



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:20 PM GMT

PDB ID : 4XM0
Title : N,N'-diacetylchitobiose deacetylase (SeMet derivative) from *Pyrococcus furiosus* in the absence of cadmium
Authors : Nakamura, T.; Niiyama, M.; Hashimoto, W.; Ida, K.; Uegaki, K.
Deposited on : 2015-01-14
Resolution : 2.80 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

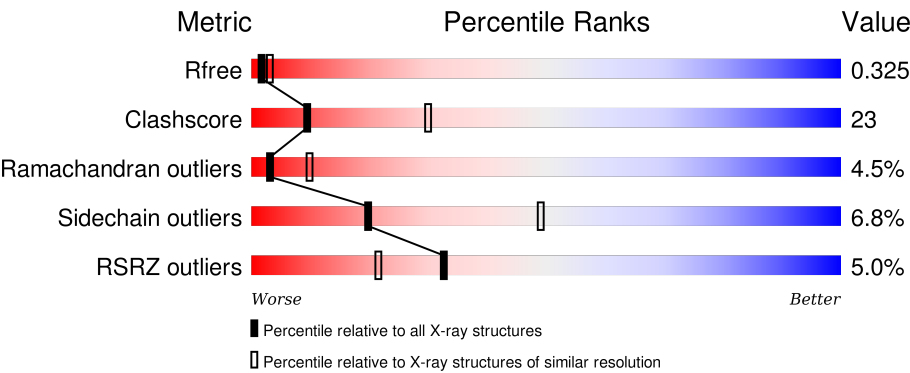
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	267	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>60%34%..</div></div>
1	B	267	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>55%36%5%.</div></div>
1	C	267	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>46%43%8%..</div></div>
1	D	267	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>55%38%..</div></div>
1	E	267	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>48%42%7%..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	267	<div><div></div><div>2%</div><div>57%</div><div>38%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12890 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	Se	0	0	0
			2162	1397	357	399	3	6			
1	B	255	Total	C	N	O	S	Se	0	0	0
			2089	1350	347	383	3	6			
1	C	262	Total	C	N	O	S	Se	0	0	0
			2147	1388	354	396	3	6			
1	D	262	Total	C	N	O	S	Se	0	0	0
			2147	1388	354	396	3	6			
1	E	262	Total	C	N	O	S	Se	0	0	0
			2147	1388	354	396	3	6			
1	F	264	Total	C	N	O	S	Se	0	0	0
			2162	1397	357	399	3	6			

- 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	4	Total 4	O 4	0	0
3	B	5	Total 5	O 5	0	0
3	C	4	Total 4	O 4	0	0
3	D	4	Total 4	O 4	0	0
3	E	3	Total 3	O 3	0	0
3	F	10	Total 10	O 10	0	0

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.

Chain A:

6% 60% 34%

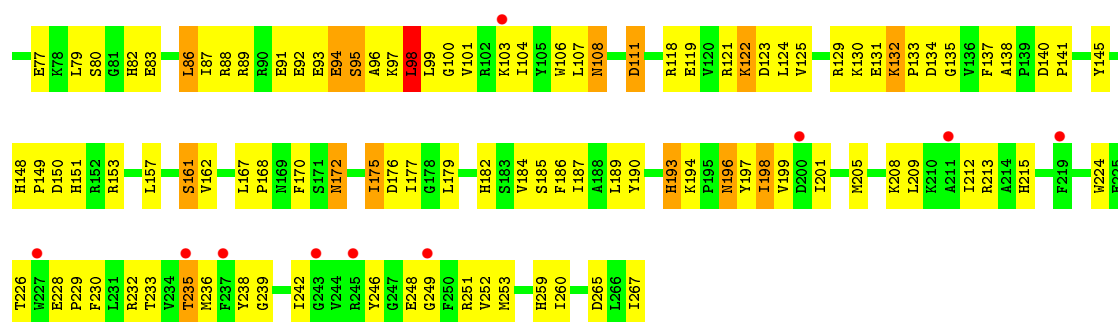
MSE PHE GLU N4 V5 S6 I7 N13 K14 K17 L24 E25 N26 P27 F28 E29 D30 K33 E38 P39 H40 P41 D42 D43 I46 G47 M48 I52 K53 E61 V62 I63 M67 I68 D69 G70 Y71 M72 G73 T74 F75 D76 E77 K78 L79 S80 H82 E83 E84 A85

L26 I37 R38 B39 R40 E91 A96 L99 G100 V101 R102 K103 V106 L107 N108 D111 R118 E119 L124 R129 K130 A131 K132 P133 D134 G135 V136 F137 A138 P139 D140 P141 V142 L143 P144 Y145 G155 L167 P168 N169 F170 S171 N172 I173 D176 I177 G178 H182

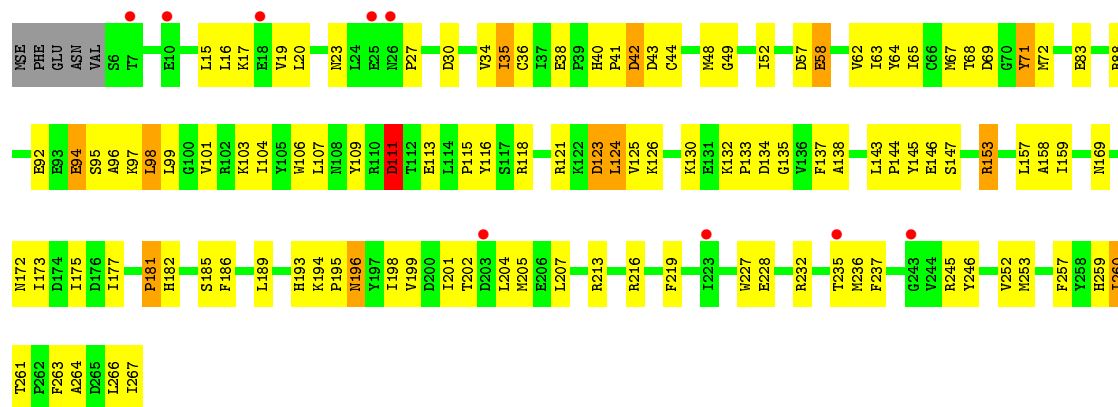
Chain B:

55% 36% 5%

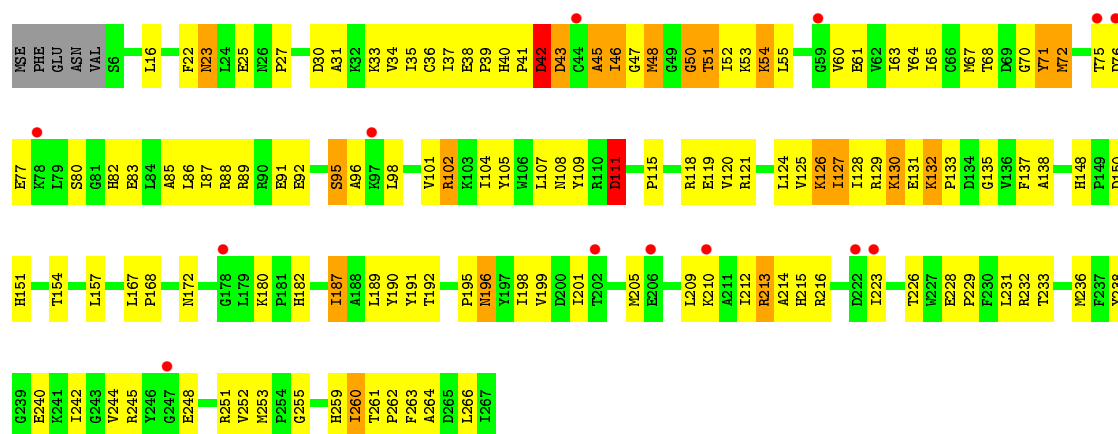
Chain C:



• Molecule 1: Uncharacterized protein

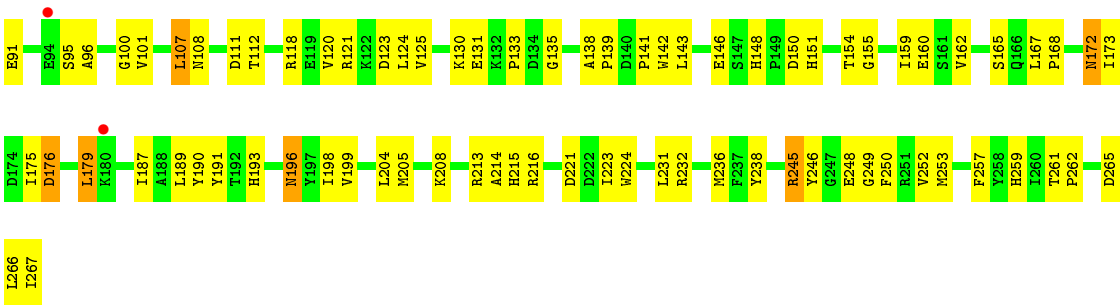


• Molecule 1: Uncharacterized protein



• Molecule 1: Uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.01Å 121.93Å 92.27Å 90.00° 114.21° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 21.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.80) 99.8 (21.66-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.22 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.262 , 0.346 0.247 , 0.325	Depositor DCC
R_{free} test set	2034 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.9	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 40595 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12890	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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, 0.375 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	0.57	0/2213	0.67	0/2985
1	B	0.56	0/2138	0.71	0/2883
1	C	0.59	0/2198	0.72	2/2964 (0.1%)
1	D	0.58	0/2198	0.72	2/2964 (0.1%)
1	E	0.59	0/2198	0.69	0/2964
1	F	0.62	0/2213	0.71	0/2985
All	All	0.59	0/13158	0.70	4/17745 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ASP	CB-CG-OD1	6.01	123.71	118.30
1	C	153	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	111	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	153	ARG	NE-CZ-NH1	5.13	122.87	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	2162	0	2134	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2089	0	2072	113	0
1	C	2147	0	2119	126	0
1	D	2147	0	2119	91	0
1	E	2147	0	2119	117	0
1	F	2162	0	2134	95	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	4	0	0	1	0
3	B	5	0	0	0	0
3	C	4	0	0	1	0
3	D	4	0	0	0	0
3	E	3	0	0	2	0
3	F	10	0	0	0	0
All	All	12890	0	12697	578	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 23.

