Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 01:30 PM EDT

PDB ID : 3NBB

Title : Crystal structure of mutant Y305F expressed in E. coli in the copper amine oxidase from hansenula polymorpha

Authors : Chen, Z.; Datta, S.; DuBois, J.L.; Klinman, J.P.; Mathews, F.S.

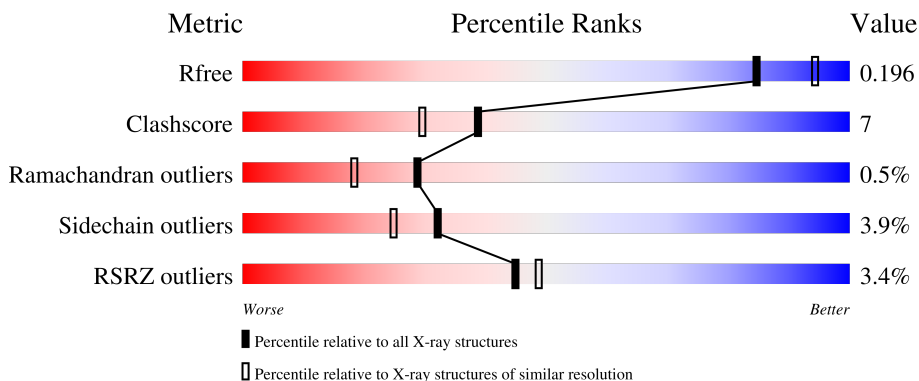Deposited on : 2010-06-03

Resolution : 2.05 Å(reported)

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 2.05 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		0.196
Clashscore		7
Ramachandran outliers		0.5%
Sidechain outliers		3.9%
RSRZ outliers		3.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
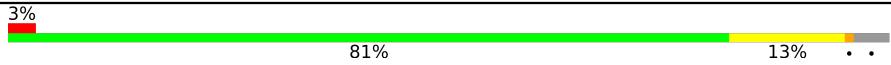
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	694	4% 81% 13% · ·
1	B	694	3% 81% 13% · ·
1	C	694	2% 79% 15% · ·
1	D	694	5% 80% 14% · ·
1	E	694	2% 80% 14% · ·

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Mol	Chain	Length	Quality of chain
1	F	694	3% ... 81% ... 13% ...

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 34758 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 Peroxisomal primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total 5263	C 3345	N 903	O 991	S 24	0	2	0
1	B	661	Total 5263	C 3345	N 903	O 991	S 24	0	2	0
1	C	661	Total 5263	C 3345	N 903	O 991	S 24	0	2	0
1	D	661	Total 5263	C 3345	N 903	O 991	S 24	0	2	0
1	E	661	Total 5263	C 3345	N 903	O 991	S 24	0	2	0
1	F	661	Total 5263	C 3345	N 903	O 991	S 24	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	PHE	TYR	engineered mutation	UNP P12807
B	305	PHE	TYR	engineered mutation	UNP P12807
C	305	PHE	TYR	engineered mutation	UNP P12807
D	305	PHE	TYR	engineered mutation	UNP P12807
E	305	PHE	TYR	engineered mutation	UNP P12807
F	305	PHE	TYR	engineered mutation	UNP P12807

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	531	Total 531	O 531	0	0
3	B	528	Total 528	O 528	0	0
3	C	531	Total 531	O 531	0	0
3	D	528	Total 528	O 528	0	0
3	E	526	Total 526	O 526	0	0
3	F	530	Total 530	O 530	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: Peroxisomal primary amine oxidase
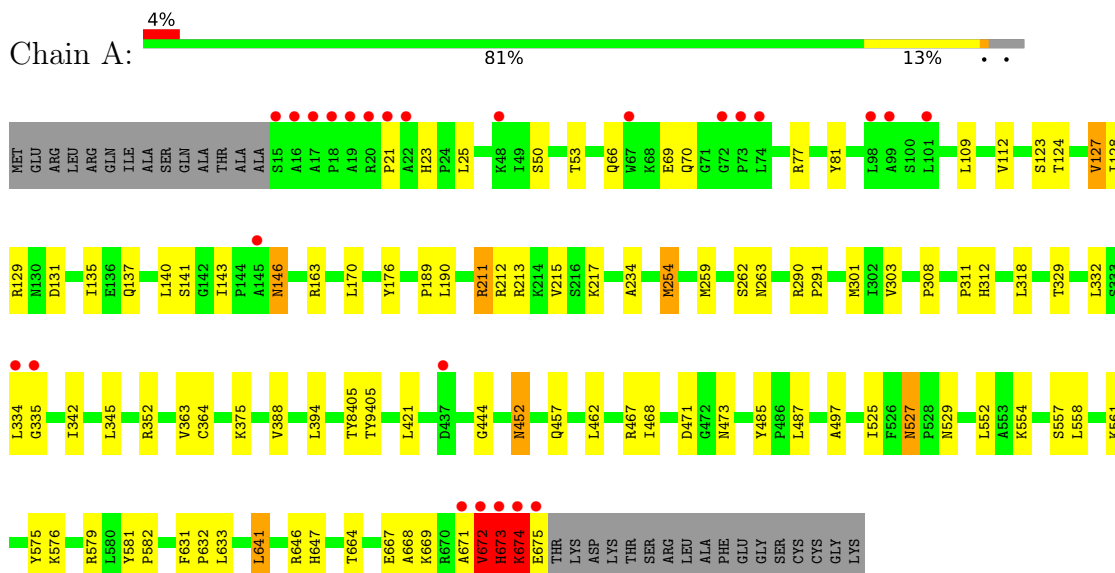
Chain A:

• Molecule 1: Peroxisomal primary amine oxidase

Chain B:

• Molecule 1: Peroxisomal primary amine oxidase

Chain C:

