WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 01:07 PM EST

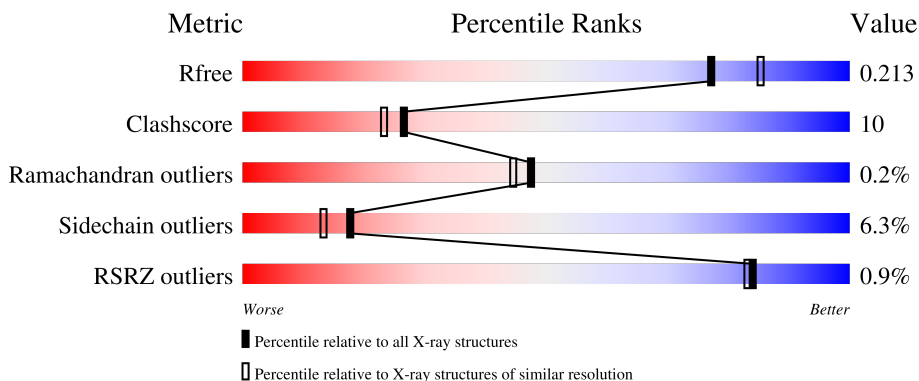|		
PDB ID	:	3U95
Title	:	Crystal structure of a putative alpha-glucosidase from Thermotoga neapolitana
Authors	:	Ha, N.C.; Jun, S.Y.; Yun, B.Y.; Yoon, B.Y.; Piao, S.
Deposited on	:	2011-10-17
Resolution	:	2.00 Å(reported)

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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
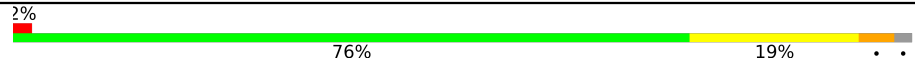
Metric	Percentile Ranks	Value
Rfree		0.213
Clashscore		10
Ramachandran outliers		0.2%
Sidechain outliers		6.3%
RSRZ outliers		0.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	477	75% 20% • •
1	B	477	.% 78% 18% • •
1	C	477	.% 73% 22% • •
1	D	477	.% 73% 22% • •
1	E	477	76% 19% • •

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Mol	Chain	Length	Quality of chain
1	F	477	

2%

76%   19%

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 25816 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 Glycoside hydrolase, family 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total 3894	C 2494	N 679	O 709	S 12	0	0	0
1	B	469	Total 3902	C 2498	N 681	O 711	S 12	0	0	0
1	C	464	Total 3860	C 2473	N 673	O 703	S 11	0	0	0
1	D	468	Total 3894	C 2494	N 679	O 709	S 12	0	0	0
1	E	466	Total 3877	C 2483	N 675	O 707	S 12	0	0	0
1	F	469	Total 3902	C 2498	N 681	O 711	S 12	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	416	THR	MET	conflict	UNP B9KAM3
A	470	LEU	-	expression tag	UNP B9KAM3
A	471	GLU	-	expression tag	UNP B9KAM3
A	472	HIS	-	expression tag	UNP B9KAM3
A	473	HIS	-	expression tag	UNP B9KAM3
A	474	HIS	-	expression tag	UNP B9KAM3
A	475	HIS	-	expression tag	UNP B9KAM3
A	476	HIS	-	expression tag	UNP B9KAM3
A	477	HIS	-	expression tag	UNP B9KAM3
B	416	THR	MET	conflict	UNP B9KAM3
B	470	LEU	-	expression tag	UNP B9KAM3
B	471	GLU	-	expression tag	UNP B9KAM3
B	472	HIS	-	expression tag	UNP B9KAM3
B	473	HIS	-	expression tag	UNP B9KAM3
B	474	HIS	-	expression tag	UNP B9KAM3
B	475	HIS	-	expression tag	UNP B9KAM3
B	476	HIS	-	expression tag	UNP B9KAM3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	477	HIS	-	expression tag	UNP B9KAM3
C	416	THR	MET	conflict	UNP B9KAM3
C	470	LEU	-	expression tag	UNP B9KAM3
C	471	GLU	-	expression tag	UNP B9KAM3
C	472	HIS	-	expression tag	UNP B9KAM3
C	473	HIS	-	expression tag	UNP B9KAM3
C	474	HIS	-	expression tag	UNP B9KAM3
C	475	HIS	-	expression tag	UNP B9KAM3
C	476	HIS	-	expression tag	UNP B9KAM3
C	477	HIS	-	expression tag	UNP B9KAM3
D	416	THR	MET	conflict	UNP B9KAM3
D	470	LEU	-	expression tag	UNP B9KAM3
D	471	GLU	-	expression tag	UNP B9KAM3
D	472	HIS	-	expression tag	UNP B9KAM3
D	473	HIS	-	expression tag	UNP B9KAM3
D	474	HIS	-	expression tag	UNP B9KAM3
D	475	HIS	-	expression tag	UNP B9KAM3
D	476	HIS	-	expression tag	UNP B9KAM3
D	477	HIS	-	expression tag	UNP B9KAM3
E	416	THR	MET	conflict	UNP B9KAM3
E	470	LEU	-	expression tag	UNP B9KAM3
E	471	GLU	-	expression tag	UNP B9KAM3
E	472	HIS	-	expression tag	UNP B9KAM3
E	473	HIS	-	expression tag	UNP B9KAM3
E	474	HIS	-	expression tag	UNP B9KAM3
E	475	HIS	-	expression tag	UNP B9KAM3
E	476	HIS	-	expression tag	UNP B9KAM3
E	477	HIS	-	expression tag	UNP B9KAM3
F	416	THR	MET	conflict	UNP B9KAM3
F	470	LEU	-	expression tag	UNP B9KAM3
F	471	GLU	-	expression tag	UNP B9KAM3
F	472	HIS	-	expression tag	UNP B9KAM3
F	473	HIS	-	expression tag	UNP B9KAM3
F	474	HIS	-	expression tag	UNP B9KAM3
F	475	HIS	-	expression tag	UNP B9KAM3
F	476	HIS	-	expression tag	UNP B9KAM3
F	477	HIS	-	expression tag	UNP B9KAM3