All (578) 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:B:162:VAL:HG11	1:B:187:ILE:HD11	1.27	1.14
1:A:170:PHE:HB2	1:B:72:MSE:HE1	1.12	1.11
1:D:253:MSE:HE2	1:D:257:PHE:HB3	1.35	1.09
1:B:187:ILE:H	1:B:254:PRO:HG3	1.12	1.08
1:B:37:ILE:CG2	1:B:67:MSE:HE1	1.84	1.07
1:B:170:PHE:HB2	1:C:72:MSE:HE1	1.47	0.97
1:A:170:PHE:HB2	1:B:72:MSE:CE	1.95	0.96
1:B:253:MSE:H	1:B:254:PRO:CD	1.80	0.93
1:B:70:GLY:O	1:B:72:MSE:N	2.02	0.93
1:F:48:MSE:HE3	1:F:250:PHE:CE1	2.03	0.93
1:B:37:ILE:HG22	1:B:67:MSE:HE1	1.47	0.92
1:F:67:MSE:HE1	1:F:124:LEU:HD11	1.51	0.92
1:A:170:PHE:CB	1:B:72:MSE:HE1	1.98	0.91
1:B:253:MSE:N	1:B:254:PRO:HD2	1.87	0.89
1:C:130:LYS:HG3	1:C:131:GLU:OE1	1.71	0.88
1:E:64:TYR:HB2	1:E:104:ILE:HG12	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:VAL:HG12	1:D:101:VAL:HG13	1.57	0.87
1:B:37:ILE:HG21	1:B:67:MSE:HE1	1.56	0.86
1:F:196:ASN:HD21	1:F:252:VAL:H	1.19	0.86
1:B:67:MSE:HE3	1:B:154:THR:HG23	1.59	0.84
1:A:172:ASN:HD22	1:A:172:ASN:H	1.21	0.84
1:B:253:MSE:N	1:B:254:PRO:CD	2.40	0.83
1:B:253:MSE:HE2	1:B:257:PHE:HB3	1.59	0.82
1:B:196:ASN:HD21	1:B:252:VAL:H	1.28	0.82
1:F:111:ASP:OD1	1:F:112:THR:HG23	1.81	0.81
1:E:35:ILE:HD12	1:E:133:PRO:HG3	1.59	0.81
1:D:44:CYS:O	1:D:48:MSE:HB3	1.79	0.81
1:E:196:ASN:HD21	1:E:252:VAL:H	1.27	0.80
1:F:143:LEU:HD23	1:F:146:GLU:HB2	1.64	0.78
1:E:213:ARG:HH22	1:E:216:ARG:HG2	1.47	0.78
1:B:253:MSE:HE1	1:B:264:ALA:HB1	1.64	0.78
1:E:151:HIS:NE2	3:E:402:HOH:O	2.07	0.78
1:C:96:ALA:HB2	1:C:104:ILE:HD11	1.67	0.77
1:D:253:MSE:CE	1:D:257:PHE:HB3	2.14	0.76
1:A:40:HIS:CD2	1:A:111:ASP:OD2	2.38	0.76
1:E:31:ALA:O	1:E:60:VAL:HG22	1.86	0.75
1:E:48:MSE:SE	1:E:137:PHE:CD1	2.89	0.75
1:B:253:MSE:H	1:B:254:PRO:HD2	1.49	0.75
1:A:40:HIS:HD2	1:A:111:ASP:OD2	1.70	0.74
1:E:150:ASP:O	1:E:154:THR:OG1	2.05	0.74
1:B:37:ILE:HG22	1:B:67:MSE:CE	2.17	0.74
1:A:196:ASN:HD21	1:A:252:VAL:H	1.34	0.74
1:C:94:GLU:O	1:C:98:LEU:HD21	1.88	0.74
1:E:48:MSE:SE	1:E:137:PHE:HD1	2.20	0.74
1:E:95:SER:HA	1:E:98:LEU:HD12	1.69	0.74
1:A:63:ILE:HG23	1:A:103:LYS:HB3	1.70	0.73
1:A:13:ASN:O	1:A:17:LYS:HG2	1.88	0.73
1:E:253:MSE:HE1	1:E:264:ALA:HB1	1.70	0.72
1:C:172:ASN:HD22	1:C:172:ASN:H	1.35	0.72
1:F:48:MSE:HE3	1:F:250:PHE:HE1	1.55	0.71
1:B:41:PRO:HD3	1:B:66:CYS:SG	2.29	0.71
1:B:162:VAL:CG1	1:B:187:ILE:HD11	2.13	0.71
1:F:96:ALA:HB1	1:F:101:VAL:HB	1.72	0.71
1:E:87:ILE:O	1:E:91:GLU:HG3	1.91	0.71
1:D:196:ASN:HD21	1:D:252:VAL:H	1.36	0.71
1:C:72:MSE:HB2	1:C:111:ASP:OD2	1.89	0.71
1:E:132:LYS:HG3	1:E:182:HIS:ND1	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:LYS:HG2	1:F:204:LEU:HD21	1.73	0.70
1:D:253:MSE:HE1	1:D:264:ALA:HB1	1.74	0.70
1:F:232:ARG:O	1:F:236:MSE:HG3	1.93	0.69
1:C:86:LEU:HD21	1:F:83:GLU:HG3	1.72	0.69
1:C:259:HIS:NE2	3:C:403:HOH:O	2.25	0.69
1:B:133:PRO:O	1:B:182:HIS:NE2	2.25	0.69
1:A:91:GLU:OE1	1:A:215:HIS:HA	1.92	0.69
1:F:39:PRO:HG2	1:F:151:HIS:CD2	2.28	0.69
1:C:209:LEU:O	1:C:213:ARG:HG3	1.93	0.69
1:C:92:GLU:HA	1:C:215:HIS:CE1	2.27	0.68
1:F:71:TYR:CD2	1:F:71:TYR:O	2.46	0.68
1:D:253:MSE:HG2	1:D:267:ILE:HD11	1.73	0.68
1:C:251:ARG:HH21	1:C:253:MSE:HE3	1.58	0.68
1:A:119:GLU:OE1	1:D:118:ARG:NH2	2.24	0.68
1:A:135:GLY:HA3	1:A:186:PHE:CE2	2.29	0.68
1:D:205:MSE:HG3	1:D:246:TYR:CD2	2.28	0.68
1:A:96:ALA:HB1	1:A:101:VAL:HB	1.75	0.68
1:B:196:ASN:HD22	1:B:196:ASN:H	1.43	0.68
1:C:251:ARG:HH21	1:C:253:MSE:CE	2.07	0.67
1:C:28:PHE:CE2	1:C:197:TYR:HE2	2.12	0.67
1:B:251:ARG:HE	1:B:253:MSE:SE	2.27	0.67
1:E:51:THR:OG1	1:E:248:GLU:OE1	2.09	0.67
1:E:48:MSE:HE3	1:E:52:ILE:HD11	1.76	0.67
1:C:48:MSE:O	1:C:52:ILE:HG13	1.95	0.67
1:B:221:ASP:O	1:B:225:GLU:HB2	1.95	0.67
1:D:147:SER:OG	1:F:159:ILE:HG21	1.95	0.66
1:A:172:ASN:HD22	1:A:172:ASN:N	1.92	0.66
1:A:72:MSE:HE1	1:C:170:PHE:HB2	1.77	0.66
1:B:162:VAL:HG12	1:B:163:ALA:N	2.11	0.66
1:E:133:PRO:O	1:E:182:HIS:NE2	2.20	0.66
1:F:53:LYS:HG2	1:F:204:LEU:CD2	2.25	0.65
1:F:216:ARG:HB2	1:F:216:ARG:NH2	2.11	0.65
1:B:187:ILE:N	1:B:254:PRO:HG3	1.98	0.65
1:B:198:ILE:HG22	1:B:199:VAL:N	2.12	0.65
1:F:141:PRO:HG3	1:F:155:GLY:HA3	1.79	0.64
1:F:143:LEU:HD13	1:F:191:TYR:O	1.96	0.64
1:E:83:GLU:O	1:E:86:LEU:N	2.32	0.63
1:D:260:ILE:HB	1:E:191:TYR:CE1	2.34	0.63
1:D:261:THR:HB	1:D:264:ALA:HB2	1.81	0.63
1:A:87:ILE:O	1:A:91:GLU:HG3	1.98	0.63
1:A:173:ILE:HG22	1:D:126:LYS:NZ	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LEU:O	1:C:108:ASN:HB2	1.98	0.62
1:F:49:GLY:HA3	1:F:208:LYS:HG3	1.82	0.62
1:B:48:MSE:HE2	1:B:52:ILE:HG12	1.81	0.62
1:A:72:MSE:HE1	1:C:170:PHE:CB	2.30	0.62
1:F:216:ARG:HH21	1:F:216:ARG:HB2	1.62	0.62
1:C:79:LEU:CD1	1:C:83:GLU:HG2	2.29	0.62
1:E:40:HIS:CE1	1:E:148:HIS:NE2	2.67	0.62
1:A:74:THR:HG22	1:A:84:LEU:HD22	1.82	0.62
1:E:40:HIS:HE1	1:E:148:HIS:NE2	1.98	0.62
1:F:141:PRO:HD2	1:F:142:TRP:CE3	2.34	0.61
1:B:48:MSE:O	1:B:52:ILE:HG13	2.00	0.61
1:D:68:THR:HA	1:D:109:TYR:O	2.00	0.61
1:D:259:HIS:HE1	1:E:151:HIS:CD2	2.18	0.61
1:A:83:GLU:HB2	1:E:86:LEU:HD22	1.81	0.61
1:A:76:ASP:O	1:A:78:LYS:N	2.32	0.61
1:E:40:HIS:HE1	1:E:148:HIS:CD2	2.19	0.61
1:D:143:LEU:HD12	1:D:144:PRO:HD2	1.83	0.61
1:C:93:GLU:C	1:C:95:SER:H	2.04	0.60
1:B:35:ILE:HD12	1:B:133:PRO:HG3	1.83	0.60
1:C:212:ILE:O	1:C:212:ILE:HG22	2.02	0.60
1:E:226:THR:O	1:E:229:PRO:HD2	2.02	0.60
1:B:107:LEU:HD11	1:B:123:ASP:HB3	1.83	0.60
1:B:162:VAL:HG11	1:B:187:ILE:CD1	2.18	0.60
1:C:97:LYS:O	1:C:99:LEU:N	2.35	0.60
1:B:67:MSE:CE	1:B:154:THR:HG23	2.31	0.60
1:E:259:HIS:HE1	1:F:151:HIS:CE1	2.20	0.60
1:D:38:GLU:HB2	1:D:43:ASP:HB2	1.83	0.60
1:E:35:ILE:CD1	1:E:133:PRO:HG3	2.30	0.59
1:C:118:ARG:NH2	1:E:119:GLU:OE1	2.34	0.59
1:A:33:LYS:HD3	1:A:63:ILE:HD11	1.84	0.59
1:E:67:MSE:SE	1:E:124:LEU:HD21	2.52	0.59
1:A:143:LEU:HD12	1:A:144:PRO:HD2	1.84	0.59
1:B:63:ILE:HG23	1:B:103:LYS:O	2.03	0.59
1:B:205:MSE:HG3	1:B:246:TYR:CD2	2.38	0.59
1:C:92:GLU:HA	1:C:215:HIS:HE1	1.66	0.59
1:F:107:LEU:O	1:F:108:ASN:HB2	2.03	0.59
1:A:48:MSE:SE	1:A:137:PHE:HB3	2.53	0.59
1:D:113:GLU:O	1:D:115:PRO:HD3	2.02	0.59
1:B:170:PHE:CB	1:C:72:MSE:HE1	2.30	0.59
1:C:87:ILE:O	1:C:91:GLU:HG3	2.02	0.58
1:C:172:ASN:ND2	1:C:172:ASN:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:HE2	1:A:212:ILE:HD11	1.85	0.58
1:E:61:GLU:OE2	1:E:102:ARG:NH2	2.37	0.58
1:A:198:ILE:HD13	1:A:249:GLY:HA2	1.85	0.58
1:B:148:HIS:HD2	1:B:149:PRO:HD2	1.68	0.58
1:E:151:HIS:CE1	3:E:402:HOH:O	2.53	0.58