• Molecule 1: Peroxisomal primary amine oxidase

Chain D:
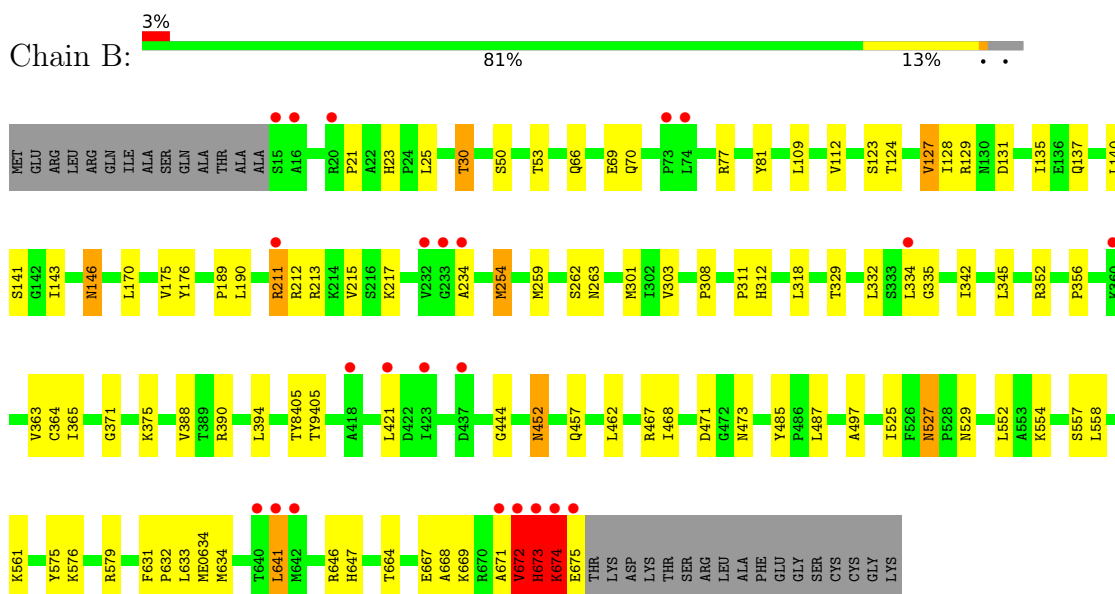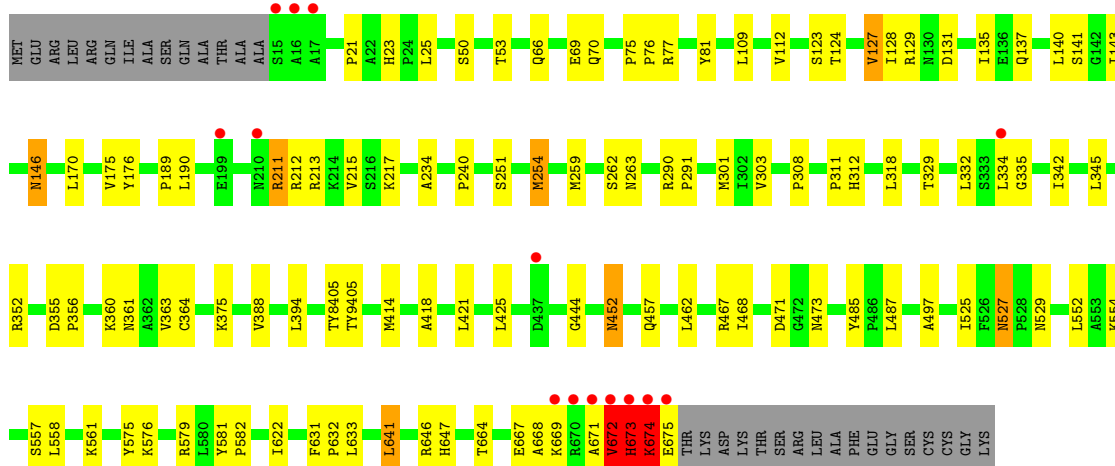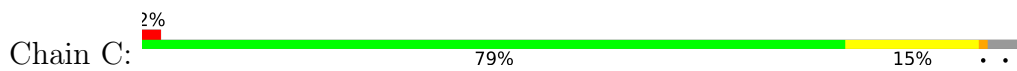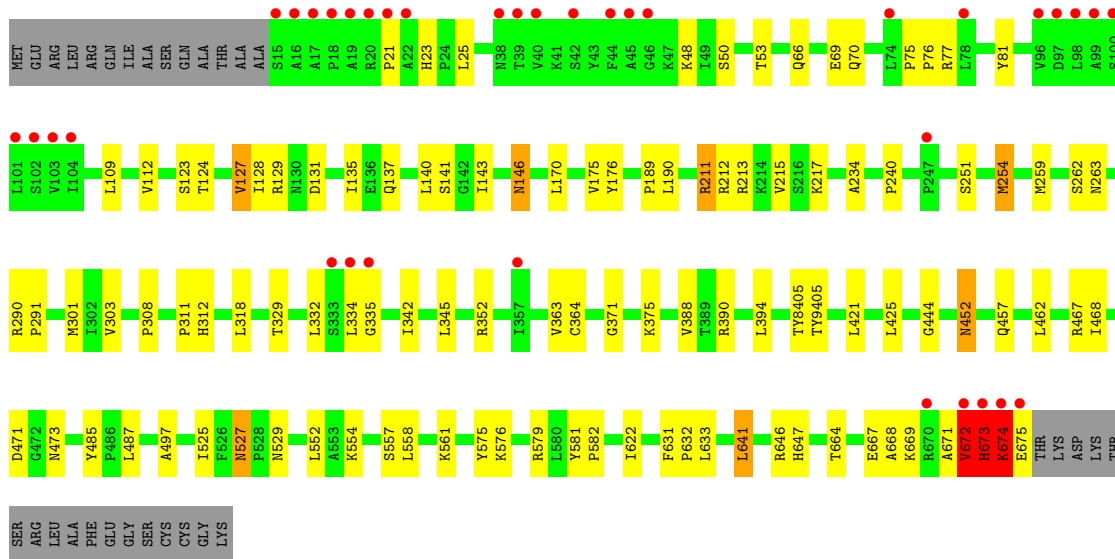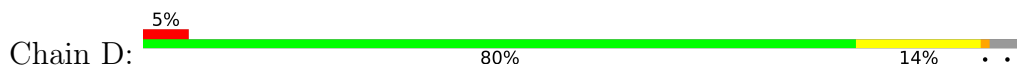
• Molecule 1: Peroxisomal primary amine oxidase

Chain E:

• Molecule 1: Peroxisomal primary amine oxidase

Chain F:
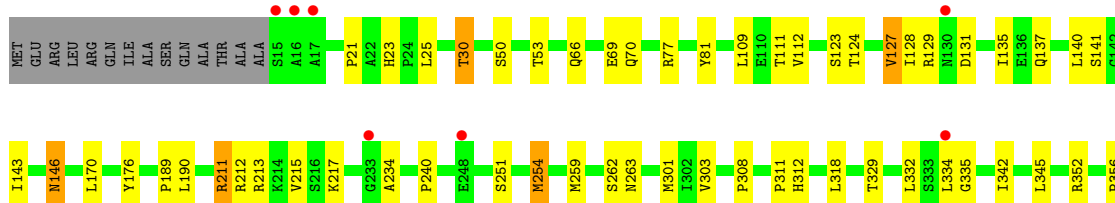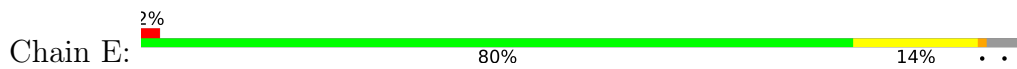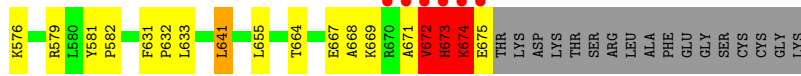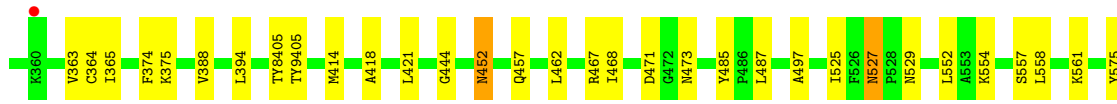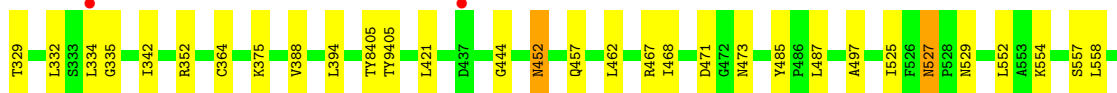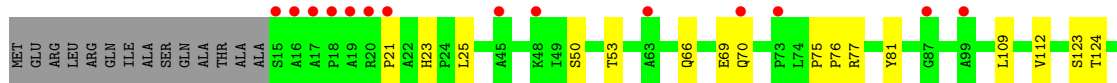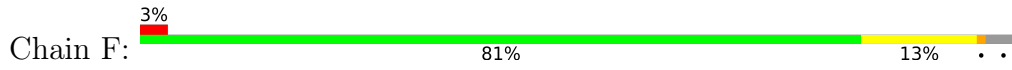
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.52Å　　232.62Å　　104.15Å 90.00°　　91.51°　　90.00°	Depositor
Resolution (Å)	36.13　–　2.05 59.94　–　2.05	Depositor EDS
% Data completeness (in resolution range)	73.3 (36.13-2.05) 73.2 (59.94-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.193　,　0.200 0.190　,　0.196	Depositor DCC
R_{free} test set	10829 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.924	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	34758	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: TY9, CU, ME0, TY8