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	444	Total 444	O 444	0	0
3	B	402	Total 402	O 402	0	0
3	C	393	Total 393	O 393	0	0
3	D	450	Total 450	O 450	0	0
3	E	431	Total 431	O 431	0	0
3	F	361	Total 361	O 361	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
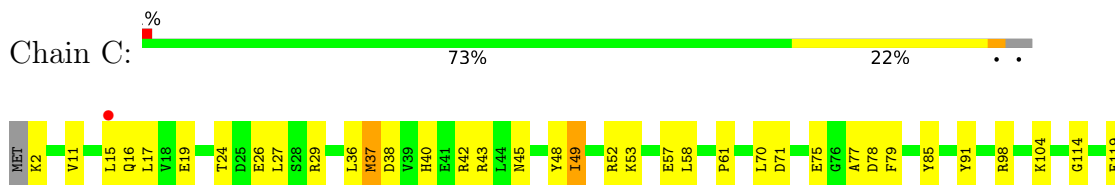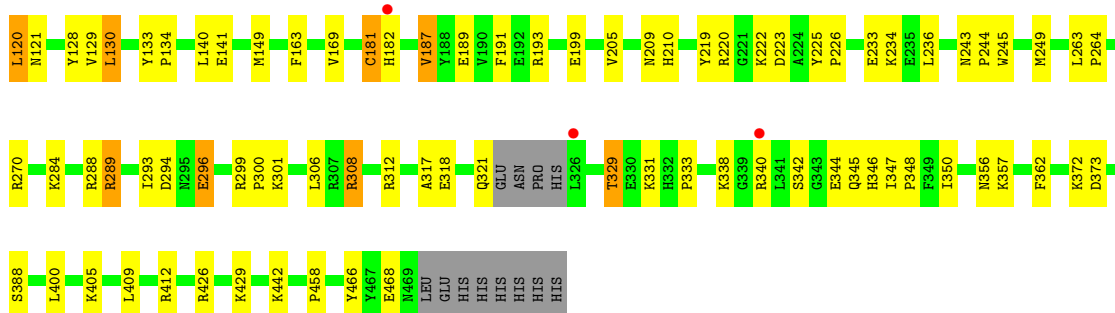
• Molecule 1: Glycoside hydrolase, family 4
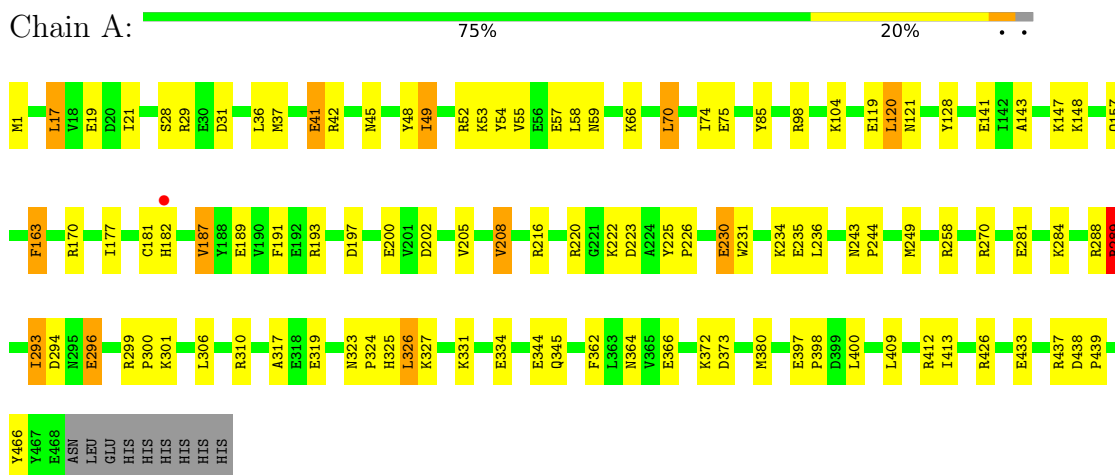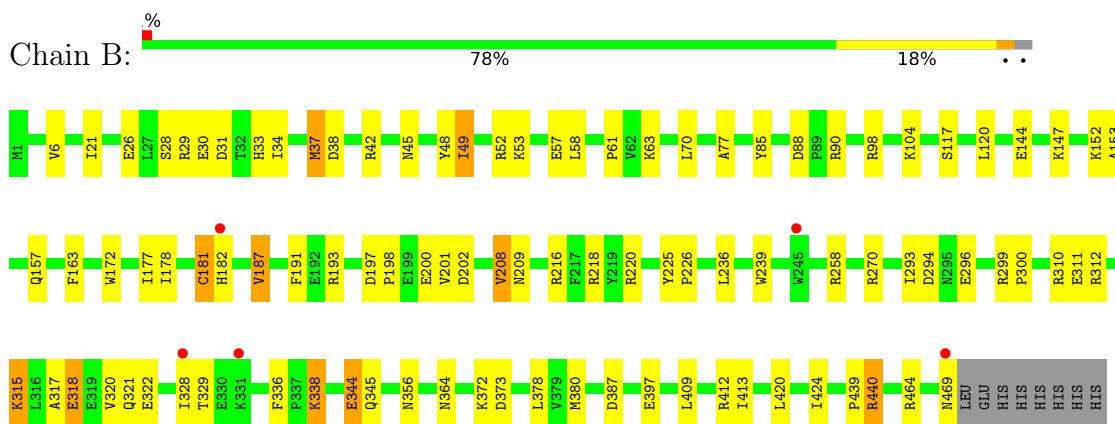
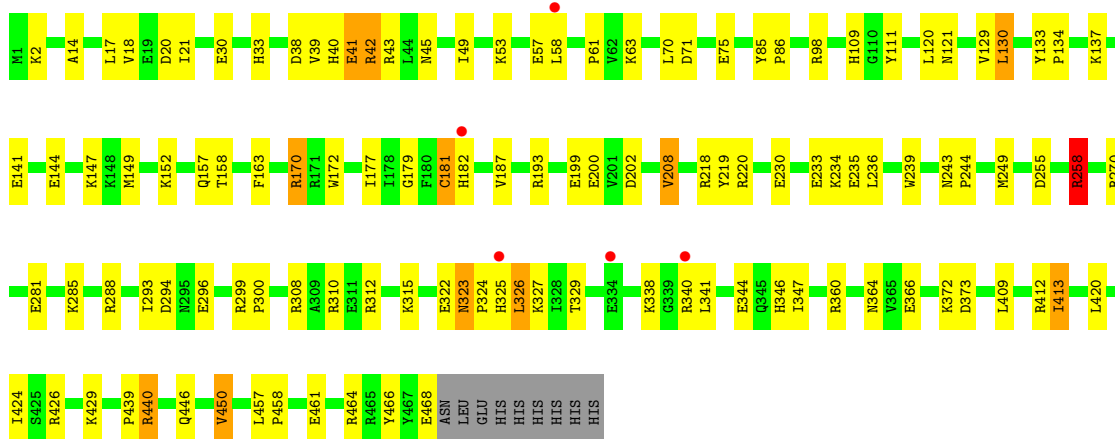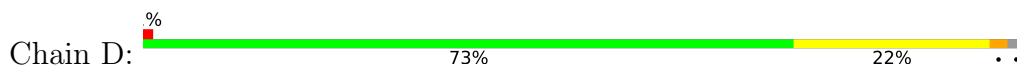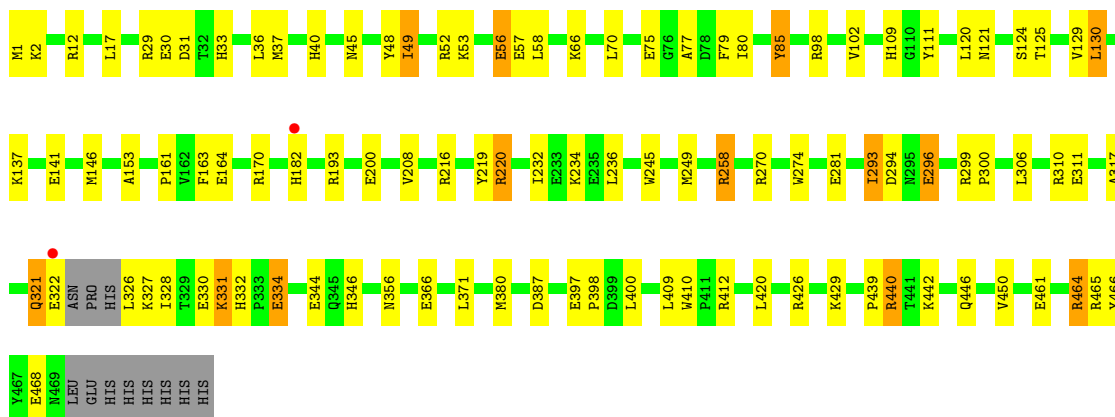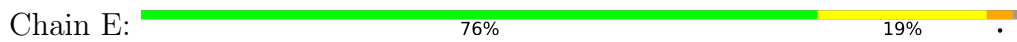• Molecule 1: Glycoside hydrolase, family 4

• Molecule 1: Glycoside hydrolase, family 4

• Molecule 1: Glycoside hydrolase, family 4

Chain D:

• Molecule 1: Glycoside hydrolase, family 4

Chain E:

• Molecule 1: Glycoside hydrolase, family 4

Chain F:
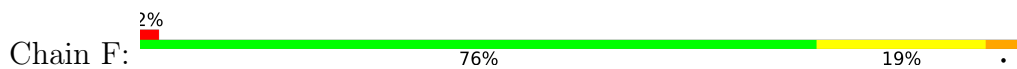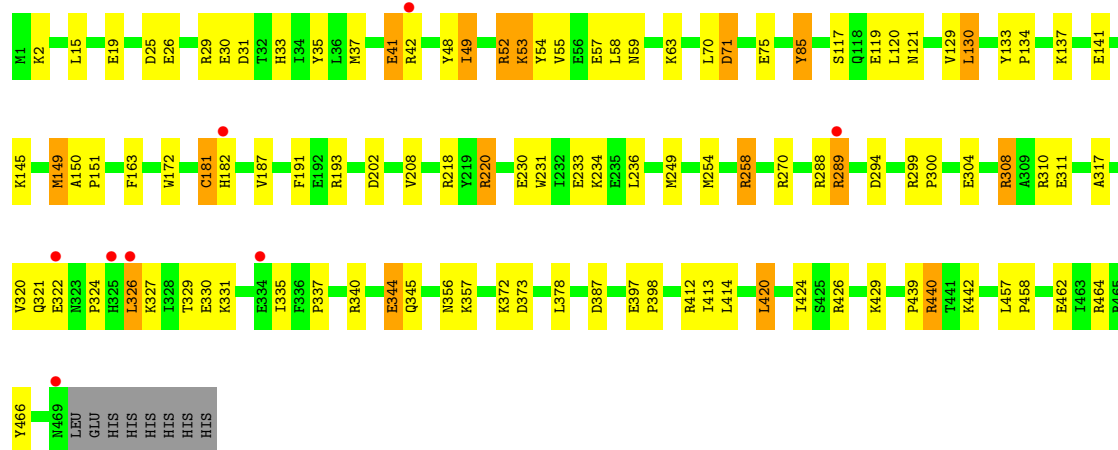
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	154.53Å 154.53Å 139.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.90 – 2.00 40.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.90-2.00) 98.9 (40.90-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.77 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.185 , 0.222 0.180 , 0.213	Depositor DCC
R_{free} test set	1985 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.1	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.024 for h,-h-k,-l 0.076 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25816	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0314e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.38	0/3994	0.53	0/5407
1	B	0.38	0/4002	0.53	0/5418
1	C	0.38	0/3957	0.52	0/5355
1	D	0.39	0/3994	0.56	2/5407 (0.0%)
1	E	0.39	0/3974	0.55	1/5377 (0.0%)
1	F	0.36	0/4002	0.52	0/5418
All	All	0.38	0/23923	0.54	3/32382 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	440	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	D	258	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	E	440	ARG	NE-CZ-NH2	-5.17	117.72	120.30

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	3894	0	3847	85	0
1	B	3902	0	3853	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3860	0	3814	97	0
1	D	3894	0	3848	73	0
1	E	3877	0	3832	77	0
1	F	3902	0	3853	81	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	444	0	0	16	0
3	B	402	0	0	12	0
3	C	393	0	0	19	0
3	D	450	0	0	14	0
3	E	431	0	0	14	0
3	F	361	0	0	17	0
All	All	25816	0	23047	476	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 10.