1:D:228:GLU:O	1:D:232:ARG:HG3	2.03	0.58
1:A:172:ASN:H	1:A:172:ASN:ND2	1.99	0.58
1:A:76:ASP:C	1:A:78:LYS:H	2.06	0.58
1:F:31:ALA:O	1:F:60:VAL:HG22	2.04	0.58
1:F:138:ALA:O	1:F:189:LEU:HA	2.03	0.58
1:E:209:LEU:O	1:E:213:ARG:CG	2.52	0.58
1:C:41:PRO:HG2	1:C:88:ARG:HE	1.68	0.58
1:E:187:ILE:HD12	1:E:187:ILE:H	1.69	0.58
1:A:33:LYS:HG3	1:A:61:GLU:HG2	1.86	0.58
1:F:91:GLU:HB3	1:F:215:HIS:HA	1.86	0.58
1:F:265:ASP:OD1	1:F:266:LEU:HG	2.02	0.58
1:A:168:PRO:HB3	1:B:77:GLU:HG2	1.86	0.58
1:E:71:TYR:HD2	1:E:72:MSE:HG2	1.69	0.58
1:E:233:THR:HA	1:E:236:MSE:HE3	1.85	0.58
1:E:38:GLU:HB2	1:E:43:ASP:HB2	1.86	0.57
1:B:253:MSE:H	1:B:254:PRO:HD3	1.66	0.57
1:D:97:LYS:C	1:D:99:LEU:H	2.07	0.57
1:D:138:ALA:O	1:D:189:LEU:HA	2.04	0.57
1:E:130:LYS:O	1:E:132:LYS:N	2.38	0.57
1:E:37:ILE:O	1:E:190:TYR:OH	2.22	0.57
1:D:193:HIS:C	1:D:195:PRO:HD3	2.25	0.57
1:B:232:ARG:O	1:B:236:MSE:HG3	2.03	0.57
1:F:253:MSE:HG2	1:F:267:ILE:HD11	1.86	0.57
1:F:139:PRO:HA	1:F:190:TYR:O	2.05	0.57
1:C:7:THR:HG22	1:C:8:PHE:H	1.70	0.57
1:A:133:PRO:HD2	1:A:182:HIS:CD2	2.39	0.56
1:C:67:MSE:SE	1:C:107:LEU:HD12	2.55	0.56
1:F:34:VAL:HG12	1:F:135:GLY:HA3	1.86	0.56
1:B:48:MSE:SE	1:B:137:PHE:CD1	3.08	0.56
1:C:122:LYS:HE3	1:E:119:GLU:OE2	2.05	0.56
1:A:214:ALA:O	1:A:216:ARG:NH2	2.39	0.56
1:D:237:PHE:CE2	1:F:262:PRO:HB2	2.41	0.56
1:D:64:TYR:HB2	1:D:104:ILE:HG12	1.88	0.56
1:A:38:GLU:HB2	1:A:43:ASP:HB2	1.88	0.56
1:D:15:LEU:HA	1:D:19:VAL:HG23	1.87	0.56
1:C:201:ILE:HG12	1:C:248:GLU:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ILE:HD12	1:A:238:TYR:HB3	1.86	0.56
1:A:74:THR:O	1:C:168:PRO:HD2	2.04	0.56
1:D:219:PHE:HE1	1:D:227:TRP:CE3	2.24	0.56
1:D:123:ASP:O	1:D:126:LYS:N	2.38	0.56
1:A:129:ARG:NH2	1:A:167:LEU:O	2.38	0.56
1:E:196:ASN:HD22	1:E:196:ASN:H	1.54	0.56
1:E:40:HIS:CD2	1:E:111:ASP:OD2	2.59	0.56
1:D:48:MSE:HE1	1:D:137:PHE:CE1	2.41	0.56
1:D:97:LYS:O	1:D:99:LEU:N	2.38	0.56
1:C:98:LEU:HD23	1:C:98:LEU:H	1.70	0.55
1:C:62:VAL:O	1:C:101:VAL:HG13	2.05	0.55
1:E:41:PRO:O	1:E:42:ASP:HB3	2.07	0.55
1:A:118:ARG:NH1	1:B:113:GLU:OE2	2.30	0.55
1:C:198:ILE:HA	1:C:249:GLY:HA2	1.89	0.55
1:A:194:LYS:HB3	1:A:251:ARG:NH1	2.21	0.55
1:C:131:GLU:HB2	1:C:133:PRO:HD3	1.89	0.55
1:D:198:ILE:HG22	1:D:199:VAL:N	2.22	0.55
1:C:97:LYS:C	1:C:99:LEU:H	2.09	0.55
1:C:135:GLY:HA3	1:C:186:PHE:CE2	2.42	0.55
1:E:259:HIS:CE1	1:F:151:HIS:CE1	2.94	0.55
1:D:196:ASN:N	1:D:196:ASN:HD22	2.03	0.55
1:D:132:LYS:HA	1:D:182:HIS:CD2	2.41	0.55
1:A:196:ASN:H	1:A:196:ASN:HD22	1.53	0.55
1:C:79:LEU:HD11	1:C:83:GLU:HG2	1.89	0.55
1:E:38:GLU:HB2	1:E:43:ASP:CB	2.37	0.55
1:A:82:HIS:O	1:E:82:HIS:HB3	2.07	0.55
1:A:130:LYS:HG2	1:D:177:ILE:HG22	1.89	0.55
1:B:196:ASN:ND2	1:B:196:ASN:H	2.05	0.54
1:E:198:ILE:HG22	1:E:199:VAL:N	2.22	0.54
1:E:40:HIS:HB3	1:E:41:PRO:HD2	1.88	0.54
1:A:237:PHE:HB2	1:C:8:PHE:CE1	2.42	0.54
1:A:41:PRO:O	1:A:42:ASP:HB3	2.06	0.54
1:D:16:LEU:HA	1:D:20:LEU:HD12	1.90	0.54
1:F:198:ILE:HD13	1:F:249:GLY:HA2	1.88	0.54
1:A:145:TYR:HE2	1:C:265:ASP:HB3	1.73	0.54
1:D:253:MSE:CE	1:D:264:ALA:HB1	2.38	0.54
1:C:91:GLU:O	1:C:94:GLU:HB2	2.08	0.54
1:C:51:THR:O	1:C:55:LEU:HG	2.08	0.54
1:F:213:ARG:NH2	1:F:221:ASP:OD2	2.41	0.54
1:E:138:ALA:O	1:E:189:LEU:HA	2.08	0.54
1:C:194:LYS:HB3	1:C:251:ARG:NH1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:ILE:HA	1:F:179:LEU:O	2.07	0.54
1:C:232:ARG:O	1:C:236:MSE:HG3	2.07	0.54
1:B:64:TYR:HB2	1:B:104:ILE:HG23	1.89	0.54
1:D:36:CYS:HB3	1:D:44:CYS:SG	2.48	0.54
1:E:115:PRO:HD2	1:E:120:VAL:HG21	1.88	0.54
1:B:182:HIS:CG	1:B:183:SER:N	2.76	0.53
1:F:52:ILE:HG23	1:F:62:VAL:HG11	1.90	0.53
1:B:40:HIS:CE1	1:B:148:HIS:CE1	2.96	0.53
1:B:228:GLU:HB3	1:B:229:PRO:HD3	1.91	0.53
1:D:196:ASN:H	1:D:196:ASN:HD22	1.57	0.53
1:E:125:VAL:HG12	1:E:129:ARG:HD2	1.90	0.53
1:A:232:ARG:O	1:A:236:MSE:HG3	2.08	0.53
1:B:123:ASP:O	1:B:126:LYS:N	2.38	0.53
1:D:38:GLU:OE1	1:D:44:CYS:HB2	2.09	0.53
1:E:82:HIS:O	1:E:85:ALA:HB3	2.08	0.53
1:B:37:ILE:CG2	1:B:67:MSE:CE	2.73	0.53
1:A:83:GLU:C	1:A:85:ALA:N	2.62	0.53
1:B:226:THR:O	1:B:229:PRO:HD2	2.09	0.53
1:A:224:TRP:CE2	1:A:228:GLU:HB2	2.44	0.53
1:C:235:THR:HB	1:C:246:TYR:HD1	1.74	0.53
1:C:32:LYS:O	1:C:60:VAL:HA	2.09	0.52
1:D:123:ASP:O	1:D:125:VAL:N	2.42	0.52
1:B:242:ILE:HG13	1:B:243:GLY:H	1.74	0.52
1:A:72:MSE:HE1	1:C:170:PHE:CA	2.39	0.52
1:B:118:ARG:O	1:B:119:GLU:C	2.46	0.52
1:A:259:HIS:NE2	3:A:402:HOH:O	2.34	0.52
1:C:198:ILE:HD13	1:C:249:GLY:HA3	1.91	0.52
1:C:175:ILE:HA	1:C:179:LEU:O	2.10	0.52
1:D:123:ASP:O	1:D:124:LEU:C	2.48	0.52
1:F:30:ASP:OD1	1:F:30:ASP:N	2.42	0.52
1:C:16:LEU:HD12	1:C:17:LYS:HG3	1.92	0.52
1:D:65:ILE:HG21	1:D:124:LEU:CD2	2.40	0.52
1:B:123:ASP:O	1:B:124:LEU:C	2.47	0.52
1:F:40:HIS:HB3	1:F:41:PRO:HD2	1.91	0.52
1:E:259:HIS:CE1	1:E:260:ILE:HG23	2.44	0.52
1:D:259:HIS:CE1	1:E:151:HIS:CD2	2.98	0.52
1:E:50:GLY:O	1:E:52:ILE:N	2.43	0.52
1:F:38:GLU:HB3	1:F:44:CYS:SG	2.50	0.52
1:A:135:GLY:HA3	1:A:186:PHE:CZ	2.45	0.52
1:C:251:ARG:NH2	1:C:253:MSE:HE3	2.24	0.52
1:E:228:GLU:HB3	1:E:229:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:TYR:HA	1:F:142:TRP:CZ2	2.45	0.51
1:C:23:ASN:OD1	1:C:23:ASN:N	2.42	0.51
1:C:198:ILE:HB	1:C:242:ILE:HG12	1.92	0.51
1:E:205:MSE:HE1	1:E:232:ARG:HG2	1.93	0.51
1:D:204:LEU:O	1:D:207:LEU:HB3	2.10	0.51
1:B:148:HIS:CD2	1:B:149:PRO:HD2	2.46	0.51
1:B:138:ALA:O	1:B:189:LEU:HA	2.11	0.51
1:D:158:ALA:O	1:D:159:ILE:C	2.49	0.51
1:E:40:HIS:CE1	1:E:148:HIS:CD2	2.99	0.51
1:B:253:MSE:HG2	1:B:267:ILE:HD11	1.93	0.51
1:E:50:GLY:HA3	1:E:201:ILE:HG21	1.91	0.51
1:C:94:GLU:C	1:C:98:LEU:HD21	2.30	0.51
1:D:34:VAL:HG23	1:D:62:VAL:HG22	1.93	0.51
1:E:213:ARG:HH12	1:E:216:ARG:HG2	1.77	0.50
1:E:213:ARG:NH2	1:E:216:ARG:HG2	2.21	0.50
1:D:44:CYS:O	1:D:48:MSE:CB	2.57	0.50
1:D:69:ASP:OD1	1:D:71:TYR:CB	2.60	0.50
1:D:38:GLU:HB3	1:D:44:CYS:SG	2.52	0.50
1:F:56:SER:OG	1:F:100:GLY:HA3	2.11	0.50
1:B:198:ILE:HG22	1:B:199:VAL:H	1.77	0.50
1:E:68:THR:HA	1:E:109:TYR:O	2.12	0.50
1:F:44:CYS:O	1:F:48:MSE:HB2	2.12	0.49
1:A:173:ILE:HG22	1:D:126:LYS:HZ2	1.76	0.49
1:E:45:ALA:O	1:E:47:GLY:N	2.45	0.49
1:F:67:MSE:HE1	1:F:124:LEU:HD21	1.93	0.49
1:C:134:ASP:O	1:C:185:SER:HB2	2.11	0.49
1:E:33:LYS:HG2	1:E:133:PRO:HB3	1.93	0.49
1:C:208:LYS:HE3	1:C:248:GLU:OE2	2.11	0.49
1:D:58:GLU:CD	1:D:58:GLU:N	2.64	0.49
1:A:72:MSE:CE	1:C:170:PHE:HB2	2.41	0.49