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	0.35	1/5371 (0.0%)	0.68	2/7307 (0.0%)
1	B	0.35	1/5371 (0.0%)	0.68	2/7307 (0.0%)
1	C	0.35	1/5371 (0.0%)	0.68	2/7307 (0.0%)
1	D	0.35	1/5371 (0.0%)	0.68	2/7307 (0.0%)
1	E	0.35	1/5371 (0.0%)	0.68	2/7307 (0.0%)
1	F	0.35	1/5371 (0.0%)	0.68	2/7307 (0.0%)
All	All	0.35	6/32226 (0.0%)	0.68	12/43842 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	672	VAL	CB-CG1	-6.08	1.40	1.52
1	D	672	VAL	CB-CG1	-6.05	1.40	1.52
1	C	672	VAL	CB-CG1	-6.05	1.40	1.52
1	F	672	VAL	CB-CG1	-6.05	1.40	1.52
1	A	672	VAL	CB-CG1	-6.04	1.40	1.52
1	E	672	VAL	CB-CG1	-6.03	1.40	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	641	LEU	CA-CB-CG	7.54	132.65	115.30
1	D	641	LEU	CA-CB-CG	7.54	132.64	115.30
1	A	641	LEU	CA-CB-CG	7.53	132.62	115.30
1	B	641	LEU	CA-CB-CG	7.53	132.61	115.30
1	E	641	LEU	CA-CB-CG	7.53	132.61	115.30
1	C	641	LEU	CA-CB-CG	7.53	132.61	115.30
1	F	525	ILE	N-CA-C	-5.07	97.32	111.00
1	A	525	ILE	N-CA-C	-5.06	97.33	111.00
1	B	525	ILE	N-CA-C	-5.06	97.34	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	525	ILE	N-CA-C	-5.06	97.35	111.00
1	C	525	ILE	N-CA-C	-5.05	97.36	111.00
1	D	525	ILE	N-CA-C	-5.05	97.37	111.00

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	5263	0	5084	75	0
1	B	5263	0	5084	78	1
1	C	5263	0	5084	82	0
1	D	5263	0	5084	80	0
1	E	5263	0	5084	84	0
1	F	5263	0	5084	82	1
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	531	0	0	2	0
3	B	528	0	0	4	0
3	C	531	0	0	2	0
3	D	528	0	0	2	0
3	E	526	0	0	2	0
3	F	530	0	0	4	0
All	All	34758	0	30504	461	1