All (476) 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:A:289:ARG:HH21	1:A:289:ARG:HG3	1.15	1.09
1:C:429:LYS:HG3	3:D:2410:HOH:O	1.48	1.09
1:A:182:HIS:CE1	1:A:344:GLU:HG3	1.94	1.03
1:F:289:ARG:HG2	3:F:2213:HOH:O	1.58	1.03
1:A:182:HIS:HE1	1:A:344:GLU:HG3	1.25	1.02
1:D:258:ARG:HH11	1:D:258:ARG:HG2	1.21	1.00
1:A:222:LYS:HD3	1:A:223:ASP:H	1.23	1.00
1:F:49:ILE:HD11	1:F:317:ALA:HB1	1.43	0.98
1:A:182:HIS:CE1	1:A:345:GLN:H	1.79	0.98
1:E:461:GLU:OE2	3:E:2103:HOH:O	1.82	0.96
1:F:48:TYR:OH	3:F:1780:HOH:O	1.85	0.95
1:D:308:ARG:NH2	3:D:2063:HOH:O	1.99	0.93
1:A:310:ARG:NH1	3:A:2217:HOH:O	1.96	0.92
1:D:429:LYS:HG3	3:D:1953:HOH:O	1.68	0.92
1:B:201:VAL:N	3:B:2090:HOH:O	1.89	0.92
1:F:26:GLU:OE1	3:F:829:HOH:O	1.91	0.89
1:A:230:GLU:OE2	1:A:234:LYS:NZ	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:TYR:OH	3:D:1779:HOH:O	1.91	0.88
1:C:270:ARG:HD2	1:C:294:ASP:OD2	1.75	0.87
1:A:49:ILE:HD11	1:A:317:ALA:HB1	1.57	0.87
1:E:245:TRP:CE2	1:E:293:ILE:HD12	2.12	0.84
1:D:285:LYS:NZ	3:D:2277:HOH:O	2.10	0.84
1:A:310:ARG:NH2	3:A:2217:HOH:O	2.08	0.83
1:B:182:HIS:CE1	1:B:344:GLU:HA	2.14	0.82
1:B:182:HIS:CE1	1:B:345:GLN:HG3	2.16	0.80
1:B:310:ARG:NH1	1:B:311:GLU:OE1	2.13	0.80
1:B:338:LYS:H	1:B:338:LYS:HZ2	1.27	0.80
1:A:412:ARG:HD3	3:A:1649:HOH:O	1.81	0.80
1:A:222:LYS:HD3	1:A:223:ASP:N	1.96	0.80
1:C:193:ARG:HD2	3:C:1683:HOH:O	1.80	0.80
1:B:29:ARG:NH2	1:B:31:ASP:OD1	2.15	0.80
1:B:338:LYS:H	1:B:338:LYS:NZ	1.81	0.79
1:F:42:ARG:NE	3:F:1478:HOH:O	2.14	0.79
1:A:197:ASP:HB3	1:A:200:GLU:HG3	1.62	0.79
1:B:469:ASN:O	3:B:2453:HOH:O	2.01	0.79
1:E:270:ARG:HD2	1:E:294:ASP:OD2	1.84	0.78
1:A:289:ARG:HH21	1:A:289:ARG:CG	1.96	0.78
1:A:289:ARG:HG3	1:A:289:ARG:NH2	1.96	0.78
3:E:1090:HOH:O	1:F:429:LYS:HG3	1.82	0.78
1:F:182:HIS:HE2	1:F:345:GLN:H	1.32	0.78
1:A:200:GLU:OE2	1:A:220:ARG:NH2	2.14	0.77
1:D:98:ARG:NH1	3:D:1576:HOH:O	2.17	0.76
1:E:200:GLU:OE2	3:E:1923:HOH:O	2.03	0.75
1:E:52:ARG:NH2	3:E:2168:HOH:O	2.19	0.75
1:C:468:GLU:OE2	3:C:2345:HOH:O	2.06	0.74
1:D:258:ARG:HG2	1:D:258:ARG:NH1	1.96	0.74
1:A:270:ARG:HD2	1:A:294:ASP:OD2	1.86	0.74
1:E:111:TYR:HE1	1:E:450:VAL:HG21	1.52	0.74
1:A:48:TYR:CZ	1:A:52:ARG:HD2	2.23	0.74
1:A:296:GLU:HG2	3:A:1091:HOH:O	1.88	0.74
1:D:33:HIS:CE1	1:D:63:LYS:HD2	2.23	0.73
1:E:446:GLN:O	1:E:450:VAL:HG23	1.87	0.73
1:E:111:TYR:CE1	1:E:450:VAL:HG21	2.23	0.73
1:F:310:ARG:NH1	1:F:311:GLU:OE1	2.21	0.73
1:F:464:ARG:NH2	3:F:499:HOH:O	2.18	0.73
1:A:409:LEU:O	1:A:413:ILE:HD13	1.88	0.72
1:D:270:ARG:HD2	1:D:294:ASP:OD2	1.90	0.72
1:C:296:GLU:HG2	3:C:1078:HOH:O	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ARG:NH2	3:D:1383:HOH:O	2.05	0.72
1:B:270:ARG:HD2	1:B:294:ASP:OD2	1.90	0.71
1:D:42:ARG:HG2	1:D:42:ARG:HH21	1.55	0.70
1:A:310:ARG:CZ	3:A:2217:HOH:O	2.30	0.70
1:B:198:PRO:C	3:B:2090:HOH:O	2.30	0.70
1:E:77:ALA:O	1:E:153:ALA:HB2	1.92	0.70
1:E:281:GLU:OE1	3:E:549:HOH:O	2.10	0.70
1:A:202:ASP:OD2	3:A:2110:HOH:O	2.10	0.69
1:C:57:GLU:OE1	1:C:329:THR:OG1	2.09	0.69
1:D:322:GLU:O	1:D:323:ASN:HB2	1.93	0.69
1:D:312:ARG:NH2	3:D:568:HOH:O	2.25	0.68
1:E:1:MET:HE1	1:E:79:PHE:HE2	1.58	0.68
1:E:310:ARG:HD3	3:E:2306:HOH:O	1.92	0.68
1:B:197:ASP:O	3:B:2090:HOH:O	2.11	0.68
1:D:258:ARG:HH11	1:D:258:ARG:CG	2.03	0.68
1:B:33:HIS:NE2	1:B:63:LYS:HD2	2.08	0.68
1:E:327:LYS:HD2	1:E:330:GLU:OE2	1.94	0.68
1:B:45:ASN:O	1:B:49:ILE:HG22	1.94	0.68
1:A:49:ILE:CD1	1:A:317:ALA:HB1	2.25	0.67
1:E:124:SER:O	1:E:125:THR:HG22	1.94	0.67
1:F:327:LYS:HB3	1:F:330:GLU:HG3	1.76	0.67
1:E:2:LYS:NZ	1:E:75:GLU:O	2.22	0.67
1:F:71:ASP:CG	3:F:2121:HOH:O	2.32	0.67
1:F:53:LYS:NZ	1:F:57:GLU:OE2	2.27	0.67
1:E:109:HIS:HB3	1:E:450:VAL:HG22	1.77	0.66
1:B:58:LEU:O	3:B:2161:HOH:O	2.14	0.66
1:C:187:VAL:HG13	1:C:191:PHE:CZ	2.30	0.66
1:E:426:ARG:HG2	1:E:466:TYR:CZ	2.30	0.66
1:A:326:LEU:HD21	1:A:331:LYS:HD2	1.78	0.66
1:D:41:GLU:HG3	1:D:42:ARG:N	2.10	0.66
1:D:255:ASP:OD1	1:D:258:ARG:NH2	2.28	0.66
1:D:446:GLN:O	1:D:450:VAL:HG23	1.96	0.66
1:F:117:SER:O	1:F:440:ARG:NH2	2.29	0.65
1:F:150:ALA:N	1:F:151:PRO:HD3	2.11	0.65
1:D:86:PRO:O	1:D:98:ARG:NH1	2.28	0.65
1:E:1:MET:N	1:E:31:ASP:O	2.29	0.65
1:E:120:LEU:HB3	1:E:412:ARG:HD3	1.77	0.65
1:F:57:GLU:OE1	1:F:329:THR:OG1	2.11	0.65
1:F:254:MET:O	1:F:258:ARG:HG2	1.96	0.65
1:B:49:ILE:HD11	1:B:320:VAL:HB	1.79	0.65
1:B:409:LEU:O	1:B:413:ILE:HG12	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LYS:NZ	1:C:57:GLU:OE2	2.30	0.65
1:C:141:GLU:OE2	3:C:2095:HOH:O	2.13	0.65
1:B:372:LYS:HD2	1:B:373:ASP:OD2	1.97	0.65
1:C:182:HIS:NE2	1:C:345:GLN:N	2.45	0.64
1:F:33:HIS:NE2	1:F:63:LYS:HD2	2.12	0.64
1:A:181:CYS:O	1:A:182:HIS:HD2	1.80	0.64
1:A:284:LYS:O	1:A:288:ARG:HA	1.97	0.63
1:A:181:CYS:C	1:A:182:HIS:CD2	2.72	0.63
1:A:281:GLU:OE2	3:C:570:HOH:O	2.16	0.63
1:D:324:PRO:O	1:D:325:HIS:HB3	1.99	0.63
1:B:200:GLU:N	3:B:2090:HOH:O	2.33	0.62
1:D:208:VAL:HG11	1:D:412:ARG:HG2	1.80	0.62
1:C:98:ARG:NH1	3:C:558:HOH:O	2.33	0.62
1:E:53:LYS:HD2	1:E:57:GLU:OE2	1.99	0.62
1:B:312:ARG:O	1:B:315:LYS:HE2	2.00	0.62
1:F:233:GLU:HG2	1:F:234:LYS:HD3	1.81	0.62
1:C:29:ARG:HA	1:C:61:PRO:HG2	1.81	0.62
1:D:200:GLU:OE1	1:D:220:ARG:NH1	2.32	0.62
1:D:152:LYS:HB3	3:D:2427:HOH:O	1.98	0.61
1:B:328:ILE:N	1:B:328:ILE:HD12	2.15	0.61
1:B:328:ILE:HD12	1:B:328:ILE:H	1.66	0.61
1:E:296:GLU:HG2	3:E:507:HOH:O	1.99	0.61
1:B:182:HIS:NE2	1:B:344:GLU:HG3	2.15	0.61
1:D:340:ARG:NH1	1:D:341:LEU:O	2.34	0.61
1:B:182:HIS:CE1	1:B:345:GLN:N	2.69	0.60
1:A:193:ARG:NH2	3:A:747:HOH:O	2.33	0.60
1:B:320:VAL:HG22	1:B:328:ILE:HD11	1.83	0.60
1:B:152:LYS:NZ	3:B:2019:HOH:O	2.33	0.60
1:E:85:TYR:OH	1:E:125:THR:OG1	2.18	0.60
1:E:442:LYS:NZ	1:F:442:LYS:HE2	2.15	0.60
1:F:372:LYS:O	1:F:373:ASP:HB2	2.01	0.60
1:A:53:LYS:HE3	1:A:57:GLU:OE2	2.02	0.60
1:A:98:ARG:HD2	1:A:128:TYR:OH	2.02	0.60
1:A:181:CYS:C	1:A:182:HIS:HD2	2.06	0.60
1:C:308:ARG:HG2	1:C:308:ARG:HH11	1.67	0.59
1:B:378:LEU:HD21	1:B:413:ILE:HD12	1.84	0.59
1:D:111:TYR:CE1	1:D:450:VAL:HG21	2.36	0.59
1:A:141:GLU:OE1	3:A:625:HOH:O	2.17	0.59
1:F:42:ARG:CZ	3:F:1478:HOH:O	2.49	0.59
1:F:145:LYS:HD3	3:F:2121:HOH:O	2.01	0.59
1:D:324:PRO:O	1:D:325:HIS:CB	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:ILE:HD11	1:E:317:ALA:O	2.02	0.59
1:F:75:GLU:HG2	3:F:2235:HOH:O	2.03	0.59
1:B:98:ARG:NH2	3:B:1651:HOH:O	1.88	0.59
1:B:328:ILE:HG22	1:B:336:PHE:CD2	2.38	0.59
1:E:109:HIS:CB	1:E:450:VAL:HG22	2.32	0.59
1:E:45:ASN:OD1	1:E:66:LYS:NZ	2.36	0.58
1:F:187:VAL:HG22	1:F:191:PHE:CZ	2.38	0.58
1:F:202:ASP:HB3	1:F:218:ARG:HB2	1.84	0.58
1:B:372:LYS:O	1:B:373:ASP:HB2	2.04	0.58
1:C:219:TYR:CE2	1:C:220:ARG:HG3	2.39	0.58
1:F:426:ARG:HG2	1:F:466:TYR:CZ	2.39	0.57
1:B:293:ILE:HG22	3:B:1664:HOH:O	2.03	0.57
1:C:40:HIS:CE1	1:C:43:ARG:HG3	2.38	0.57
1:C:114:GLY:HA3	3:C:635:HOH:O	2.04	0.57
1:D:20:ASP:HB2	1:D:347:ILE:HG13	1.85	0.57
1:D:372:LYS:O	1:D:373:ASP:HB2	2.03	0.57
1:A:319:GLU:OE2	1:A:331:LYS:NZ	2.38	0.57
1:E:442:LYS:HZ2	1:F:442:LYS:HE2	1.67	0.57
1:F:322:GLU:O	1:F:324:PRO:HD3	2.04	0.57
1:D:17:LEU:O	1:D:21:ILE:HG13	2.05	0.56
1:C:49:ILE:HD11	1:C:317:ALA:HB1	1.87	0.56