1:B:205:MSE:HG3	1:B:246:TYR:CG	2.48	0.49
1:D:196:ASN:N	1:D:196:ASN:ND2	2.58	0.49
1:B:170:PHE:HB2	1:C:72:MSE:CE	2.31	0.49
1:F:190:TYR:O	1:F:191:TYR:HB2	2.13	0.49
1:A:196:ASN:ND2	1:A:251:ARG:HA	2.27	0.49
1:E:212:ILE:HD13	1:E:231:LEU:HD22	1.94	0.49
1:E:34:VAL:HG12	1:E:135:GLY:HA3	1.95	0.49
1:C:253:MSE:HG2	1:C:267:ILE:HD11	1.94	0.49
1:A:118:ARG:HD3	1:B:113:GLU:OE2	2.13	0.49
1:F:46:ILE:HG23	1:F:231:LEU:HD21	1.95	0.49
1:B:36:CYS:HA	1:B:137:PHE:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:TYR:OH	1:B:131:GLU:OE2	2.31	0.48
1:A:80:SER:HB3	1:E:89:ARG:HH11	1.78	0.48
1:E:23:ASN:N	1:E:23:ASN:HD22	2.11	0.48
1:C:129:ARG:NH2	1:C:167:LEU:O	2.46	0.48
1:A:131:GLU:O	1:A:132:LYS:C	2.50	0.48
1:B:107:LEU:O	1:B:108:ASN:HB2	2.13	0.48
1:D:135:GLY:HA3	1:D:186:PHE:CZ	2.47	0.48
1:E:190:TYR:CD2	1:E:191:TYR:CD2	3.02	0.48
1:B:64:TYR:CB	1:B:104:ILE:HG23	2.43	0.48
1:F:205:MSE:HE3	1:F:208:LYS:HB3	1.95	0.48
1:A:173:ILE:HD11	1:D:107:LEU:HD23	1.96	0.48
1:B:262:PRO:O	1:C:193:HIS:HB2	2.14	0.48
1:A:200:ASP:OD2	1:A:244:VAL:HG11	2.12	0.48
1:E:195:PRO:HG3	1:E:238:TYR:CE1	2.48	0.48
1:C:97:LYS:O	1:C:100:GLY:N	2.40	0.48
1:A:83:GLU:O	1:A:86:LEU:N	2.47	0.48
1:E:16:LEU:HD22	1:E:22:PHE:HB3	1.96	0.48
1:B:227:TRP:O	1:B:231:LEU:HG	2.12	0.48
1:C:55:LEU:O	1:C:60:VAL:HB	2.13	0.48
1:B:229:PRO:O	1:B:233:THR:OG1	2.27	0.48
1:D:236:MSE:HE1	1:F:6:SER:O	2.13	0.48
1:B:86:LEU:HD21	1:D:83:GLU:HG3	1.96	0.48
1:C:95:SER:HA	1:C:98:LEU:HG	1.95	0.48
1:F:69:ASP:OD1	1:F:71:TYR:HB2	2.14	0.48
1:B:48:MSE:HE2	1:B:52:ILE:CG1	2.44	0.48
1:D:69:ASP:OD1	1:D:71:TYR:HB2	2.14	0.48
1:B:41:PRO:O	1:B:42:ASP:CG	2.51	0.48
1:F:69:ASP:C	1:F:69:ASP:OD1	2.53	0.48
1:E:129:ARG:NH2	1:E:167:LEU:O	2.46	0.48
1:E:63:ILE:HG21	1:E:105:TYR:HE2	1.77	0.48
1:F:95:SER:HB2	1:F:214:ALA:HB3	1.95	0.48
1:C:138:ALA:O	1:C:189:LEU:HA	2.14	0.48
1:A:48:MSE:O	1:A:52:ILE:HG13	2.14	0.47
1:F:205:MSE:HG2	1:F:246:TYR:CE2	2.49	0.47
1:C:121:ARG:HB3	1:C:170:PHE:HZ	1.78	0.47
1:E:92:GLU:HB2	1:E:215:HIS:HE1	1.79	0.47
1:C:233:THR:HA	1:C:236:MSE:HE2	1.95	0.47
1:D:201:ILE:HD12	1:D:205:MSE:HG2	1.96	0.47
1:C:49:GLY:O	1:C:99:LEU:HD22	2.13	0.47
1:E:167:LEU:HA	1:E:168:PRO:HD2	1.68	0.47
1:F:131:GLU:HB2	1:F:133:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:MSE:HB3	1:B:72:MSE:HE3	1.75	0.47
1:C:36:CYS:HA	1:C:137:PHE:HB2	1.97	0.47
1:A:173:ILE:CG2	1:D:126:LYS:HZ1	2.26	0.47
1:A:173:ILE:HG22	1:D:126:LYS:HZ1	1.79	0.47
1:C:39:PRO:HA	1:C:67:MSE:HB2	1.95	0.47
1:C:71:TYR:CD2	1:C:71:TYR:O	2.67	0.47
1:C:228:GLU:N	1:C:229:PRO:CD	2.78	0.47
1:C:63:ILE:HD12	1:C:131:GLU:HG3	1.97	0.47
1:E:132:LYS:HG3	1:E:182:HIS:CE1	2.49	0.47
1:A:96:ALA:CB	1:A:101:VAL:HB	2.44	0.47
1:C:54:LYS:O	1:C:54:LYS:HG2	2.15	0.47
1:A:140:ASP:HA	1:A:141:PRO:HD3	1.82	0.47
1:C:123:ASP:O	1:C:124:LEU:C	2.53	0.47
1:E:67:MSE:HA	1:E:107:LEU:HD12	1.96	0.47
1:C:41:PRO:O	1:C:42:ASP:OD2	2.32	0.47
1:F:257:PHE:CE2	1:F:267:ILE:HG12	2.49	0.47
1:C:198:ILE:HG22	1:C:199:VAL:H	1.80	0.47
1:F:198:ILE:HG22	1:F:199:VAL:N	2.30	0.47
1:F:67:MSE:HE2	1:F:154:THR:HG23	1.97	0.46
1:B:162:VAL:HG12	1:B:163:ALA:H	1.80	0.46
1:E:196:ASN:N	1:E:196:ASN:HD22	2.11	0.46
1:D:259:HIS:CE1	1:D:260:ILE:HG23	2.50	0.46
1:E:55:LEU:O	1:E:60:VAL:HB	2.15	0.46
1:F:213:ARG:HD2	1:F:224:TRP:CD2	2.50	0.46
1:C:205:MSE:O	1:C:209:LEU:HG	2.16	0.46
1:B:175:ILE:H	1:B:175:ILE:HD12	1.80	0.46
1:E:261:THR:HA	1:E:262:PRO:HD2	1.84	0.46
1:A:24:LEU:HA	1:A:27:PRO:HG3	1.98	0.46
1:B:253:MSE:CE	1:B:264:ALA:HB1	2.38	0.46
1:F:39:PRO:CG	1:F:151:HIS:CD2	2.98	0.46
1:B:182:HIS:CG	1:B:183:SER:H	2.34	0.46
1:E:96:ALA:HB1	1:E:101:VAL:HB	1.98	0.46
1:E:130:LYS:C	1:E:132:LYS:H	2.18	0.46
1:B:259:HIS:HE1	1:C:151:HIS:CD2	2.33	0.46
1:B:149:PRO:O	1:B:153:ARG:HG3	2.16	0.46
1:A:89:ARG:HG3	1:A:106:TRP:CE2	2.51	0.46
1:C:119:GLU:OE1	1:E:118:ARG:NH2	2.41	0.46
1:D:35:ILE:HG13	1:D:133:PRO:HG3	1.98	0.46
1:D:41:PRO:O	1:D:42:ASP:HB3	2.15	0.46
1:C:93:GLU:C	1:C:95:SER:N	2.69	0.46
1:C:196:ASN:HD21	1:C:252:VAL:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:PHE:HB2	1:E:266:LEU:HD12	1.98	0.46
1:D:260:ILE:HB	1:E:191:TYR:HE1	1.80	0.45
1:D:92:GLU:HB3	1:D:106:TRP:HH2	1.80	0.45
1:E:259:HIS:HE1	1:F:151:HIS:ND1	2.12	0.45
1:A:196:ASN:N	1:A:196:ASN:HD22	2.13	0.45
1:A:227:TRP:HA	1:A:230:PHE:HB3	1.98	0.45
1:F:172:ASN:HD22	1:F:173:ILE:N	2.15	0.45
1:B:198:ILE:CG2	1:B:199:VAL:N	2.78	0.45
1:D:40:HIS:HD2	1:D:68:THR:OG1	1.99	0.45
1:D:144:PRO:HD3	1:D:193:HIS:CE1	2.51	0.45
1:E:41:PRO:O	1:E:42:ASP:CB	2.63	0.45
1:C:53:LYS:C	1:C:55:LEU:H	2.19	0.45
1:D:253:MSE:HE2	1:D:257:PHE:CB	2.26	0.45
1:A:118:ARG:O	1:A:119:GLU:C	2.55	0.45
1:A:240:GLU:OE1	1:C:8:PHE:HB3	2.17	0.45
1:F:198:ILE:HD12	1:F:238:TYR:HB3	1.97	0.45
1:C:131:GLU:O	1:C:132:LYS:HB2	2.16	0.45
1:D:96:ALA:HB1	1:D:101:VAL:HB	1.98	0.45
1:B:42:ASP:HB3	1:B:215:HIS:CE1	2.50	0.45
1:C:69:ASP:OD2	1:F:82:HIS:CE1	2.70	0.45
1:C:87:ILE:O	1:C:91:GLU:CG	2.64	0.45
1:A:172:ASN:N	1:A:172:ASN:ND2	2.61	0.45
1:F:236:MSE:HE3	1:F:245:ARG:HD3	1.98	0.45
1:C:48:MSE:SE	1:C:137:PHE:CD1	3.19	0.45
1:B:148:HIS:CD2	1:B:150:ASP:HB2	2.52	0.45
1:A:67:MSE:SE	1:A:124:LEU:HD21	2.67	0.45
1:E:157:LEU:HD23	1:E:157:LEU:HA	1.76	0.45
1:F:121:ARG:NH2	1:F:160:GLU:OE1	2.44	0.45
1:D:175:ILE:HD12	1:D:181:PRO:HD3	1.97	0.45
1:B:15:LEU:HD21	1:C:230:PHE:HA	1.98	0.45
1:D:263:PHE:HB2	1:D:266:LEU:HD12	1.98	0.45
1:E:50:GLY:O	1:E:51:THR:C	2.55	0.44
1:C:86:LEU:HD12	1:C:89:ARG:HH11	1.81	0.44
1:A:89:ARG:HG3	1:A:106:TRP:CZ2	2.52	0.44
1:B:135:GLY:HA3	1:B:186:PHE:CE2	2.52	0.44
1:D:63:ILE:HG23	1:D:103:LYS:O	2.17	0.44
1:D:94:GLU:O	1:D:96:ALA:N	2.51	0.44
1:A:72:MSE:HE1	1:C:170:PHE:HA	1.99	0.44
1:E:45:ALA:O	1:E:46:ILE:C	2.55	0.44
1:B:131:GLU:O	1:B:132:LYS:C	2.56	0.44
1:A:205:MSE:HG2	1:A:246:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:PRO:CB	1:F:151:HIS:CD2	3.00	0.44
1:C:48:MSE:HG3	1:C:190:TYR:CG	2.51	0.44
1:E:195:PRO:HG3	1:E:238:TYR:HE1	1.82	0.44
1:D:169:ASN:HD21	1:E:80:SER:HA	1.81	0.44
1:C:48:MSE:HE2	1:C:52:ILE:CG1	2.46	0.44
1:B:65:ILE:HG23	1:B:107:LEU:HD23	1.99	0.44
1:E:187:ILE:N	1:E:187:ILE:HD12	2.31	0.44
1:B:167:LEU:HA	1:B:168:PRO:HD2	1.80	0.44
1:B:119:GLU:CD	1:F:118:ARG:HE	2.21	0.44
1:A:140:ASP:HB2	1:A:189:LEU:HB3	2.00	0.44
1:D:41:PRO:O	1:D:88:ARG:NH2	2.46	0.44
1:F:162:VAL:HG21	1:F:187:ILE:HG12	1.98	0.44
1:B:196:ASN:HD22	1:B:196:ASN:N	2.06	0.44