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 (461) 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:F:669:LYS:HD3	1:F:675:GLU:OE2	1.26	1.28
1:E:23:HIS:HD2	1:E:25:LEU:H	1.11	0.97
1:F:23:HIS:HD2	1:F:25:LEU:H	1.11	0.95
1:B:23:HIS:HD2	1:B:25:LEU:H	1.11	0.95
1:D:217:LYS:HB2	1:D:217:LYS:NZ	1.82	0.94
1:D:23:HIS:HD2	1:D:25:LEU:H	1.11	0.92
1:A:23:HIS:HD2	1:A:25:LEU:H	1.11	0.91
1:C:23:HIS:HD2	1:C:25:LEU:H	1.11	0.91
1:F:669:LYS:O	1:F:672:VAL:HG12	1.75	0.86
1:B:669:LYS:O	1:B:672:VAL:HG12	1.75	0.86
1:C:669:LYS:O	1:C:672:VAL:HG12	1.75	0.86
1:A:669:LYS:O	1:A:672:VAL:HG12	1.75	0.85
1:E:669:LYS:O	1:E:672:VAL:HG12	1.75	0.85
1:D:669:LYS:O	1:D:672:VAL:HG12	1.75	0.85
1:A:217:LYS:HB2	1:A:217:LYS:NZ	1.92	0.85
1:C:217:LYS:HB2	1:C:217:LYS:NZ	1.92	0.85
1:E:673:HIS:O	1:E:674:LYS:HG2	1.77	0.85
1:F:673:HIS:O	1:F:674:LYS:HG2	1.77	0.85
1:B:673:HIS:O	1:B:674:LYS:HG2	1.77	0.84
1:C:217:LYS:HB2	1:C:217:LYS:HZ2	1.41	0.84
1:E:217:LYS:HB2	1:E:217:LYS:NZ	1.92	0.84
1:C:673:HIS:O	1:C:674:LYS:HG2	1.77	0.84
1:B:217:LYS:HB2	1:B:217:LYS:NZ	1.92	0.84
1:A:673:HIS:O	1:A:674:LYS:HG2	1.77	0.83
1:E:30:THR:HG22	1:E:356:PRO:HB3	1.59	0.83
1:F:217:LYS:NZ	1:F:217:LYS:HB2	1.92	0.83
1:F:669:LYS:CD	1:F:675:GLU:OE2	2.21	0.82
1:D:217:LYS:HB2	1:D:217:LYS:HZ2	1.43	0.81
1:A:137:GLN:OE1	1:A:212:ARG:NH2	2.14	0.79
1:F:137:GLN:OE1	1:F:212:ARG:NH2	2.14	0.78
1:B:137:GLN:OE1	1:B:212:ARG:NH2	2.14	0.77
1:E:137:GLN:OE1	1:E:212:ARG:NH2	2.14	0.76
1:A:468:ILE:H	1:A:473:ASN:HD21	1.36	0.74
1:C:468:ILE:H	1:C:473:ASN:HD21	1.36	0.73
1:E:468:ILE:H	1:E:473:ASN:HD21	1.36	0.73
1:C:137:GLN:OE1	1:C:212:ARG:NH2	2.14	0.73
1:D:527:ASN:HD22	1:D:529:ASN:H	1.37	0.73
1:B:527:ASN:HD22	1:B:529:ASN:H	1.37	0.73
1:A:527:ASN:HD22	1:A:529:ASN:H	1.37	0.73
1:F:527:ASN:HD22	1:F:529:ASN:H	1.37	0.73
1:F:468:ILE:H	1:F:473:ASN:HD21	1.36	0.73
1:E:527:ASN:HD22	1:E:529:ASN:H	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:ASN:HD22	1:C:529:ASN:H	1.37	0.72
1:D:468:ILE:H	1:D:473:ASN:HD21	1.36	0.72
1:B:468:ILE:H	1:B:473:ASN:HD21	1.36	0.72
1:D:137:GLN:OE1	1:D:212:ARG:NH2	2.14	0.72
1:E:30:THR:HG22	1:E:356:PRO:CB	2.20	0.71
1:B:217:LYS:HB2	1:B:217:LYS:HZ3	1.54	0.71
1:D:673:HIS:O	1:D:674:LYS:HE2	1.91	0.69
1:E:217:LYS:HB2	1:E:217:LYS:HZ3	1.57	0.69
1:F:217:LYS:HB2	1:F:217:LYS:HZ2	1.55	0.67
1:B:30:THR:HG23	3:B:1536:HOH:O	1.94	0.67
1:C:21:PRO:HG3	1:C:77:ARG:CZ	2.25	0.67
1:B:217:LYS:HZ3	1:B:217:LYS:CB	2.08	0.66
1:E:124:THR:O	1:E:127:VAL:HG13	1.96	0.66
1:A:21:PRO:HG3	1:A:77:ARG:CZ	2.25	0.66
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.25	0.66
1:F:124:THR:O	1:F:127:VAL:HG13	1.96	0.66
1:E:21:PRO:HG3	1:E:77:ARG:CZ	2.25	0.66
1:F:21:PRO:HG3	1:F:77:ARG:CZ	2.25	0.66
1:D:124:THR:O	1:D:127:VAL:HG13	1.96	0.66
1:D:21:PRO:HG3	1:D:77:ARG:CZ	2.25	0.65
1:A:124:THR:O	1:A:127:VAL:HG13	1.96	0.65
1:C:124:THR:O	1:C:127:VAL:HG13	1.96	0.65
1:B:124:THR:O	1:B:127:VAL:HG13	1.96	0.65
1:A:217:LYS:HB2	1:A:217:LYS:HZ3	1.62	0.64
1:E:217:LYS:NZ	1:E:217:LYS:CB	2.60	0.64
1:A:575:TYR:O	1:A:576:LYS:HD2	1.99	0.63
1:E:217:LYS:HZ3	1:E:217:LYS:CB	2.11	0.63
1:A:217:LYS:NZ	1:A:217:LYS:CB	2.60	0.63
1:B:575:TYR:O	1:B:576:LYS:HD2	1.99	0.63
1:C:527:ASN:HD21	1:C:529:ASN:HB2	1.64	0.63
1:F:575:TYR:O	1:F:576:LYS:HD2	1.99	0.62
1:B:527:ASN:HD21	1:B:529:ASN:HB2	1.64	0.62
1:C:575:TYR:O	1:C:576:LYS:HD2	1.99	0.62
1:F:217:LYS:NZ	1:F:217:LYS:CB	2.60	0.62
1:D:575:TYR:O	1:D:576:LYS:HD2	1.99	0.62
1:E:575:TYR:O	1:E:576:LYS:HD2	1.99	0.62
1:A:217:LYS:HB2	1:A:217:LYS:HZ2	1.63	0.62
1:F:527:ASN:HD21	1:F:529:ASN:HB2	1.64	0.62
1:A:527:ASN:HD21	1:A:529:ASN:HB2	1.64	0.61
1:D:217:LYS:NZ	1:D:217:LYS:CB	2.60	0.61
1:F:334:LEU:HD13	1:F:335:GLY:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:PRO:HB3	1:B:497:ALA:HB2	1.81	0.61
1:A:334:LEU:HD13	1:A:335:GLY:N	2.16	0.61
1:D:527:ASN:HD21	1:D:529:ASN:HB2	1.64	0.61
1:D:334:LEU:HD13	1:D:335:GLY:N	2.16	0.61
1:E:527:ASN:HD21	1:E:529:ASN:HB2	1.64	0.60
1:D:217:LYS:HB2	1:D:217:LYS:HZ3	1.64	0.60
1:A:234:ALA:HB1	3:A:1174:HOH:O	2.01	0.60
1:A:254:MET:HE3	1:A:259:MET:HA	1.83	0.60
1:E:334:LEU:HD13	1:E:335:GLY:N	2.16	0.60
1:F:234:ALA:HB1	3:F:1174:HOH:O	2.01	0.60
1:B:234:ALA:HB1	3:B:1174:HOH:O	2.01	0.60
1:C:217:LYS:NZ	1:C:217:LYS:CB	2.60	0.60
1:D:254:MET:HE3	1:D:259:MET:HA	1.83	0.60
1:E:234:ALA:HB1	3:E:1174:HOH:O	2.01	0.60
1:B:334:LEU:HD13	1:B:335:GLY:N	2.16	0.60
1:F:254:MET:HE3	1:F:259:MET:HA	1.83	0.60
1:B:254:MET:HE3	1:B:259:MET:HA	1.84	0.59
1:E:254:MET:HE3	1:E:259:MET:HA	1.84	0.59
1:F:23:HIS:CD2	1:F:25:LEU:H	2.04	0.59
1:F:527:ASN:ND2	1:F:529:ASN:H	2.01	0.59
1:B:527:ASN:ND2	1:B:529:ASN:H	2.01	0.59
1:C:334:LEU:HD13	1:C:335:GLY:N	2.16	0.59
1:D:234:ALA:HB1	3:D:1174:HOH:O	2.01	0.59
1:A:497:ALA:HB2	1:B:308:PRO:HB3	1.85	0.59
1:C:527:ASN:ND2	1:C:529:ASN:H	2.01	0.59
1:C:23:HIS:CD2	1:C:25:LEU:H	2.04	0.59
1:C:234:ALA:HB1	3:C:1174:HOH:O	2.01	0.58
1:B:190:LEU:CD2	1:B:215:VAL:HG22	2.34	0.58
1:E:527:ASN:ND2	1:E:529:ASN:H	2.00	0.58
1:C:124:THR:HA	1:C:127:VAL:CG1	2.34	0.58
1:C:190:LEU:CD2	1:C:215:VAL:HG22	2.34	0.58
1:E:124:THR:HA	1:E:127:VAL:CG1	2.34	0.58
1:F:190:LEU:CD2	1:F:215:VAL:HG22	2.34	0.58
1:B:124:THR:HA	1:B:127:VAL:CG1	2.34	0.57
1:D:124:THR:HA	1:D:127:VAL:CG1	2.34	0.57
1:A:375:LYS:HG3	1:A:388:VAL:HG22	1.86	0.57
1:D:631:PHE:CG	1:D:632:PRO:HA	2.39	0.57
1:F:124:THR:HA	1:F:127:VAL:CG1	2.34	0.57
1:A:190:LEU:CD2	1:A:215:VAL:HG22	2.34	0.57
1:C:254:MET:HE3	1:C:259:MET:HA	1.84	0.57
1:A:527:ASN:ND2	1:A:529:ASN:H	2.00	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:LEU:CD2	1:E:215:VAL:HG22	2.34	0.57
1:E:375:LYS:HG3	1:E:388:VAL:HG22	1.87	0.57
1:F:245:THR:HA	3:F:1508:HOH:O	2.04	0.57
1:C:631:PHE:CG	1:C:632:PRO:HA	2.40	0.57
1:A:217:LYS:HZ3	1:A:217:LYS:CB	2.15	0.57
1:C:375:LYS:HG3	1:C:388:VAL:HG22	1.87	0.57
1:D:375:LYS:HG3	1:D:388:VAL:HG22	1.87	0.57
1:E:217:LYS:HB2	1:E:217:LYS:HZ2	1.67	0.57
1:D:190:LEU:HD22	1:D:215:VAL:HG22	1.87	0.57
1:D:664:THR:OG1	1:D:667:GLU:HG3	2.05	0.57
1:E:631:PHE:CG	1:E:632:PRO:HA	2.39	0.57
1:A:124:THR:HA	1:A:127:VAL:CG1	2.34	0.57
1:D:190:LEU:CD2	1:D:215:VAL:HG22	2.34	0.57
1:F:631:PHE:CG	1:F:632:PRO:HA	2.40	0.57
1:B:217:LYS:NZ	1:B:217:LYS:CB	2.60	0.56
1:D:527:ASN:HD22	1:D:527:ASN:C	2.09	0.56
1:A:190:LEU:HD22	1:A:215:VAL:HG22	1.87	0.56
1:A:631:PHE:CG	1:A:632:PRO:HA	2.40	0.56
1:D:527:ASN:ND2	1:D:529:ASN:H	2.00	0.56
1:E:23:HIS:CD2	1:E:25:LEU:H	2.04	0.56
1:F:190:LEU:HD22	1:F:215:VAL:HG22	1.87	0.56
1:F:375:LYS:HG3	1:F:388:VAL:HG22	1.86	0.56
1:B:190:LEU:HD22	1:B:215:VAL:HG22	1.87	0.56
1:B:631:PHE:CG	1:B:632:PRO:HA	2.40	0.56
1:B:664:THR:OG1	1:B:667:GLU:HG3	2.05	0.56
1:E:497:ALA:HB2	1:F:308:PRO:HB3	1.88	0.56
1:C:527:ASN:HD22	1:C:527:ASN:C	2.09	0.56
1:C:123:SER:O	1:C:127:VAL:HG12	2.06	0.56
1:D:673:HIS:O	1:D:674:LYS:CE	2.53	0.56