1:D:426:ARG:HG2	1:D:466:TYR:CZ	2.40	0.56
1:C:48:TYR:CZ	1:C:52:ARG:HD2	2.41	0.56
1:C:48:TYR:OH	1:C:52:ARG:NH1	2.34	0.56
1:D:409:LEU:O	1:D:413:ILE:HG23	2.06	0.56
1:E:1:MET:HE1	1:E:79:PHE:CE2	2.40	0.56
1:C:187:VAL:HG13	1:C:191:PHE:CE2	2.41	0.56
1:F:270:ARG:HD2	1:F:294:ASP:OD2	2.05	0.56
1:B:30:GLU:HA	1:B:61:PRO:O	2.04	0.55
1:C:426:ARG:HG2	1:C:466:TYR:CZ	2.41	0.55
1:A:243:ASN:HB2	1:A:244:PRO:CD	2.36	0.55
1:E:48:TYR:CG	1:E:66:LYS:HD3	2.41	0.55
1:C:193:ARG:HG3	1:C:249:MET:HG3	1.89	0.55
1:F:220:ARG:HD3	3:F:2280:HOH:O	2.07	0.55
1:A:200:GLU:HB3	1:A:220:ARG:HH12	1.71	0.55
1:A:299:ARG:HB3	1:A:300:PRO:HD3	1.88	0.55
1:C:223:ASP:O	1:C:226:PRO:HD2	2.05	0.55
1:D:172:TRP:CE2	1:D:424:ILE:HD12	2.41	0.55
1:E:400:LEU:HD13	1:E:409:LEU:HD11	1.88	0.55
1:A:426:ARG:HG2	1:A:466:TYR:CZ	2.41	0.55
1:D:360:ARG:HD3	3:D:1473:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLU:HB2	3:A:2157:HOH:O	2.06	0.55
1:C:119:GLU:O	1:C:120:LEU:HB2	2.06	0.55
1:C:58:LEU:HD21	1:C:338:LYS:HG2	1.89	0.55
1:C:372:LYS:O	1:C:373:ASP:HB2	2.07	0.55
1:A:119:GLU:O	1:A:120:LEU:HB2	2.07	0.54
1:E:429:LYS:NZ	3:E:2124:HOH:O	2.39	0.54
1:F:378:LEU:HD21	1:F:413:ILE:CD1	2.38	0.54
1:A:372:LYS:O	1:A:373:ASP:HB2	2.07	0.54
1:E:33:HIS:CD2	3:E:1967:HOH:O	2.61	0.54
1:F:41:GLU:HG3	1:F:42:ARG:N	2.22	0.54
1:F:119:GLU:O	1:F:120:LEU:HB2	2.08	0.54
1:E:321:GLN:HB3	1:E:322:GLU:OE2	2.08	0.54
1:C:233:GLU:HB3	1:C:234:LYS:HD2	1.90	0.53
1:A:41:GLU:HG3	1:A:42:ARG:N	2.22	0.53
1:C:312:ARG:NH1	3:C:2122:HOH:O	2.41	0.53
1:B:42:ARG:HA	1:B:42:ARG:NE	2.24	0.53
1:B:182:HIS:CE1	1:B:345:GLN:H	2.26	0.53
1:D:45:ASN:O	1:D:49:ILE:HG12	2.08	0.53
1:F:182:HIS:NE2	1:F:344:GLU:HG3	2.24	0.53
1:E:129:VAL:O	1:E:130:LEU:HB2	2.09	0.53
1:C:234:LYS:HD2	1:C:234:LYS:N	2.24	0.53
1:B:193:ARG:NH2	3:B:1855:HOH:O	2.42	0.53
1:D:243:ASN:HB2	1:D:244:PRO:HD2	1.90	0.53
1:B:26:GLU:OE1	1:B:26:GLU:N	2.42	0.53
1:B:216:ARG:HD3	1:B:397:GLU:O	2.09	0.52
1:C:98:ARG:NE	3:C:1375:HOH:O	2.43	0.52
1:A:182:HIS:CD2	1:A:345:GLN:HE21	2.26	0.52
1:E:245:TRP:NE1	1:E:293:ILE:HD12	2.23	0.52
1:F:397:GLU:HA	1:F:398:PRO:C	2.28	0.52
1:A:98:ARG:NH2	3:A:1053:HOH:O	2.42	0.52
1:C:222:LYS:HG2	1:C:223:ASP:H	1.74	0.52
1:E:80:ILE:HD12	1:E:146:MET:SD	2.50	0.52
1:F:372:LYS:HA	3:F:2232:HOH:O	2.10	0.52
1:A:1:MET:N	1:A:31:ASP:O	2.42	0.52
1:C:75:GLU:HB2	1:C:149:MET:CE	2.39	0.52
1:D:33:HIS:HE1	1:D:63:LYS:HD2	1.71	0.52
1:D:42:ARG:HG2	1:D:42:ARG:NH2	2.24	0.52
1:E:45:ASN:O	1:E:49:ILE:HG23	2.10	0.52
1:C:181:CYS:SG	1:C:182:HIS:N	2.83	0.52
1:B:6:VAL:HA	1:B:37:MET:HG3	1.92	0.51
1:C:37:MET:HE2	1:C:38:ASP:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:VAL:CG1	1:C:191:PHE:CE2	2.93	0.51
1:F:172:TRP:CZ2	1:F:424:ILE:HG12	2.45	0.51
1:D:30:GLU:HG3	1:D:61:PRO:HB2	1.93	0.51
1:E:344:GLU:HG2	1:E:346:HIS:ND1	2.25	0.51
1:A:193:ARG:HG3	1:A:249:MET:HG3	1.93	0.51
1:B:53:LYS:NZ	1:B:57:GLU:OE2	2.37	0.51
1:C:308:ARG:HH11	1:C:308:ARG:CG	2.23	0.51
1:E:344:GLU:HG2	1:E:346:HIS:CE1	2.46	0.51
1:A:397:GLU:HA	1:A:398:PRO:C	2.31	0.51
1:C:53:LYS:O	1:C:57:GLU:HG3	2.11	0.51
1:C:98:ARG:HD2	1:C:128:TYR:OH	2.10	0.51
1:D:53:LYS:O	1:D:57:GLU:HG3	2.10	0.51
1:A:244:PRO:HB2	1:A:293:ILE:HG12	1.93	0.51
1:F:54:TYR:O	1:F:58:LEU:HD23	2.11	0.51
1:E:442:LYS:HE3	1:F:442:LYS:NZ	2.26	0.50
1:C:400:LEU:HD13	1:C:409:LEU:HD11	1.92	0.50
1:D:133:TYR:HB3	1:D:134:PRO:HD3	1.93	0.50
1:D:310:ARG:NE	3:D:1521:HOH:O	2.39	0.50
1:E:331:LYS:HD2	1:E:332:HIS:NE2	2.27	0.50
1:A:289:ARG:NH2	1:A:289:ARG:CG	2.65	0.50
1:E:29:ARG:NH1	1:E:31:ASP:OD1	2.45	0.50
1:F:181:CYS:C	1:F:182:HIS:ND1	2.65	0.50
1:F:424:ILE:HD11	3:F:520:HOH:O	2.12	0.50
1:D:258:ARG:NH2	3:D:549:HOH:O	2.44	0.50
1:A:310:ARG:HD3	3:A:814:HOH:O	2.11	0.49
1:E:232:ILE:HD13	1:E:258:ARG:NH1	2.27	0.49
1:E:397:GLU:HA	1:E:398:PRO:C	2.32	0.49
1:C:45:ASN:O	1:C:49:ILE:HG23	2.11	0.49
1:C:24:THR:HB	1:C:27:LEU:HB2	1.94	0.49
1:B:378:LEU:HD21	1:B:413:ILE:CD1	2.42	0.49
1:E:326:LEU:HD23	1:E:327:LYS:N	2.27	0.49
1:A:400:LEU:HD13	1:A:409:LEU:HD11	1.95	0.49
1:C:98:ARG:CZ	3:C:558:HOH:O	2.60	0.49
1:D:464:ARG:NH1	1:D:468:GLU:OE2	2.46	0.49
1:E:310:ARG:NH1	1:E:311:GLU:OE1	2.45	0.49
1:E:468:GLU:OE2	3:E:2426:HOH:O	2.18	0.49
1:C:344:GLU:CG	1:C:346:HIS:HD1	2.26	0.49
1:D:144:GLU:OE1	1:D:147:LYS:HE2	2.12	0.49
1:F:335:ILE:C	1:F:337:PRO:HD3	2.33	0.49
1:B:172:TRP:CZ2	1:B:424:ILE:HG12	2.48	0.49
1:F:193:ARG:HE	1:F:193:ARG:HA	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ILE:HD12	1:B:317:ALA:HA	1.94	0.48
1:C:49:ILE:HD11	1:C:317:ALA:O	2.14	0.48
1:C:284:LYS:O	1:C:288:ARG:HA	2.13	0.48
1:B:37:MET:HE2	1:B:38:ASP:N	2.28	0.48
1:B:310:ARG:HD3	3:B:1425:HOH:O	2.13	0.48
1:B:144:GLU:OE1	1:B:147:LYS:HE2	2.13	0.48
1:D:2:LYS:NZ	1:D:75:GLU:O	2.44	0.48
1:D:170:ARG:HD3	1:D:366:GLU:OE2	2.13	0.48
1:C:182:HIS:CD2	1:C:345:GLN:HG3	2.49	0.48
1:E:120:LEU:HD23	1:E:412:ARG:HG2	1.94	0.48
1:C:372:LYS:NZ	1:C:373:ASP:OD2	2.42	0.48
1:D:243:ASN:HB2	1:D:244:PRO:CD	2.44	0.48
1:B:42:ARG:HH21	1:B:45:ASN:ND2	2.12	0.48
1:C:26:GLU:OE1	1:C:26:GLU:N	2.30	0.48
1:F:33:HIS:CD2	1:F:63:LYS:HD2	2.48	0.48
1:B:181:CYS:SG	1:B:182:HIS:N	2.87	0.48
1:C:49:ILE:HD11	1:C:317:ALA:C	2.34	0.48
1:F:464:ARG:NE	3:F:1930:HOH:O	1.95	0.48
1:F:71:ASP:OD2	3:F:2121:HOH:O	2.20	0.47
1:A:141:GLU:OE2	3:A:776:HOH:O	2.20	0.47
1:C:356:ASN:OD1	1:C:388:SER:OG	2.15	0.47
1:A:48:TYR:CE2	1:A:52:ARG:HD2	2.49	0.47
1:A:170:ARG:HD3	1:A:366:GLU:OE2	2.14	0.47
1:D:157:GLN:HB2	1:D:177:ILE:HD11	1.96	0.47
1:A:243:ASN:HB2	1:A:244:PRO:HD2	1.96	0.47
1:C:412:ARG:NE	3:C:1570:HOH:O	2.45	0.47
1:D:137:LYS:O	1:D:141:GLU:HG3	2.14	0.47
1:D:322:GLU:O	1:D:323:ASN:CB	2.62	0.47
1:B:364:ASN:HA	1:B:380:MET:O	2.14	0.47
1:D:40:HIS:CE1	1:D:43:ARG:HG3	2.50	0.47
1:D:53:LYS:NZ	1:D:326:LEU:O	2.47	0.47
1:A:208:VAL:HG11	1:A:412:ARG:HG2	1.96	0.47
1:F:412:ARG:HD2	3:F:553:HOH:O	2.14	0.47
1:E:334:GLU:H	1:E:334:GLU:CD	2.18	0.47
1:D:179:GLY:HA3	1:D:364:ASN:HB2	1.96	0.46
1:D:299:ARG:HB3	1:D:300:PRO:HD3	1.97	0.46
1:F:193:ARG:HG3	1:F:249:MET:HG3	1.97	0.46
1:F:304:GLU:HG3	1:F:308:ARG:HE	1.80	0.46
1:B:177:ILE:C	1:B:178:ILE:HD12	2.35	0.46
1:A:222:LYS:CD	1:A:223:ASP:N	2.73	0.46
1:B:117:SER:O	1:B:440:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LYS:NZ	3:A:1244:HOH:O	2.48	0.46
1:B:88:ASP:OD2	1:B:90:ARG:NH1	2.49	0.46
1:C:299:ARG:HB3	1:C:300:PRO:HD3	1.97	0.46
1:D:344:GLU:HG2	1:D:346:HIS:ND1	2.31	0.46
1:C:209:ASN:O	1:C:412:ARG:NH2	2.48	0.46
1:D:439:PRO:HD2	3:D:532:HOH:O	2.15	0.46
1:F:30:GLU:OE2	1:F:63:LYS:HE3	2.15	0.46
1:F:85:TYR:OH	3:F:559:HOH:O	2.17	0.46
1:B:208:VAL:HG11	1:B:412:ARG:HG2	1.98	0.46
1:A:70:LEU:HD22	1:A:74:ILE:CD1	2.46	0.46
1:C:98:ARG:HD2	1:C:128:TYR:CZ	2.51	0.46
1:D:235:GLU:CD	3:D:2149:HOH:O	2.54	0.46
1:D:329:THR:HB	1:D:338:LYS:HE2	1.98	0.46
1:E:49:ILE:HD11	1:E:317:ALA:C	2.37	0.46
1:E:219:TYR:CE2	1:E:220:ARG:HG3	2.51	0.46
1:B:320:VAL:CG2	1:B:328:ILE:HD11	2.45	0.45
1:C:37:MET:CE	1:C:38:ASP:N	2.79	0.45
1:C:301:LYS:HE2	1:C:301:LYS:HB2	1.78	0.45
1:E:464:ARG:NH2	3:E:2038:HOH:O	2.47	0.45
1:B:157:GLN:HB2	1:B:177:ILE:HD11	1.98	0.45
1:C:405:LYS:HE2	3:C:626:HOH:O	2.16	0.45
