:29:PRO:HD3	1.91	0.40
1:A:188:LEU:HD11	1:A:197:LEU:HD11	2.04	0.40
1:C:257:PHE:N	1:C:258:PRO:HD3	2.37	0.40
1:E:75:GLN:HG2	1:E:122:GLU:HG2	2.02	0.40
1:F:37:GLY:HA2	1:F:224:PRO:O	2.22	0.40
1:F:171:PHE:CZ	1:F:173:GLY:HA2	2.56	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	256/260 (98%)	247 (96%)	9 (4%)	0	100	100
1	B	255/260 (98%)	249 (98%)	6 (2%)	0	100	100
1	C	255/260 (98%)	248 (97%)	7 (3%)	0	100	100
1	D	255/260 (98%)	248 (97%)	7 (3%)	0	100	100
1	E	255/260 (98%)	248 (97%)	6 (2%)	1 (0%)	30	16
1	F	254/260 (98%)	248 (98%)	6 (2%)	0	100	100
All	All	1530/1560 (98%)	1488 (97%)	41 (3%)	1 (0%)	48	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	124	SER

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	211/215 (98%)	210 (100%)	1 (0%)	81	73
1	B	211/215 (98%)	209 (99%)	2 (1%)	70	59
1	C	210/215 (98%)	209 (100%)	1 (0%)	81	73
1	D	210/215 (98%)	210 (100%)	0	100	100
1	E	208/215 (97%)	207 (100%)	1 (0%)	81	73
1	F	207/215 (96%)	207 (100%)	0	100	100
All	All	1257/1290 (97%)	1252 (100%)	5 (0%)	84	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LEU
1	B	35	GLN
1	B	212	ASP
1	C	158	LYS

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Mol	Chain	Res	Type
1	E	212	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	76	GLN
1	A	83	HIS
1	A	165	GLN
1	B	35	GLN
1	B	123	ASN
1	B	165	GLN
1	B	247	GLN
1	C	76	GLN
1	D	247	GLN
1	E	69	GLN
1	E	76	GLN
1	E	83	HIS
1	F	120	HIS
1	F	247	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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
4	CAC	D	303	2,3	2,4,4	2.55	2 (100%)	4,6,6	0.34	0
4	CAC	C	303	2,3	2,4,4	2.60	2 (100%)	4,6,6	0.36	0
4	CAC	F	303	2,3	2,4,4	2.56	2 (100%)	4,6,6	0.41	0
4	CAC	A	303	2,3	2,4,4	2.71	2 (100%)	4,6,6	0.53	0
4	CAC	B	303	2,3	2,4,4	2.54	2 (100%)	4,6,6	0.26	0
4	CAC	E	303	2,3	2,4,4	2.66	2 (100%)	4,6,6	0.31	0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	CAC	AS-C2	2.88	1.97	1.90
4	F	303	CAC	AS-C2	2.73	1.96	1.90
4	E	303	CAC	AS-C2	2.71	1.96	1.90
4	C	303	CAC	AS-C2	2.69	1.96	1.90
4	D	303	CAC	AS-C2	2.63	1.96	1.90
4	E	303	CAC	AS-C1	2.61	1.96	1.90
4	B	303	CAC	AS-C2	2.55	1.96	1.90
4	B	303	CAC	AS-C1	2.53	1.96	1.90
4	A	303	CAC	AS-C1	2.53	1.96	1.90
4	C	303	CAC	AS-C1	2.51	1.96	1.90
4	D	303	CAC	AS-C1	2.46	1.96	1.90
4	F	303	CAC	AS-C1	2.36	1.95	1.90