1:E:123:SER:O	1:E:127:VAL:HG12	2.06	0.56
1:E:190:LEU:HD22	1:E:215:VAL:HG22	1.87	0.56
1:A:664:THR:OG1	1:A:667:GLU:HG3	2.05	0.56
1:B:375:LYS:HG3	1:B:388:VAL:HG22	1.86	0.56
1:F:527:ASN:HD22	1:F:527:ASN:C	2.09	0.56
1:B:217:LYS:HB2	1:B:217:LYS:HZ2	1.70	0.56
1:F:217:LYS:HB2	1:F:217:LYS:HZ3	1.69	0.56
1:C:190:LEU:HD22	1:C:215:VAL:HG22	1.87	0.56
1:C:664:THR:OG1	1:C:667:GLU:HG3	2.05	0.56
1:F:123:SER:O	1:F:127:VAL:HG12	2.06	0.55
1:F:664:THR:OG1	1:F:667:GLU:HG3	2.05	0.55
1:A:123:SER:O	1:A:127:VAL:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:ASN:HD22	1:E:527:ASN:C	2.09	0.55
1:E:664:THR:OG1	1:E:667:GLU:HG3	2.05	0.55
1:A:23:HIS:CD2	1:A:25:LEU:H	2.04	0.55
1:A:211:ARG:HD3	1:A:213:ARG:HD2	1.89	0.55
1:B:176:TYR:CE1	1:B:189:PRO:HB3	2.42	0.55
1:A:527:ASN:HD22	1:A:527:ASN:C	2.09	0.55
1:B:123:SER:O	1:B:127:VAL:HG12	2.06	0.55
1:C:211:ARG:HD3	1:C:213:ARG:HD2	1.89	0.55
1:E:176:TYR:CE1	1:E:189:PRO:HB3	2.42	0.55
1:D:123:SER:O	1:D:127:VAL:HG12	2.06	0.55
1:E:211:ARG:HD3	1:E:213:ARG:HD2	1.89	0.55
1:D:176:TYR:CE1	1:D:189:PRO:HB3	2.42	0.55
1:C:176:TYR:CE1	1:C:189:PRO:HB3	2.42	0.54
1:F:50:SER:HB2	1:F:352:ARG:HG3	1.90	0.54
1:B:527:ASN:HD22	1:B:527:ASN:C	2.09	0.54
1:D:50:SER:HB2	1:D:352:ARG:HG3	1.90	0.54
1:C:468:ILE:N	1:C:473:ASN:HD21	2.06	0.54
1:C:50:SER:HB2	1:C:352:ARG:HG3	1.90	0.54
1:B:50:SER:HB2	1:B:352:ARG:HG3	1.90	0.54
1:D:211:ARG:HD3	1:D:213:ARG:HD2	1.89	0.54
1:B:23:HIS:CD2	1:B:25:LEU:H	2.04	0.53
1:E:69:GLU:CD	1:E:467:ARG:HH22	2.11	0.53
1:F:69:GLU:CD	1:F:467:ARG:HH22	2.11	0.53
1:B:211:ARG:HD3	1:B:213:ARG:HD2	1.89	0.53
1:B:557:SER:O	1:B:561:LYS:HG3	2.09	0.53
1:C:69:GLU:CD	1:C:467:ARG:HH22	2.11	0.53
1:E:308:PRO:HB3	1:F:497:ALA:HB2	1.89	0.53
1:E:557:SER:O	1:E:561:LYS:HG3	2.09	0.53
1:B:468:ILE:N	1:B:473:ASN:HD21	2.06	0.53
1:C:631:PHE:CD1	1:C:632:PRO:HA	2.44	0.53
1:D:23:HIS:CD2	1:D:25:LEU:H	2.04	0.53
1:F:211:ARG:HD3	1:F:213:ARG:HD2	1.89	0.53
1:A:176:TYR:CE1	1:A:189:PRO:HB3	2.42	0.53
1:B:457:GLN:HE22	1:B:552:LEU:H	1.57	0.53
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.44	0.53
1:E:631:PHE:CD1	1:E:632:PRO:HA	2.44	0.53
1:F:176:TYR:CE1	1:F:189:PRO:HB3	2.42	0.53
1:A:50:SER:HB2	1:A:352:ARG:HG3	1.90	0.53
1:A:69:GLU:CD	1:A:467:ARG:HH22	2.11	0.53
1:F:457:GLN:HE22	1:F:552:LEU:H	1.57	0.53
1:F:557:SER:O	1:F:561:LYS:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:HG21	1:A:364:CYS:HB2	1.91	0.53
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.44	0.53
1:B:69:GLU:CD	1:B:467:ARG:HH22	2.11	0.53
1:A:557:SER:O	1:A:561:LYS:HG3	2.09	0.53
1:C:308:PRO:HB3	1:D:497:ALA:HB2	1.91	0.53
1:D:457:GLN:HE22	1:D:552:LEU:H	1.57	0.53
1:C:457:GLN:HE22	1:C:552:LEU:H	1.57	0.52
1:D:557:SER:O	1:D:561:LYS:HG3	2.09	0.52
1:E:342:ILE:HG21	1:E:364:CYS:HB2	1.91	0.52
1:F:468:ILE:N	1:F:473:ASN:HD21	2.06	0.52
1:D:69:GLU:CD	1:D:467:ARG:HH22	2.11	0.52
1:E:457:GLN:HE22	1:E:552:LEU:H	1.57	0.52
1:A:457:GLN:HE22	1:A:552:LEU:H	1.57	0.52
1:F:631:PHE:CD1	1:F:632:PRO:HA	2.44	0.52
1:E:50:SER:HB2	1:E:352:ARG:HG3	1.90	0.52
1:C:557:SER:O	1:C:561:LYS:HG3	2.09	0.52
1:C:497:ALA:HB2	1:D:308:PRO:HB3	1.92	0.52
1:F:217:LYS:CB	1:F:217:LYS:HZ3	2.22	0.52
1:D:631:PHE:CD1	1:D:632:PRO:HA	2.44	0.52
1:B:342:ILE:HG21	1:B:364:CYS:HB2	1.91	0.51
1:C:342:ILE:HG21	1:C:364:CYS:HB2	1.91	0.51
1:F:342:ILE:HG21	1:F:364:CYS:HB2	1.91	0.51
1:B:672:VAL:HG13	1:B:673:HIS:N	2.26	0.51
1:A:672:VAL:HG13	1:A:673:HIS:N	2.26	0.51
1:C:672:VAL:HG13	1:C:673:HIS:N	2.26	0.51
1:E:672:VAL:HG13	1:E:673:HIS:N	2.25	0.51
1:D:342:ILE:HG21	1:D:364:CYS:HB2	1.91	0.51
1:F:468:ILE:H	1:F:473:ASN:ND2	2.08	0.50
1:F:672:VAL:HG13	1:F:673:HIS:N	2.26	0.50
1:D:50:SER:HB2	1:D:352:ARG:CG	2.42	0.50
1:B:468:ILE:H	1:B:473:ASN:ND2	2.08	0.50
1:D:672:VAL:HG13	1:D:673:HIS:N	2.26	0.50
1:E:301:MET:O	1:E:318:LEU:HA	2.12	0.50
1:B:50:SER:HB2	1:B:352:ARG:CG	2.42	0.50
1:D:301:MET:O	1:D:318:LEU:HA	2.12	0.50
1:C:301:MET:O	1:C:318:LEU:HA	2.12	0.49
1:A:50:SER:HB2	1:A:352:ARG:CG	2.42	0.49
1:C:50:SER:HB2	1:C:352:ARG:CG	2.42	0.49
1:A:301:MET:O	1:A:318:LEU:HA	2.12	0.49
1:A:468:ILE:N	1:A:473:ASN:HD21	2.06	0.49
1:B:576:LYS:HB2	1:B:579:ARG:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:SER:HB2	1:F:352:ARG:CG	2.42	0.49
1:C:468:ILE:H	1:C:473:ASN:ND2	2.08	0.49
1:C:668:ALA:O	1:C:672:VAL:HB	2.13	0.49
1:E:50:SER:HB2	1:E:352:ARG:CG	2.42	0.49
1:D:468:ILE:N	1:D:473:ASN:HD21	2.06	0.48
1:E:576:LYS:HB2	1:E:579:ARG:HD2	1.95	0.48
1:F:301:MET:O	1:F:318:LEU:HA	2.12	0.48
1:E:668:ALA:O	1:E:672:VAL:HB	2.13	0.48
1:A:141:SER:O	1:A:215:VAL:HG23	2.14	0.48
1:A:576:LYS:HB2	1:A:579:ARG:HD2	1.95	0.48
1:E:468:ILE:N	1:E:473:ASN:HD21	2.06	0.48
1:A:668:ALA:O	1:A:672:VAL:HB	2.13	0.48
1:D:468:ILE:H	1:D:473:ASN:ND2	2.08	0.48
1:D:668:ALA:O	1:D:672:VAL:HB	2.14	0.48
1:B:301:MET:O	1:B:318:LEU:HA	2.12	0.48
1:C:576:LYS:HB2	1:C:579:ARG:HD2	1.95	0.48
1:C:141:SER:O	1:C:215:VAL:HG23	2.14	0.48
1:F:668:ALA:O	1:F:672:VAL:HB	2.13	0.48
1:E:128:ILE:HG13	1:E:129:ARG:N	2.29	0.48
1:E:581:TYR:HA	1:E:582:PRO:HD2	1.78	0.48
1:F:245:THR:CA	3:F:1508:HOH:O	2.61	0.48
1:A:554:LYS:HE2	1:B:485:TYR:O	2.14	0.48
1:C:554:LYS:HE2	1:D:485:TYR:O	2.14	0.48
1:F:128:ILE:HG13	1:F:129:ARG:N	2.29	0.48
1:D:576:LYS:HB2	1:D:579:ARG:HD2	1.95	0.47
1:A:128:ILE:HG13	1:A:129:ARG:N	2.29	0.47
1:B:141:SER:O	1:B:215:VAL:HG23	2.14	0.47
1:C:128:ILE:HG13	1:C:129:ARG:N	2.29	0.47
1:C:669:LYS:HB3	1:C:675:GLU:HG2	1.96	0.47
1:F:576:LYS:HB2	1:F:579:ARG:HD2	1.95	0.47
1:B:668:ALA:O	1:B:672:VAL:HB	2.14	0.47
1:F:141:SER:O	1:F:215:VAL:HG23	2.14	0.47
1:D:141:SER:O	1:D:215:VAL:HG23	2.14	0.47
1:D:254:MET:HE3	1:D:259:MET:CA	2.44	0.47
1:E:669:LYS:HB3	1:E:675:GLU:HG2	1.96	0.47
1:F:669:LYS:HB3	1:F:675:GLU:HG2	1.97	0.47
1:A:143:ILE:HG13	1:A:215:VAL:HG21	1.97	0.47
1:D:342:ILE:CG2	1:D:364:CYS:HB2	2.45	0.47
1:B:143:ILE:HG13	1:B:215:VAL:HG21	1.97	0.47
1:B:342:ILE:CG2	1:B:364:CYS:HB2	2.45	0.47
1:E:143:ILE:HG13	1:E:215:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:669:LYS:O	1:E:672:VAL:CG1	2.57	0.47
1:F:143:ILE:HG13	1:F:215:VAL:HG21	1.97	0.47
1:E:141:SER:O	1:E:215:VAL:HG23	2.14	0.46
1:D:128:ILE:HG13	1:D:129:ARG:N	2.29	0.46
1:D:669:LYS:HB3	1:D:675:GLU:HG2	1.96	0.46
1:A:669:LYS:HB3	1:A:675:GLU:HG2	1.96	0.46
1:B:669:LYS:HB3	1:B:675:GLU:HG2	1.96	0.46
1:B:128:ILE:HG13	1:B:129:ARG:N	2.29	0.46
1:B:254:MET:HE1	1:B:259:MET:HB2	1.98	0.46
1:C:69:GLU:OE2	1:C:467:ARG:NH2	2.49	0.46
1:E:468:ILE:H	1:E:473:ASN:ND2	2.08	0.46
1:C:254:MET:HE1	1:C:259:MET:HB2	1.96	0.46
1:C:342:ILE:CG2	1:C:364:CYS:HB2	2.45	0.46
1:E:69:GLU:OE2	1:E:467:ARG:NH2	2.49	0.46
1:B:69:GLU:OE2	1:B:467:ARG:NH2	2.49	0.46
1:C:360:LYS:HE2	1:C:361:ASN:OD1	2.15	0.46
1:E:254:MET:HE1	1:E:259:MET:HB2	1.96	0.46
1:A:69:GLU:OE2	1:A:467:ARG:NH2	2.49	0.46
1:B:30:THR:CG2	3:B:1536:HOH:O	2.58	0.46