1:E:137:LYS:HE2	1:E:141:GLU:OE2	2.17	0.45
1:A:182:HIS:CE1	1:A:345:GLN:N	2.65	0.45
1:D:312:ARG:HA	1:D:315:LYS:HE3	1.97	0.45
1:E:193:ARG:HG3	1:E:249:MET:HG3	1.99	0.45
1:A:104:LYS:HB3	3:A:1043:HOH:O	2.15	0.45
1:D:129:VAL:O	1:D:130:LEU:HB2	2.16	0.45
1:E:293:ILE:HG12	1:E:293:ILE:O	2.16	0.45
1:A:45:ASN:OD1	1:A:66:LYS:NZ	2.50	0.45
1:A:438:ASP:HA	1:A:439:PRO:HD3	1.86	0.45
1:C:141:GLU:HG3	3:C:542:HOH:O	2.16	0.45
1:F:133:TYR:HB3	1:F:134:PRO:HD3	1.97	0.45
1:C:182:HIS:CE1	1:C:344:GLU:HG3	2.52	0.45
1:E:40:HIS:HB2	3:E:1094:HOH:O	2.16	0.45
1:E:125:THR:HG21	3:E:958:HOH:O	2.16	0.45
1:B:318:GLU:O	1:B:322:GLU:HG2	2.17	0.45
1:E:322:GLU:OE2	1:E:322:GLU:N	2.50	0.45
1:F:193:ARG:NH2	1:F:231:TRP:HE1	2.14	0.45
1:C:331:LYS:O	1:C:333:PRO:HD3	2.17	0.44
1:E:439:PRO:HA	1:F:439:PRO:HA	1.99	0.44
1:D:38:ASP:OD1	1:D:39:VAL:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:ARG:O	1:F:55:VAL:HG22	2.17	0.44
1:F:420:LEU:O	1:F:424:ILE:HG13	2.18	0.44
1:B:225:TYR:N	1:B:226:PRO:CD	2.81	0.44
1:C:210:HIS:HB2	1:C:412:ARG:HH22	1.82	0.44
1:B:202:ASP:HB3	1:B:218:ARG:HB2	2.00	0.44
1:C:29:ARG:CA	1:C:61:PRO:HG2	2.47	0.44
1:C:245:TRP:CZ3	3:C:1569:HOH:O	2.68	0.44
1:E:299:ARG:HB3	1:E:300:PRO:HD3	1.98	0.44
1:F:182:HIS:CD2	1:F:344:GLU:HG3	2.52	0.44
1:A:157:GLN:HB2	1:A:177:ILE:HD11	1.99	0.44
1:F:2:LYS:HE3	1:F:35:TYR:CD1	2.53	0.44
1:B:328:ILE:H	1:B:328:ILE:CD1	2.29	0.44
1:C:71:ASP:HB3	1:C:149:MET:HE3	2.00	0.44
1:C:219:TYR:CD2	1:C:220:ARG:HG3	2.53	0.44
1:C:233:GLU:HG2	3:C:1413:HOH:O	2.17	0.44
1:E:216:ARG:HD3	1:E:397:GLU:O	2.18	0.44
1:E:274:TRP:CD1	1:E:439:PRO:HG2	2.53	0.44
1:F:182:HIS:HD2	1:F:344:GLU:HA	1.82	0.44
1:C:11:VAL:O	1:C:15:LEU:HG	2.18	0.43
1:C:15:LEU:O	1:C:19:GLU:HG3	2.18	0.43
1:E:56:GLU:HG3	1:E:57:GLU:N	2.30	0.43
1:C:289:ARG:CD	1:F:462:GLU:HG3	2.48	0.43
1:C:42:ARG:HA	1:C:42:ARG:NE	2.33	0.43
1:C:79:PHE:CE2	1:C:350:ILE:HG23	2.53	0.43
1:D:71:ASP:HB3	1:D:149:MET:HE1	1.99	0.43
1:F:53:LYS:O	1:F:57:GLU:HG3	2.19	0.43
1:A:181:CYS:SG	1:A:182:HIS:N	2.92	0.43
1:C:129:VAL:O	1:C:130:LEU:HB2	2.18	0.43
1:C:243:ASN:HB2	1:C:244:PRO:CD	2.49	0.43
1:F:182:HIS:CE1	1:F:345:GLN:HB2	2.54	0.43
1:F:230:GLU:O	1:F:234:LYS:HE2	2.18	0.43
1:A:187:VAL:HG22	1:A:191:PHE:CZ	2.53	0.43
1:B:356:ASN:OD1	1:B:387:ASP:HB2	2.18	0.43
1:C:289:ARG:HD3	1:F:462:GLU:CD	2.39	0.43
1:A:205:VAL:HG22	1:A:362:PHE:CE2	2.54	0.43
1:B:209:ASN:O	1:B:412:ARG:NH2	2.52	0.43
1:C:347:ILE:N	1:C:348:PRO:CD	2.82	0.43
1:C:442:LYS:NZ	3:C:1851:HOH:O	2.51	0.43
1:C:182:HIS:HE1	1:C:346:HIS:CE1	2.36	0.43
1:F:230:GLU:HG3	1:F:234:LYS:CE	2.48	0.43
1:B:187:VAL:HG22	1:B:191:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:TRP:HB3	1:F:414:LEU:HD11	2.01	0.43
1:A:70:LEU:HD22	1:A:74:ILE:HD11	2.00	0.42
1:A:104:LYS:HG3	3:A:545:HOH:O	2.19	0.42
1:E:109:HIS:CG	1:E:450:VAL:HG22	2.55	0.42
1:A:163:PHE:CE2	1:A:208:VAL:HG22	2.54	0.42
1:A:372:LYS:NZ	1:A:372:LYS:HB3	2.34	0.42
1:A:45:ASN:O	1:A:49:ILE:HG12	2.19	0.42
1:A:222:LYS:CD	1:A:223:ASP:H	2.11	0.42
1:B:299:ARG:HB3	1:B:300:PRO:HD3	2.01	0.42
1:C:49:ILE:CD1	1:C:317:ALA:HB1	2.47	0.42
1:A:143:ALA:O	1:A:147:LYS:HG3	2.19	0.42
1:A:270:ARG:CD	1:A:294:ASP:OD2	2.62	0.42
1:A:433:GLU:O	1:A:437:ARG:HG2	2.20	0.42
1:B:193:ARG:HH12	1:B:239:TRP:HE1	1.65	0.42
1:C:225:TYR:N	1:C:226:PRO:CD	2.83	0.42
1:F:182:HIS:HE2	1:F:344:GLU:HG3	1.83	0.42
1:C:16:GLN:OE1	1:C:342:SER:HB2	2.20	0.42
1:D:326:LEU:C	1:D:327:LYS:HE3	2.40	0.42
1:B:464:ARG:NH1	3:B:2233:HOH:O	2.52	0.42
1:C:140:LEU:HD23	1:C:169:VAL:HG22	2.02	0.42
1:C:193:ARG:CD	3:C:1683:HOH:O	2.55	0.42
1:D:202:ASP:HB3	1:D:218:ARG:HB2	2.02	0.42
1:F:75:GLU:OE1	1:F:149:MET:HG2	2.19	0.42
1:D:293:ILE:HG13	1:D:293:ILE:O	2.20	0.42
1:E:49:ILE:HD11	1:E:317:ALA:CA	2.50	0.42
1:E:125:THR:O	1:E:125:THR:HG23	2.20	0.42
1:F:317:ALA:O	1:F:320:VAL:HG22	2.20	0.42
1:A:216:ARG:HD3	1:A:397:GLU:O	2.20	0.41
1:C:318:GLU:O	1:C:321:GLN:HB3	2.20	0.41
1:E:161:PRO:HG2	1:E:164:GLU:HB2	2.02	0.41
1:F:230:GLU:HG3	1:F:234:LYS:NZ	2.35	0.41
1:A:17:LEU:O	1:A:21:ILE:HG13	2.20	0.41
1:A:364:ASN:HA	1:A:380:MET:O	2.20	0.41
1:C:263:LEU:HD12	1:C:264:PRO:HD2	2.02	0.41
1:D:14:ALA:O	1:D:18:VAL:HG23	2.21	0.41
1:E:170:ARG:HD3	1:E:366:GLU:OE2	2.21	0.41
1:F:326:LEU:HD21	1:F:331:LYS:HD2	2.01	0.41
1:A:323:ASN:C	1:A:325:HIS:H	2.23	0.41
1:B:53:LYS:HG2	1:B:328:ILE:HD13	2.02	0.41
1:C:2:LYS:HD3	1:C:77:ALA:HA	2.03	0.41
1:E:53:LYS:HG3	1:E:328:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:ALA:N	1:F:151:PRO:CD	2.83	0.41
1:A:231:TRP:CE2	1:A:235:GLU:HB2	2.55	0.41
1:C:37:MET:HE2	1:C:38:ASP:H	1.84	0.41
1:C:205:VAL:HG22	1:C:362:PHE:CE2	2.54	0.41
1:D:181:CYS:SG	1:D:182:HIS:N	2.93	0.41
1:D:457:LEU:HA	1:D:458:PRO:HD3	1.91	0.41
1:A:225:TYR:N	1:A:226:PRO:CD	2.84	0.41
1:B:48:TYR:O	1:B:52:ARG:HG3	2.19	0.41
1:B:77:ALA:O	1:B:153:ALA:HB2	2.21	0.41
1:C:26:GLU:H	1:C:26:GLU:CD	2.21	0.41
1:F:15:LEU:O	1:F:19:GLU:HG3	2.21	0.41
1:F:29:ARG:NH2	1:F:31:ASP:OD1	2.38	0.41
1:C:199:GLU:CD	3:C:2175:HOH:O	2.58	0.41
1:E:245:TRP:CZ2	1:E:293:ILE:HD12	2.55	0.41
1:C:75:GLU:HB2	1:C:149:MET:HE2	2.01	0.41
1:A:409:LEU:O	1:A:413:ILE:CD1	2.64	0.41
1:B:21:ILE:HG21	1:B:34:ILE:HD11	2.02	0.41
1:B:57:GLU:OE1	1:B:329:THR:OG1	2.29	0.41
1:C:288:ARG:HB3	1:C:289:ARG:H	1.75	0.41
1:D:109:HIS:HB2	1:D:450:VAL:HG13	2.02	0.41
1:D:111:TYR:HE1	1:D:450:VAL:HG21	1.82	0.41
1:E:12:ARG:HA	1:E:12:ARG:HD2	1.95	0.41
1:E:98:ARG:NH1	3:E:568:HOH:O	2.54	0.41
1:F:457:LEU:HA	1:F:458:PRO:HD3	1.93	0.41
1:B:182:HIS:CE1	1:B:344:GLU:CA	2.95	0.41
1:D:158:THR:HG21	1:D:346:HIS:HE2	1.86	0.41
1:C:133:TYR:HB3	1:C:134:PRO:HD3	2.03	0.40
1:C:344:GLU:HG2	1:C:346:HIS:HD1	1.86	0.40
1:E:371:LEU:HD12	1:E:380:MET:SD	2.61	0.40
1:F:129:VAL:O	1:F:130:LEU:HB2	2.19	0.40
1:F:356:ASN:OD1	1:F:387:ASP:HB2	2.21	0.40
1:F:440:ARG:HB2	3:F:1332:HOH:O	2.21	0.40
1:A:323:ASN:O	1:A:325:HIS:N	2.54	0.40
1:C:245:TRP:HH2	3:C:1569:HOH:O	2.02	0.40
1:D:193:ARG:HG3	1:D:249:MET:HG3	2.02	0.40
1:E:356:ASN:OD1	1:E:387:ASP:HB2	2.21	0.40
1:A:19:GLU:HG2	1:A:54:TYR:CZ	2.56	0.40
1:E:48:TYR:CD1	1:E:66:LYS:HB3	2.56	0.40
1:F:193:ARG:HA	1:F:193:ARG:NE	2.36	0.40
1:C:91:TYR:CE1	1:C:458:PRO:HB2	2.57	0.40
1:E:49:ILE:HD11	1:E:317:ALA:HB1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:ARG:HB3	1:F:300:PRO:HD3	2.02	0.40
1:A:52:ARG:O	1:A:55:VAL:HG22	2.22	0.40
3:A:1917:HOH:O	1:B:439:PRO:HG3	2.22	0.40
1:C:75:GLU:HA	1:C:149:MET:HB3	2.04	0.40
1:C:357:LYS:HA	1:C:357:LYS:HD2	1.89	0.40
1:D:193:ARG:NH2	1:D:239:TRP:CD1	2.90	0.40
1:D:344:GLU:HG2	1:D:346:HIS:CE1	2.56	0.40
1:F:137:LYS:O	1:F:141:GLU:HG3	2.21	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	466/477 (98%)	453 (97%)	11 (2%)	2 (0%)	34	30
1	B	467/477 (98%)	449 (96%)	18 (4%)	0	100	100
1	C	460/477 (96%)	441 (96%)	18 (4%)	1 (0%)	47	44
1	D	466/477 (98%)	452 (97%)	13 (3%)	1 (0%)	47	44
1	E	462/477 (97%)	445 (96%)	17 (4%)	0	100	100
1	F	467/477 (98%)	449 (96%)	17 (4%)	1 (0%)	47	44
All	All	2788/2862 (97%)	2689 (96%)	94 (3%)	5 (0%)	47	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ARG
1	D	323	ASN
1	F	289	ARG
1	C	289	ARG
1	A	324	PRO