1:E:71:TYR:HB3	1:E:111:ASP:HB2	2.00	0.44
1:D:67:MSE:SE	1:D:124:LEU:HD21	2.68	0.44
1:C:50:GLY:H	1:C:208:LYS:CE	2.30	0.44
1:E:63:ILE:HG21	1:E:105:TYR:CE2	2.52	0.44
1:E:118:ARG:O	1:E:121:ARG:HB2	2.18	0.44
1:B:89:ARG:NH2	1:B:106:TRP:CD1	2.86	0.44
1:E:201:ILE:HD12	1:E:205:MSE:HG2	1.99	0.44
1:D:67:MSE:SE	1:D:124:LEU:HD11	2.68	0.44
1:A:139:PRO:O	1:A:155:GLY:HA3	2.18	0.44
1:F:38:GLU:HB2	1:F:43:ASP:HB2	1.99	0.44
1:C:52:ILE:HG23	1:C:62:VAL:HG11	1.99	0.44
1:A:260:ILE:HA	1:B:143:LEU:HD21	1.99	0.44
1:B:162:VAL:CG1	1:B:163:ALA:N	2.81	0.43
1:C:89:ARG:HG2	1:C:106:TRP:CZ2	2.53	0.43
1:A:41:PRO:O	1:A:42:ASP:CB	2.65	0.43
1:A:53:LYS:HB2	1:A:99:LEU:CD2	2.48	0.43
1:B:70:GLY:O	1:B:71:TYR:C	2.57	0.43
1:E:38:GLU:O	1:E:67:MSE:HG2	2.19	0.43
1:E:126:LYS:O	1:E:128:ILE:N	2.51	0.43
1:C:35:ILE:HA	1:C:63:ILE:O	2.18	0.43
1:B:42:ASP:HB3	1:B:215:HIS:CD2	2.53	0.43
1:C:212:ILE:O	1:C:212:ILE:CG2	2.65	0.43
1:D:97:LYS:C	1:D:99:LEU:N	2.72	0.43
1:D:146:GLU:OE2	1:F:259:HIS:HA	2.18	0.43
1:F:14:LYS:O	1:F:19:VAL:HG23	2.18	0.43
1:C:48:MSE:SE	1:C:137:PHE:CG	3.21	0.43
1:E:107:LEU:O	1:E:108:ASN:HB2	2.18	0.43
1:E:65:ILE:HD11	1:E:127:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:TRP:CE3	1:C:145:TYR:HD1	2.36	0.43
1:C:69:ASP:OD2	1:F:82:HIS:HE1	2.01	0.43
1:C:148:HIS:NE2	1:C:150:ASP:OD2	2.35	0.43
1:B:196:ASN:ND2	1:B:196:ASN:N	2.66	0.43
1:E:70:GLY:HA3	1:E:88:ARG:HD3	2.00	0.43
1:E:91:GLU:CD	1:E:215:HIS:HA	2.39	0.43
1:B:135:GLY:HA3	1:B:186:PHE:CZ	2.53	0.43
1:D:52:ILE:HG23	1:D:62:VAL:HG11	2.00	0.43
1:C:49:GLY:HA2	1:C:52:ILE:HD12	2.00	0.43
1:F:35:ILE:CD1	1:F:133:PRO:HG3	2.48	0.43
1:C:140:ASP:OD1	1:C:141:PRO:HD2	2.19	0.43
1:B:38:GLU:HA	1:B:39:PRO:HD3	1.87	0.43
1:D:121:ARG:HG3	1:D:157:LEU:HD22	2.01	0.43
1:C:38:GLU:HB2	1:C:43:ASP:HB2	2.01	0.43
1:B:212:ILE:HG22	1:B:224:TRP:HZ3	1.83	0.42
1:B:71:TYR:CD2	1:B:110:ARG:HD3	2.54	0.42
1:E:38:GLU:HA	1:E:39:PRO:HD2	1.78	0.42
1:F:120:VAL:O	1:F:121:ARG:C	2.57	0.42
1:B:177:ILE:HB	1:F:130:LYS:HD3	2.01	0.42
1:C:46:ILE:HG22	1:C:46:ILE:O	2.19	0.42
1:C:213:ARG:HG2	1:C:224:TRP:CZ3	2.54	0.42
1:A:48:MSE:HE3	1:A:48:MSE:HB2	1.96	0.42
1:B:39:PRO:HG2	1:B:151:HIS:CD2	2.54	0.42
1:F:125:VAL:HG13	1:F:165:SER:HA	1.99	0.42
1:E:262:PRO:O	1:F:193:HIS:HB2	2.19	0.42
1:F:35:ILE:HD11	1:F:133:PRO:HG3	2.02	0.42
1:D:41:PRO:O	1:D:42:ASP:CB	2.67	0.42
1:A:245:ARG:HD2	1:A:246:TYR:CZ	2.54	0.42
1:E:120:VAL:HG12	1:E:120:VAL:O	2.20	0.42
1:D:63:ILE:HG23	1:D:103:LYS:HB3	2.02	0.42
1:C:162:VAL:HG11	1:C:187:ILE:HD11	2.02	0.42
1:E:70:GLY:O	1:E:72:MSE:N	2.53	0.42
1:A:205:MSE:O	1:A:205:MSE:HG3	2.20	0.42
1:F:38:GLU:HA	1:F:39:PRO:HD3	1.93	0.42
1:F:67:MSE:CE	1:F:124:LEU:HD11	2.36	0.42
1:C:175:ILE:O	1:C:177:ILE:N	2.52	0.42
1:F:35:ILE:HA	1:F:63:ILE:O	2.20	0.42
1:C:133:PRO:O	1:C:182:HIS:NE2	2.47	0.42
1:B:48:MSE:HB2	1:B:48:MSE:HE3	1.79	0.42
1:D:194:LYS:N	1:D:195:PRO:HD3	2.35	0.42
1:A:167:LEU:HA	1:A:168:PRO:HD2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:TYR:CD2	1:C:71:TYR:C	2.93	0.42
1:A:28:PHE:O	1:A:30:ASP:N	2.53	0.42
1:F:232:ARG:HD3	1:F:246:TYR:OH	2.20	0.42
1:F:141:PRO:HD2	1:F:142:TRP:CZ3	2.54	0.42
1:A:83:GLU:O	1:A:84:LEU:C	2.57	0.42
1:F:253:MSE:CG	1:F:267:ILE:HD11	2.50	0.42
1:F:196:ASN:H	1:F:196:ASN:HD22	1.67	0.41
1:E:130:LYS:C	1:E:132:LYS:N	2.74	0.41
1:E:209:LEU:O	1:E:213:ARG:HG2	2.20	0.41
1:A:83:GLU:O	1:A:85:ALA:N	2.53	0.41
1:F:15:LEU:HA	1:F:19:VAL:HB	2.03	0.41
1:F:167:LEU:HA	1:F:168:PRO:HD3	1.86	0.41
1:D:36:CYS:HB2	1:D:64:TYR:HD1	1.84	0.41
1:E:196:ASN:ND2	1:E:251:ARG:HA	2.35	0.41
1:E:36:CYS:HA	1:E:137:PHE:HB2	2.02	0.41
1:E:242:ILE:HD13	1:E:244:VAL:HG22	2.02	0.41
1:A:245:ARG:HD2	1:A:246:TYR:CE2	2.55	0.41
1:A:202:THR:HA	1:A:246:TYR:HB2	2.01	0.41
1:B:38:GLU:HG2	1:B:44:CYS:SG	2.59	0.41
1:B:14:LYS:O	1:B:19:VAL:HG23	2.20	0.41
1:F:148:HIS:HD2	1:F:150:ASP:H	1.68	0.41
1:F:53:LYS:HE3	1:F:57:ASP:OD2	2.20	0.41
1:D:145:TYR:HA	1:F:142:TRP:CE2	2.56	0.41
1:C:148:HIS:CD2	1:C:150:ASP:HB2	2.55	0.41
1:B:69:ASP:O	1:B:71:TYR:N	2.46	0.41
1:F:232:ARG:O	1:F:236:MSE:CG	2.66	0.41
1:C:125:VAL:HG21	1:C:170:PHE:CE2	2.55	0.41
1:A:74:THR:CG2	1:A:84:LEU:HD22	2.50	0.41
1:F:37:ILE:HG21	1:F:67:MSE:HE2	2.02	0.41
1:F:111:ASP:O	1:F:112:THR:OG1	2.34	0.41
1:E:190:TYR:HD2	1:E:191:TYR:CD2	2.38	0.41
1:C:82:HIS:O	1:C:83:GLU:C	2.59	0.41
1:B:107:LEU:HD12	1:B:123:ASP:OD2	2.20	0.41
1:A:198:ILE:HD13	1:A:249:GLY:CA	2.49	0.41
1:C:56:SER:OG	1:C:100:GLY:O	2.38	0.41
1:C:22:PHE:HZ	1:C:252:VAL:HG12	1.85	0.41
1:D:72:MSE:HG2	1:D:111:ASP:HB3	2.03	0.41
1:B:253:MSE:HB2	1:B:258:TYR:CE2	2.55	0.41
1:C:132:LYS:N	1:C:133:PRO:CD	2.84	0.41
1:E:148:HIS:NE2	1:E:150:ASP:OD2	2.53	0.41
1:E:92:GLU:HB2	1:E:215:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:MSE:SE	1:B:137:PHE:HD1	2.54	0.41
1:C:140:ASP:HA	1:C:189:LEU:HD22	2.03	0.41
1:B:95:SER:O	1:B:98:LEU:HB2	2.20	0.41
1:C:27:PRO:HD2	1:C:197:TYR:CZ	2.56	0.41
1:C:62:VAL:HB	1:C:101:VAL:HG22	2.03	0.41
1:C:53:LYS:HD3	1:C:99:LEU:HA	2.02	0.41
1:B:202:THR:HA	1:B:246:TYR:HB2	2.02	0.41
1:B:236:MSE:HE3	1:B:245:ARG:HG3	2.03	0.41
1:F:261:THR:HA	1:F:262:PRO:HD3	1.89	0.41
1:A:221:ASP:O	1:A:225:GLU:HG2	2.21	0.41
1:B:264:ALA:O	1:B:267:ILE:HG12	2.22	0.40
1:E:260:ILE:O	1:E:262:PRO:HD3	2.21	0.40
1:D:205:MSE:HG3	1:D:246:TYR:HD2	1.84	0.40
1:C:193:HIS:CG	1:C:193:HIS:O	2.75	0.40
1:C:148:HIS:HA	1:C:149:PRO:HD2	1.69	0.40
1:D:116:TYR:HB2	1:D:153:ARG:HD3	2.02	0.40
1:A:69:ASP:OD1	1:A:71:TYR:HB2	2.21	0.40
1:E:53:LYS:C	1:E:55:LEU:H	2.23	0.40
1:C:97:LYS:C	1:C:99:LEU:N	2.75	0.40
1:B:49:GLY:HA2	1:B:52:ILE:HD12	2.03	0.40
1:E:198:ILE:HB	1:E:242:ILE:HG12	2.03	0.40
1:C:157:LEU:O	1:C:161:SER:HB2	2.20	0.40
1:A:107:LEU:HD12	1:D:173:ILE:HD11	2.03	0.40
1:F:173:ILE:HA	1:F:176:ASP:HB2	2.04	0.40
1:E:36:CYS:HB3	1:E:48:MSE:HE1	2.02	0.40
1:D:72:MSE:O	1:F:167:LEU:HD13	2.22	0.40
1:F:38:GLU:OE1	1:F:43:ASP:N	2.54	0.40
1:F:198:ILE:HA	1:F:248:GLU:O	2.22	0.40
1:A:141:PRO:HD2	1:A:142:TRP:CE3	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	262/267 (98%)	228 (87%)	29 (11%)	5 (2%)	10	32
1	B	253/267 (95%)	206 (81%)	37 (15%)	10 (4%)	4	12
1	C	260/267 (97%)	200 (77%)	43 (16%)	17 (6%)	1	4
1	D	260/267 (97%)	213 (82%)	34 (13%)	13 (5%)	3	8
1	E	260/267 (97%)	206 (79%)	35 (14%)	19 (7%)	1	3
1	F	262/267 (98%)	213 (81%)	43 (16%)	6 (2%)	8	26
All	All	1557/1602 (97%)	1266 (81%)	221 (14%)	70 (4%)	3	10