1:C:262:SER:O	1:C:263:ASN:HB2	2.16	0.46
1:B:444:GLY:HA3	1:B:452:ASN:HD21	1.81	0.46
1:D:262:SER:O	1:D:263:ASN:HB2	2.16	0.46
1:E:240:PRO:HD2	1:F:251:SER:HB3	1.97	0.46
1:E:655:LEU:HD11	1:F:632:PRO:HD2	1.98	0.46
1:A:342:ILE:CG2	1:A:364:CYS:HB2	2.45	0.46
1:E:342:ILE:CG2	1:E:364:CYS:HB2	2.45	0.46
1:F:69:GLU:OE2	1:F:467:ARG:NH2	2.49	0.45
1:C:143:ILE:HG13	1:C:215:VAL:HG21	1.97	0.45
1:E:554:LYS:HE2	1:F:485:TYR:O	2.17	0.45
1:F:262:SER:O	1:F:263:ASN:HB2	2.16	0.45
1:F:444:GLY:HA3	1:F:452:ASN:HD21	1.82	0.45
1:A:66:GLN:HG2	1:A:70:GLN:NE2	2.32	0.45
1:E:66:GLN:HG2	1:E:70:GLN:NE2	2.32	0.45
1:F:342:ILE:CG2	1:F:364:CYS:HB2	2.45	0.45
1:C:240:PRO:HD2	1:D:251:SER:HB3	1.97	0.45
1:D:143:ILE:HG13	1:D:215:VAL:HG21	1.97	0.45
1:A:467:ARG:HD2	1:A:471:ASP:OD1	2.17	0.45
1:B:262:SER:O	1:B:263:ASN:HB2	2.16	0.45
1:B:467:ARG:HD2	1:B:471:ASP:OD1	2.17	0.45
1:B:669:LYS:O	1:B:672:VAL:CG1	2.57	0.45
1:D:467:ARG:HD2	1:D:471:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:467:ARG:HD2	1:F:471:ASP:OD1	2.17	0.45
1:C:467:ARG:HD2	1:C:471:ASP:OD1	2.17	0.45
1:B:66:GLN:HG2	1:B:70:GLN:NE2	2.32	0.45
1:E:262:SER:O	1:E:263:ASN:HB2	2.16	0.45
1:F:303:VAL:HA	1:F:457:GLN:O	2.17	0.45
1:A:581:TYR:HA	1:A:582:PRO:HD2	1.78	0.45
1:D:66:GLN:HG2	1:D:70:GLN:NE2	2.32	0.45
1:F:671:ALA:O	1:F:672:VAL:C	2.56	0.45
1:A:262:SER:O	1:A:263:ASN:HB2	2.16	0.45
1:D:69:GLU:OE2	1:D:467:ARG:NH2	2.49	0.45
1:D:444:GLY:HA3	1:D:452:ASN:HD21	1.81	0.45
1:E:671:ALA:O	1:E:672:VAL:C	2.56	0.45
1:D:303:VAL:HA	1:D:457:GLN:O	2.17	0.45
1:C:444:GLY:HA3	1:C:452:ASN:HD21	1.82	0.44
1:D:671:ALA:O	1:D:672:VAL:C	2.56	0.44
1:A:312:HIS:HD2	3:A:1323:HOH:O	2.01	0.44
1:A:669:LYS:O	1:A:672:VAL:CG1	2.57	0.44
1:A:468:ILE:H	1:A:473:ASN:ND2	2.08	0.44
1:B:303:VAL:HA	1:B:457:GLN:O	2.17	0.44
1:C:66:GLN:HG2	1:C:70:GLN:NE2	2.31	0.44
1:C:303:VAL:HA	1:C:457:GLN:O	2.17	0.44
1:A:303:VAL:HA	1:A:457:GLN:O	2.17	0.44
1:A:444:GLY:HA3	1:A:452:ASN:HD21	1.82	0.44
1:C:131:ASP:O	1:C:135:ILE:HG13	2.18	0.44
1:D:131:ASP:O	1:D:135:ILE:HG13	2.18	0.44
1:F:669:LYS:C	1:F:672:VAL:HG12	2.38	0.44
1:C:669:LYS:C	1:C:672:VAL:HG12	2.38	0.44
1:F:66:GLN:HG2	1:F:70:GLN:NE2	2.32	0.44
1:E:485:TYR:O	1:F:554:LYS:HE2	2.17	0.44
1:F:131:ASP:O	1:F:135:ILE:HG13	2.18	0.44
1:F:312:HIS:HD2	3:F:1323:HOH:O	2.01	0.44
1:A:131:ASP:O	1:A:135:ILE:HG13	2.18	0.44
1:C:671:ALA:O	1:C:672:VAL:C	2.56	0.44
1:E:312:HIS:HD2	3:E:1323:HOH:O	2.01	0.44
1:A:671:ALA:O	1:A:672:VAL:C	2.56	0.44
1:D:53:THR:O	1:D:81:TYR:HA	2.18	0.44
1:D:312:HIS:HD2	3:D:1323:HOH:O	2.01	0.44
1:E:53:THR:O	1:E:81:TYR:HA	2.18	0.44
1:E:444:GLY:HA3	1:E:452:ASN:HD21	1.82	0.44
1:E:467:ARG:HD2	1:E:471:ASP:OD1	2.17	0.44
1:F:669:LYS:O	1:F:672:VAL:CG1	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:MET:HE3	1:A:259:MET:CA	2.46	0.43
1:E:303:VAL:HA	1:E:457:GLN:O	2.17	0.43
1:B:671:ALA:O	1:B:672:VAL:C	2.56	0.43
1:B:669:LYS:C	1:B:672:VAL:HG12	2.38	0.43
1:D:527:ASN:HD21	1:D:529:ASN:HD22	1.67	0.43
1:F:527:ASN:HD21	1:F:529:ASN:HD22	1.67	0.43
1:B:312:HIS:HD2	3:B:1323:HOH:O	2.01	0.43
1:C:254:MET:HE3	1:C:259:MET:CA	2.48	0.43
1:C:527:ASN:HD21	1:C:529:ASN:HD22	1.66	0.43
1:E:254:MET:HE3	1:E:259:MET:CA	2.48	0.43
1:F:254:MET:HE1	1:F:259:MET:HB2	1.99	0.43
1:D:290:ARG:HA	1:D:291:PRO:HD3	1.89	0.43
1:D:669:LYS:O	1:D:672:VAL:CG1	2.57	0.43
1:A:53:THR:O	1:A:81:TYR:HA	2.18	0.43
1:E:131:ASP:O	1:E:135:ILE:HG13	2.18	0.43
1:C:312:HIS:HD2	3:C:1323:HOH:O	2.01	0.43
1:C:53:THR:O	1:C:81:TYR:HA	2.18	0.43
1:F:146:ASN:N	1:F:146:ASN:HD22	2.17	0.43
1:F:254:MET:HE3	1:F:259:MET:CA	2.47	0.42
1:D:669:LYS:C	1:D:672:VAL:HG12	2.38	0.42
1:B:131:ASP:O	1:B:135:ILE:HG13	2.18	0.42
1:C:485:TYR:O	1:D:554:LYS:HE2	2.18	0.42
1:B:53:THR:O	1:B:81:TYR:HA	2.18	0.42
1:A:146:ASN:N	1:A:146:ASN:HD22	2.17	0.42
1:A:673:HIS:O	1:A:674:LYS:CG	2.60	0.42
1:E:527:ASN:HD21	1:E:529:ASN:HD22	1.67	0.42
1:F:53:THR:O	1:F:81:TYR:HA	2.18	0.42
1:F:75:PRO:HA	1:F:76:PRO:HD3	1.95	0.42
1:B:146:ASN:HD22	1:B:146:ASN:N	2.17	0.42
1:C:334:LEU:HD13	1:C:334:LEU:C	2.40	0.42
1:A:485:TYR:O	1:B:554:LYS:HE2	2.19	0.42
1:D:75:PRO:HA	1:D:76:PRO:HD3	1.95	0.42
1:A:334:LEU:HD13	1:A:334:LEU:C	2.40	0.42
1:D:146:ASN:N	1:D:146:ASN:HD22	2.17	0.42
1:D:671:ALA:O	1:D:673:HIS:N	2.53	0.42
1:E:671:ALA:O	1:E:673:HIS:N	2.53	0.42
1:B:334:LEU:HD13	1:B:334:LEU:C	2.40	0.42
1:E:251:SER:HB3	1:F:240:PRO:HD2	2.02	0.42
1:F:334:LEU:HD13	1:F:334:LEU:C	2.40	0.42
1:A:254:MET:HE1	1:A:259:MET:HB2	2.02	0.41
1:B:254:MET:HE3	1:B:259:MET:CA	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:671:ALA:O	1:C:673:HIS:N	2.53	0.41
1:D:334:LEU:HD13	1:D:334:LEU:C	2.40	0.41
1:B:527:ASN:HD21	1:B:529:ASN:HD22	1.66	0.41
1:C:75:PRO:HA	1:C:76:PRO:HD3	1.95	0.41
1:B:646:ARG:O	1:B:647:HIS:HB2	2.21	0.41
1:B:671:ALA:O	1:B:673:HIS:N	2.53	0.41
1:E:146:ASN:N	1:E:146:ASN:HD22	2.17	0.41
1:C:146:ASN:N	1:C:146:ASN:HD22	2.17	0.41
1:C:669:LYS:O	1:C:672:VAL:CG1	2.57	0.41
1:D:48:LYS:HE3	1:D:48:LYS:HB2	1.94	0.41
1:F:671:ALA:O	1:F:673:HIS:N	2.53	0.41
1:A:646:ARG:O	1:A:647:HIS:HB2	2.21	0.41
1:B:345:LEU:HB2	1:B:363:VAL:HB	2.03	0.41
1:E:374:PHE:CD1	1:F:633:LEU:HD13	2.56	0.41
1:E:414:MET:HE3	1:E:418:ALA:HB3	2.02	0.41
1:A:345:LEU:HB2	1:A:363:VAL:HB	2.03	0.41
1:A:527:ASN:HD21	1:A:529:ASN:HD22	1.67	0.41
1:D:425:LEU:HD12	1:D:622:ILE:HD11	2.03	0.41
1:A:671:ALA:O	1:A:673:HIS:N	2.53	0.41
1:C:345:LEU:HB2	1:C:363:VAL:HB	2.03	0.41
1:D:345:LEU:HB2	1:D:363:VAL:HB	2.03	0.41
1:E:345:LEU:HB2	1:E:363:VAL:HB	2.03	0.41
1:C:355:ASP:HA	1:C:356:PRO:HD3	1.94	0.41
1:F:646:ARG:O	1:F:647:HIS:HB2	2.21	0.41
1:B:175:VAL:HG11	1:B:190:LEU:HD12	2.03	0.41
1:B:634[A]:ME0:H7	1:B:634[A]:ME0:HB	1.89	0.41
1:C:251:SER:HB3	1:D:240:PRO:HD2	2.02	0.41
1:C:290:ARG:HA	1:C:291:PRO:HD3	1.89	0.41
1:C:646:ARG:O	1:C:647:HIS:HB2	2.21	0.41
1:D:646:ARG:O	1:D:647:HIS:HB2	2.21	0.41
1:E:673:HIS:O	1:E:674:LYS:CG	2.60	0.41
1:A:290:ARG:HA	1:A:291:PRO:HD3	1.89	0.40
1:C:175:VAL:HG11	1:C:190:LEU:HD12	2.03	0.40
1:C:414:MET:HE3	1:C:418:ALA:HB3	2.03	0.40
1:E:334:LEU:HD13	1:E:334:LEU:C	2.40	0.40
1:E:669:LYS:C	1:E:672:VAL:HG12	2.38	0.40
1:C:425:LEU:HD12	1:C:622:ILE:HD11	2.03	0.40
1:C:527:ASN:ND2	1:C:529:ASN:HB2	2.34	0.40
1:C:581:TYR:HA	1:C:582:PRO:HD2	1.78	0.40
1:D:581:TYR:HA	1:D:582:PRO:HD2	1.78	0.40
1:B:259:MET:CE	1:B:365:ILE:HG21	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:HD2	1:E:111:THR:HG21	2.03	0.40
1:B:371:GLY:HA2	1:B:390:ARG:HH12	1.87	0.40
1:E:259:MET:CE	1:E:365:ILE:HG21	2.52	0.40
1:E:672:VAL:CG1	1:E:673:HIS:N	2.85	0.40
1:C:674:LYS:O	1:C:675:GLU:HB2	2.22	0.40
1:D:175:VAL:HG11	1:D:190:LEU:HD12	2.03	0.40
1:D:371:GLY:HA2	1:D:390:ARG:HH12	1.87	0.40
1:E:632:PRO:HD2	1:F:655:LEU:HD11	2.03	0.40
1:F:672:VAL:CG1	1:F:673:HIS:N	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:PRO:O	1:F:675:GLU:O[2_556]	2.18	0.02