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	418/427 (98%)	390 (93%)	28 (7%)	16	11
1	B	419/427 (98%)	397 (95%)	22 (5%)	22	18
1	C	414/427 (97%)	392 (95%)	22 (5%)	22	18
1	D	418/427 (98%)	390 (93%)	28 (7%)	16	11
1	E	416/427 (97%)	387 (93%)	29 (7%)	15	10
1	F	419/427 (98%)	391 (93%)	28 (7%)	16	11
All	All	2504/2562 (98%)	2347 (94%)	157 (6%)	18	13

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	28	SER
1	A	29	ARG
1	A	36	LEU
1	A	37	MET
1	A	41	GLU
1	A	49	ILE
1	A	58	LEU
1	A	59	ASN
1	A	70	LEU
1	A	75	GLU
1	A	85	TYR
1	A	120	LEU
1	A	121	ASN
1	A	148	LYS
1	A	163	PHE
1	A	187	VAL
1	A	189	GLU
1	A	208	VAL
1	A	230	GLU
1	A	236	LEU
1	A	258	ARG

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Mol	Chain	Res	Type
1	A	289	ARG
1	A	293	ILE
1	A	296	GLU
1	A	306	LEU
1	A	326	LEU
1	A	327	LYS
1	B	28	SER
1	B	37	MET
1	B	49	ILE
1	B	70	LEU
1	B	85	TYR
1	B	104	LYS
1	B	120	LEU
1	B	163	PHE
1	B	181	CYS
1	B	187	VAL
1	B	208	VAL
1	B	220	ARG
1	B	236	LEU
1	B	258	ARG
1	B	296	GLU
1	B	315	LYS
1	B	318	GLU
1	B	321	GLN
1	B	338	LYS
1	B	344	GLU
1	B	420	LEU
1	B	440	ARG
1	C	17	LEU
1	C	36	LEU
1	C	37	MET
1	C	49	ILE
1	C	70	LEU
1	C	78	ASP
1	C	85	TYR
1	C	104	LYS
1	C	120	LEU
1	C	121	ASN
1	C	130	LEU
1	C	163	PHE
1	C	181	CYS
1	C	187	VAL