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	42	ASP
1	A	77	GLU
1	B	71	TYR
1	B	162	VAL
1	B	254	PRO
1	B	260	ILE
1	C	94	GLU
1	C	98	LEU
1	D	94	GLU
1	D	98	LEU
1	E	42	ASP
1	E	45	ALA
1	E	46	ILE
1	F	42	ASP
1	B	42	ASP
1	C	24	LEU
1	C	58	GLU
1	C	71	TYR
1	C	77	GLU
1	C	176	ASP
1	C	184	VAL
1	D	42	ASP
1	D	49	GLY
1	D	95	SER
1	D	124	LEU
1	E	50	GLY
1	E	51	THR
1	E	71	TYR
1	E	95	SER

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Mol	Chain	Res	Type
1	E	111	ASP
1	E	127	ILE
1	E	131	GLU
1	E	240	GLU
1	F	49	GLY
1	A	28	PHE
1	B	184	VAL
1	B	243	GLY
1	B	253	MSE
1	C	22	PHE
1	C	57	ASP
1	D	111	ASP
1	D	245	ARG
1	E	126	LYS
1	F	71	TYR
1	C	54	LYS
1	C	108	ASN
1	C	239	GLY
1	D	130	LYS
1	D	181	PRO
1	E	25	GLU
1	E	54	LYS
1	E	130	LYS
1	F	179	LEU
1	B	58	GLU
1	C	132	LYS
1	C	238	TYR
1	D	27	PRO
1	D	123	ASP
1	F	176	ASP
1	E	27	PRO
1	E	214	ALA
1	C	175	ILE
1	C	260	ILE
1	E	255	GLY
1	B	27	PRO
1	E	260	ILE
1	F	46	ILE
1	A	132	LYS
1	D	260	ILE