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	657/694 (95%)	629 (96%)	25 (4%)	3 (0%)	29	18
1	B	657/694 (95%)	629 (96%)	25 (4%)	3 (0%)	29	18
1	C	657/694 (95%)	629 (96%)	25 (4%)	3 (0%)	29	18
1	D	657/694 (95%)	630 (96%)	24 (4%)	3 (0%)	29	18
1	E	657/694 (95%)	629 (96%)	25 (4%)	3 (0%)	29	18
1	F	657/694 (95%)	629 (96%)	25 (4%)	3 (0%)	29	18
All	All	3942/4164 (95%)	3775 (96%)	149 (4%)	18 (0%)	29	18

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	674	LYS
1	B	674	LYS
1	C	674	LYS
1	D	674	LYS
1	E	674	LYS
1	F	674	LYS
1	A	672	VAL
1	A	673	HIS
1	B	672	VAL
1	B	673	HIS
1	C	672	VAL
1	C	673	HIS
1	D	672	VAL
1	D	673	HIS
1	E	672	VAL
1	E	673	HIS
1	F	672	VAL
1	F	673	HIS

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	569/593 (96%)	547 (96%)	22 (4%)	32	25
1	B	569/593 (96%)	546 (96%)	23 (4%)	31	24
1	C	569/593 (96%)	547 (96%)	22 (4%)	32	25
1	D	569/593 (96%)	547 (96%)	22 (4%)	32	25
1	E	569/593 (96%)	546 (96%)	23 (4%)	31	24
1	F	569/593 (96%)	547 (96%)	22 (4%)	32	25
All	All	3414/3558 (96%)	3280 (96%)	134 (4%)	32	25