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Mol	Chain	Res	Type
1	C	189	GLU
1	C	236	LEU
1	C	293	ILE
1	C	296	GLU
1	C	306	LEU
1	C	308	ARG
1	C	329	THR
1	C	340	ARG
1	D	41	GLU
1	D	42	ARG
1	D	58	LEU
1	D	70	LEU
1	D	85	TYR
1	D	120	LEU
1	D	121	ASN
1	D	130	LEU
1	D	163	PHE
1	D	170	ARG
1	D	181	CYS
1	D	187	VAL
1	D	199	GLU
1	D	208	VAL
1	D	230	GLU
1	D	233	GLU
1	D	234	LYS
1	D	236	LEU
1	D	258	ARG
1	D	281	GLU
1	D	288	ARG
1	D	296	GLU
1	D	326	LEU
1	D	413	ILE
1	D	420	LEU
1	D	440	ARG
1	D	450	VAL
1	D	461	GLU
1	E	17	LEU
1	E	30	GLU
1	E	36	LEU
1	E	37	MET
1	E	49	ILE
1	E	56	GLU

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Mol	Chain	Res	Type
1	E	58	LEU
1	E	70	LEU
1	E	85	TYR
1	E	102	VAL
1	E	121	ASN
1	E	130	LEU
1	E	163	PHE
1	E	182	HIS
1	E	208	VAL
1	E	220	ARG
1	E	234	LYS
1	E	236	LEU
1	E	258	ARG
1	E	293	ILE
1	E	296	GLU
1	E	306	LEU
1	E	321	GLN
1	E	331	LYS
1	E	334	GLU
1	E	420	LEU
1	E	440	ARG
1	E	464	ARG
1	E	465	ARG
1	F	25	ASP
1	F	37	MET
1	F	41	GLU
1	F	49	ILE
1	F	52	ARG
1	F	53	LYS
1	F	59	ASN
1	F	70	LEU
1	F	71	ASP
1	F	85	TYR
1	F	121	ASN
1	F	130	LEU
1	F	149	MET
1	F	163	PHE
1	F	181	CYS
1	F	208	VAL
1	F	220	ARG
1	F	236	LEU
1	F	258	ARG

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Mol	Chain	Res	Type
1	F	288	ARG
1	F	308	ARG
1	F	321	GLN
1	F	326	LEU
1	F	340	ARG
1	F	344	GLU
1	F	357	LYS
1	F	420	LEU
1	F	440	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	HIS
1	D	33	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 monosaccharides 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	468/477 (98%)	-0.21	1 (0%) 95	94	15, 26, 50, 72	0
1	B	469/477 (98%)	-0.14	5 (1%) 80	79	14, 28, 56, 69	0
1	C	464/477 (97%)	-0.05	4 (0%) 84	83	15, 29, 60, 74	0
1	D	468/477 (98%)	-0.17	5 (1%) 80	79	14, 27, 53, 71	0
1	E	466/477 (97%)	-0.19	2 (0%) 92	92	14, 26, 52, 74	0
1	F	469/477 (98%)	-0.11	8 (1%) 70	68	15, 29, 57, 80	0
All	All	2804/2862 (97%)	-0.14	25 (0%) 84	83	14, 28, 57, 80	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	HIS	5.5
1	B	328	ILE	5.1
1	C	326	LEU	4.9
1	F	182	HIS	4.8
1	D	325	HIS	4.0
1	B	182	HIS	3.4
1	F	289	ARG	3.3
1	F	469	ASN	3.2
1	C	182	HIS	3.0
1	C	340	ARG	2.9
1	F	326	LEU	2.9
1	F	42	ARG	2.8
1	D	58	LEU	2.6
1	D	334	GLU	2.6
1	F	325	HIS	2.5
1	E	182	HIS	2.5
1	D	182	HIS	2.5
1	F	334	GLU	2.4
1	E	322	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	245	TRP	2.3
1	C	15	LEU	2.2
1	B	331	LYS	2.2
1	B	469	ASN	2.2
1	D	340	ARG	2.2
1	F	322	GLU	2.1

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 monosaccharides 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
2	MN	A	601	1/1	0.98	0.04	55,55,55,55	0
2	MN	C	500	1/1	0.98	0.03	51,51,51,51	0
2	MN	D	600	1/1	0.98	0.04	58,58,58,58	0
2	MN	B	602	1/1	0.99	0.03	48,48,48,48	0
2	MN	E	600	1/1	0.99	0.03	51,51,51,51	0
2	MN	F	600	1/1	0.99	0.04	52,52,52,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.