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	303	CAC	1	0
4	A	303	CAC	1	0
4	B	303	CAC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	303	CAC	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, 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	258/260 (99%)	0.69	29 (11%)	10 11	12, 24, 47, 59	0
1	B	257/260 (98%)	0.61	24 (9%)	14 16	14, 22, 43, 56	0
1	C	257/260 (98%)	0.61	23 (8%)	15 17	13, 23, 44, 54	0
1	D	257/260 (98%)	0.56	20 (7%)	19 22	12, 23, 43, 53	0
1	E	257/260 (98%)	0.52	17 (6%)	24 29	11, 21, 41, 56	0
1	F	256/260 (98%)	0.44	19 (7%)	20 24	12, 20, 41, 58	0
All	All	1542/1560 (98%)	0.57	132 (8%)	16 19	11, 22, 44, 59	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	172	LEU	6.7
1	A	172	LEU	6.4
1	F	171	PHE	5.9
1	D	176	ILE	5.7
1	D	174	PHE	5.0
1	D	171	PHE	5.0
1	A	170	GLY	4.9
1	E	173	GLY	4.9
1	E	171	PHE	4.8
1	F	170	GLY	4.7
1	B	174	PHE	4.6
1	E	170	GLY	4.6
1	E	176	ILE	4.5
1	A	21	ALA	4.5
1	B	173	GLY	4.4
1	D	172	LEU	4.4
1	B	171	PHE	4.4
1	E	259	PRO	4.3
1	A	174	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	172	LEU	4.3
1	B	170	GLY	4.3
1	C	259	PRO	4.2
1	D	175	ASP	4.2
1	F	174	PHE	4.2
1	B	259	PRO	4.1
1	E	3	LYS	4.1
1	C	174	PHE	4.0
1	A	259	PRO	3.9
1	B	3	LYS	3.9
1	A	22	GLY	3.8
1	B	172	LEU	3.8
1	B	176	ILE	3.7
1	A	168	PRO	3.7
1	B	202	ASP	3.7
1	E	174	PHE	3.7
1	A	201	VAL	3.7
1	C	21	ALA	3.6
1	B	175	ASP	3.6
1	C	3	LYS	3.5
1	A	173	GLY	3.5
1	A	171	PHE	3.5
1	C	175	ASP	3.5
1	A	165	GLN	3.5
1	A	163	ILE	3.4
1	C	176	ILE	3.4
1	F	173	GLY	3.4
1	D	197	LEU	3.3
1	F	176	ILE	3.3
1	C	172	LEU	3.3
1	D	259	PRO	3.2
1	D	3	LYS	3.2
1	F	175	ASP	3.2
1	D	161	ALA	3.1
1	C	22	GLY	3.0
1	E	161	ALA	3.0
1	C	171	PHE	3.0
1	D	164	GLN	3.0
1	A	176	ILE	3.0
1	D	169	GLU	3.0
1	B	161	ALA	2.9
1	C	167	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	165	GLN	2.9
1	F	198	ASP	2.8
1	A	203	HIS	2.8
1	A	169	GLU	2.8
1	E	206	ALA	2.8
1	F	162	VAL	2.7
1	B	167	TYR	2.7
1	F	161	ALA	2.7
1	C	160	PRO	2.7
1	F	254	ARG	2.6
1	F	259	PRO	2.6
1	C	193	ASP	2.6
1	D	198	ASP	2.6
1	B	164	GLN	2.6
1	C	173	GLY	2.6
1	B	21	ALA	2.6
1	E	169	GLU	2.6
1	D	255	GLU	2.5
1	D	206	ALA	2.5
1	D	227	LEU	2.5
1	D	219	ALA	2.5
1	F	167	TYR	2.5
1	A	164	GLN	2.4
1	F	165	GLN	2.4
1	C	159	ASP	2.4
1	C	258	PRO	2.4
1	A	20	ALA	2.4
1	E	193	ASP	2.4
1	C	165	GLN	2.3
1	B	159	ASP	2.3
1	D	201	VAL	2.3
1	C	23	ASP	2.3
1	B	160	PRO	2.3
1	A	197	LEU	2.3
1	B	165	GLN	2.3
1	E	247	GLN	2.3
1	A	157	VAL	2.3
1	B	255	GLU	2.3
1	C	169	GLU	2.3
1	B	60	ILE	2.2
1	D	200	VAL	2.2
1	A	219	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	212	ASP	2.2
1	F	197	LEU	2.2
1	D	163	ILE	2.2
1	B	168	PRO	2.2
1	F	168	PRO	2.2
1	A	195	VAL	2.2
1	F	159	ASP	2.2
1	E	255	GLU	2.2
1	A	166	LEU	2.2
1	B	158	LYS	2.2
1	E	60	ILE	2.2
1	A	161	ALA	2.1
1	A	230	ALA	2.1
1	C	254	ARG	2.1
1	A	79	GLY	2.1
1	F	177	GLU	2.1
1	C	61	GLY	2.1
1	C	168	PRO	2.1
1	B	157	VAL	2.1
1	E	235	ARG	2.1
1	A	204	PRO	2.1
1	A	167	TYR	2.1
1	B	25	VAL	2.0
1	C	212	ASP	2.0
1	D	165	GLN	2.0
1	A	121	TYR	2.0
1	B	163	ILE	2.0
1	A	212	ASP	2.0
1	C	20	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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
4	CAC	A	303	5/5	0.94	0.20	38,38,40,40	0
2	MN	F	300	1/1	0.95	0.16	36,36,36,36	0
2	MN	B	300	1/1	0.96	0.13	39,39,39,39	0
2	MN	D	300	1/1	0.96	0.15	40,40,40,40	0
4	CAC	C	303	5/5	0.96	0.16	35,37,38,39	0
4	CAC	D	303	5/5	0.96	0.14	32,33,35,36	0
4	CAC	E	303	5/5	0.96	0.15	34,34,36,37	0
4	CAC	B	303	5/5	0.97	0.16	30,30,35,35	0
4	CAC	F	303	5/5	0.98	0.13	26,30,32,34	0
3	ZN	E	301	1/1	0.99	0.04	25,25,25,25	0
2	MN	A	300	1/1	0.99	0.09	34,34,34,34	0
2	MN	E	300	1/1	0.99	0.11	33,33,33,33	0
2	MN	C	300	1/1	0.99	0.10	31,31,31,31	0
3	ZN	A	301	1/1	0.99	0.03	27,27,27,27	0
3	ZN	B	301	1/1	0.99	0.02	26,26,26,26	0
3	ZN	D	301	1/1	0.99	0.02	26,26,26,26	0
3	ZN	C	301	1/1	1.00	0.01	25,25,25,25	0
3	ZN	F	301	1/1	1.00	0.02	24,24,24,24	0

6.5 Other polymers

There are no such residues in this entry.