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	236/232 (102%)	222 (94%)	14 (6%)	24	57
1	B	228/232 (98%)	215 (94%)	13 (6%)	25	58
1	C	234/232 (101%)	215 (92%)	19 (8%)	15	39
1	D	234/232 (101%)	218 (93%)	16 (7%)	20	49
1	E	234/232 (101%)	212 (91%)	22 (9%)	11	31
1	F	236/232 (102%)	224 (95%)	12 (5%)	29	63
All	All	1402/1392 (101%)	1306 (93%)	96 (7%)	20	49

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	40	HIS
1	A	42	ASP
1	A	71	TYR
1	A	78	LYS
1	A	108	ASN
1	A	172	ASN
1	A	176	ASP
1	A	196	ASN
1	A	221	ASP
1	A	231	LEU
1	A	241	LYS
1	A	244	VAL
1	A	245	ARG
1	B	30	ASP
1	B	58	GLU
1	B	75	THR
1	B	113	GLU
1	B	119	GLU
1	B	165	SER
1	B	193	HIS
1	B	196	ASN

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Mol	Chain	Res	Type
1	B	202	THR
1	B	205	MSE
1	B	226	THR
1	B	252	VAL
1	B	265	ASP
1	C	7	THR
1	C	16	LEU
1	C	23	ASN
1	C	42	ASP
1	C	48	MSE
1	C	71	TYR
1	C	80	SER
1	C	86	LEU
1	C	95	SER
1	C	98	LEU
1	C	103	LYS
1	C	122	LYS
1	C	161	SER
1	C	172	ASN
1	C	193	HIS
1	C	196	ASN
1	C	198	ILE
1	C	226	THR
1	C	235	THR
1	D	17	LYS
1	D	23	ASN
1	D	30	ASP
1	D	35	ILE
1	D	57	ASP
1	D	58	GLU
1	D	71	TYR
1	D	98	LEU
1	D	134	ASP
1	D	172	ASN
1	D	185	SER
1	D	196	ASN
1	D	202	THR
1	D	213	ARG
1	D	216	ARG
1	D	235	THR
1	E	23	ASN
1	E	30	ASP

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Mol	Chain	Res	Type
1	E	42	ASP
1	E	43	ASP
1	E	48	MSE
1	E	54	LYS
1	E	72	MSE
1	E	75	THR
1	E	76	ASP
1	E	77	GLU
1	E	102	ARG
1	E	111	ASP
1	E	132	LYS
1	E	172	ASN
1	E	180	LYS
1	E	187	ILE
1	E	192	THR
1	E	196	ASN
1	E	210	LYS
1	E	213	ARG
1	E	223	ILE
1	E	245	ARG
1	F	5	VAL
1	F	23	ASN
1	F	24	LEU
1	F	25	GLU
1	F	30	ASP
1	F	42	ASP
1	F	107	LEU
1	F	123	ASP
1	F	172	ASN
1	F	196	ASN
1	F	223	ILE
1	F	245	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	148	HIS
1	A	166	GLN
1	A	172	ASN
1	A	196	ASN
1	B	148	HIS

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Mol	Chain	Res	Type
1	B	169	ASN
1	B	196	ASN
1	C	108	ASN
1	C	172	ASN
1	C	196	ASN
1	C	215	HIS
1	D	13	ASN
1	D	23	ASN
1	D	82	HIS
1	D	108	ASN
1	D	169	ASN
1	D	172	ASN
1	D	196	ASN
1	E	40	HIS
1	E	169	ASN
1	E	196	ASN
1	E	215	HIS
1	F	23	ASN
1	F	26	ASN
1	F	82	HIS
1	F	108	ASN
1	F	172	ASN
1	F	196	ASN

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 carbohydrates 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	258/267 (96%)	0.24	16 (6%) 24 15	26, 64, 94, 97	0
1	B	249/267 (93%)	0.24	14 (5%) 28 18	18, 63, 99, 110	0
1	C	256/267 (95%)	0.35	19 (7%) 17 9	26, 70, 115, 121	0
1	D	256/267 (95%)	0.21	9 (3%) 48 35	27, 62, 100, 110	0
1	E	256/267 (95%)	0.33	13 (5%) 32 21	25, 67, 93, 99	0
1	F	258/267 (96%)	0.02	6 (2%) 64 52	18, 58, 84, 88	0
All	All	1533/1602 (95%)	0.23	77 (5%) 32 21	18, 65, 99, 121	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	GLU	4.6
1	A	6	SER	4.4
1	C	227	TRP	4.4
1	E	206	GLU	4.2
1	B	227	TRP	4.2
1	E	202	THR	4.2
1	C	243	GLY	4.0
1	C	237	PHE	3.9
1	D	25	GLU	3.9
1	C	32	LYS	3.8
1	B	180	LYS	3.7
1	C	47	GLY	3.5
1	A	221	ASP	3.5
1	E	97	LYS	3.4
1	B	24	LEU	3.4
1	C	7	THR	3.3
1	A	227	TRP	3.1
1	D	243	GLY	3.1
1	B	16	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	103	LYS	3.1
1	A	47	GLY	3.1
1	D	235	THR	3.0
1	E	59	GLY	2.9
1	A	75	THR	2.9
1	D	223	ILE	2.9
1	B	178	GLY	2.9
1	C	11	ALA	2.8
1	C	245	ARG	2.8
1	C	249	GLY	2.8
1	D	18	GLU	2.7
1	E	247	GLY	2.7
1	F	7	THR	2.7
1	D	7	THR	2.7
1	F	6	SER	2.6
1	B	233	THR	2.6
1	C	235	THR	2.6
1	E	223	ILE	2.6
1	A	29	GLU	2.5
1	A	223	ILE	2.5
1	A	46	ILE	2.5
1	A	178	GLY	2.5
1	C	44	CYS	2.4
1	C	6	SER	2.4
1	C	26	ASN	2.4
1	F	59	GLY	2.4
1	C	36	CYS	2.4
1	A	7	THR	2.4
1	E	44	CYS	2.3
1	B	210	LYS	2.3
1	D	26	ASN	2.3
1	D	203	ASP	2.3
1	F	10	GLU	2.3
1	C	103	LYS	2.3
1	C	219	PHE	2.3
1	E	178	GLY	2.3
1	E	76	ASP	2.3
1	A	76	ASP	2.2
1	C	211	ALA	2.2
1	B	18	GLU	2.2
1	B	102	ARG	2.2
1	E	222	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	180	LYS	2.1
1	B	94	GLU	2.1
1	C	200	ASP	2.1
1	A	208	LYS	2.1
1	F	94	GLU	2.1
1	A	194	LYS	2.1
1	C	35	ILE	2.1
1	A	26	ASN	2.1
1	B	231	LEU	2.1
1	E	78	LYS	2.1
1	A	14	LYS	2.1
1	E	75	THR	2.1
1	A	243	GLY	2.1
1	E	210	LYS	2.0
1	B	19	VAL	2.0
1	B	22	PHE	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	D	301	1/1	0.99	0.10	-1.15	40,40,40,40	0
2	ZN	F	301	1/1	0.96	0.12	-1.67	54,54,54,54	0
2	ZN	E	301	1/1	0.98	0.07	-2.69	50,50,50,50	0
2	ZN	A	301	1/1	0.98	0.08	-3.56	52,52,52,52	0
2	ZN	B	301	1/1	0.99	0.07	-4.82	40,40,40,40	0
2	ZN	C	301	1/1	0.98	0.08	-	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.