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	LEU

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Mol	Chain	Res	Type
1	A	112	VAL
1	A	127	VAL
1	A	140	LEU
1	A	146	ASN
1	A	170	LEU
1	A	211	ARG
1	A	254	MET
1	A	311	PRO
1	A	329	THR
1	A	332	LEU
1	A	394	LEU
1	A	421	LEU
1	A	452	ASN
1	A	462	LEU
1	A	487	LEU
1	A	527	ASN
1	A	558	LEU
1	A	633	LEU
1	A	641	LEU
1	A	673	HIS
1	A	674	LYS
1	B	30	THR
1	B	109	LEU
1	B	112	VAL
1	B	127	VAL
1	B	140	LEU
1	B	146	ASN
1	B	170	LEU
1	B	211	ARG
1	B	254	MET
1	B	311	PRO
1	B	329	THR
1	B	332	LEU
1	B	394	LEU
1	B	421	LEU
1	B	452	ASN
1	B	462	LEU
1	B	487	LEU
1	B	527	ASN
1	B	558	LEU
1	B	633	LEU
1	B	641	LEU

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Mol	Chain	Res	Type
1	B	673	HIS
1	B	674	LYS
1	C	109	LEU
1	C	112	VAL
1	C	127	VAL
1	C	140	LEU
1	C	146	ASN
1	C	170	LEU
1	C	211	ARG
1	C	254	MET
1	C	311	PRO
1	C	329	THR
1	C	332	LEU
1	C	394	LEU
1	C	421	LEU
1	C	452	ASN
1	C	462	LEU
1	C	487	LEU
1	C	527	ASN
1	C	558	LEU
1	C	633	LEU
1	C	641	LEU
1	C	673	HIS
1	C	674	LYS
1	D	109	LEU
1	D	112	VAL
1	D	127	VAL
1	D	140	LEU
1	D	146	ASN
1	D	170	LEU
1	D	211	ARG
1	D	254	MET
1	D	311	PRO
1	D	329	THR
1	D	332	LEU
1	D	394	LEU
1	D	421	LEU
1	D	452	ASN
1	D	462	LEU
1	D	487	LEU
1	D	527	ASN
1	D	558	LEU

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Mol	Chain	Res	Type
1	D	633	LEU
1	D	641	LEU
1	D	673	HIS
1	D	674	LYS
1	E	30	THR
1	E	109	LEU
1	E	112	VAL
1	E	127	VAL
1	E	140	LEU
1	E	146	ASN
1	E	170	LEU
1	E	211	ARG
1	E	254	MET
1	E	311	PRO
1	E	329	THR
1	E	332	LEU
1	E	394	LEU
1	E	421	LEU
1	E	452	ASN
1	E	462	LEU
1	E	487	LEU
1	E	527	ASN
1	E	558	LEU
1	E	633	LEU
1	E	641	LEU
1	E	673	HIS
1	E	674	LYS
1	F	109	LEU
1	F	112	VAL
1	F	127	VAL
1	F	140	LEU
1	F	146	ASN
1	F	170	LEU
1	F	211	ARG
1	F	254	MET
1	F	311	PRO
1	F	329	THR
1	F	332	LEU
1	F	394	LEU
1	F	421	LEU
1	F	452	ASN
1	F	462	LEU

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Mol	Chain	Res	Type
1	F	487	LEU
1	F	527	ASN
1	F	558	LEU
1	F	633	LEU
1	F	641	LEU
1	F	673	HIS
1	F	674	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	70	GLN
1	A	146	ASN
1	A	218	HIS
1	A	286	HIS
1	A	288	ASN
1	A	294	HIS
1	A	312	HIS
1	A	330	ASN
1	A	361	ASN
1	A	382	ASN
1	A	450	ASN
1	A	452	ASN
1	A	457	GLN
1	A	473	ASN
1	A	527	ASN
1	A	547	GLN
1	B	23	HIS
1	B	70	GLN
1	B	146	ASN
1	B	218	HIS
1	B	286	HIS
1	B	288	ASN
1	B	294	HIS
1	B	312	HIS
1	B	330	ASN
1	B	361	ASN
1	B	382	ASN
1	B	450	ASN
1	B	452	ASN
1	B	457	GLN

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Mol	Chain	Res	Type
1	B	473	ASN
1	B	527	ASN
1	B	547	GLN
1	C	23	HIS
1	C	70	GLN
1	C	146	ASN
1	C	218	HIS
1	C	243	ASN
1	C	286	HIS
1	C	288	ASN
1	C	294	HIS
1	C	312	HIS
1	C	330	ASN
1	C	361	ASN
1	C	382	ASN
1	C	450	ASN
1	C	452	ASN
1	C	457	GLN
1	C	473	ASN
1	C	527	ASN
1	C	547	GLN
1	D	23	HIS
1	D	70	GLN
1	D	146	ASN
1	D	218	HIS
1	D	243	ASN
1	D	286	HIS
1	D	288	ASN
1	D	294	HIS
1	D	312	HIS
1	D	330	ASN
1	D	361	ASN
1	D	382	ASN
1	D	450	ASN
1	D	452	ASN
1	D	457	GLN
1	D	473	ASN
1	D	527	ASN
1	D	547	GLN
1	E	23	HIS
1	E	70	GLN
1	E	146	ASN

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Mol	Chain	Res	Type
1	E	218	HIS
1	E	243	ASN
1	E	286	HIS
1	E	288	ASN
1	E	294	HIS
1	E	312	HIS
1	E	330	ASN
1	E	361	ASN
1	E	382	ASN
1	E	450	ASN
1	E	452	ASN
1	E	457	GLN
1	E	473	ASN
1	E	527	ASN
1	E	547	GLN
1	F	23	HIS
1	F	70	GLN
1	F	146	ASN
1	F	218	HIS
1	F	243	ASN
1	F	286	HIS
1	F	288	ASN
1	F	294	HIS
1	F	312	HIS
1	F	330	ASN
1	F	361	ASN
1	F	382	ASN
1	F	450	ASN
1	F	452	ASN
1	F	457	GLN
1	F	473	ASN
1	F	527	ASN
1	F	547	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	TY9	F	405[B]	-	13,16,17	4.61	8 (61%)	14,21,23	1.97	4 (28%)
1	TY9	A	405[B]	-	13,16,17	4.61	8 (61%)	14,21,23	1.97	4 (28%)
1	TY9	C	405[B]	-	13,16,17	4.61	8 (61%)	14,21,23	1.96	4 (28%)
1	TY9	E	405[B]	-	13,16,17	4.60	8 (61%)	14,21,23	1.96	4 (28%)
1	ME0	E	634[A]	1	5,8,9	0.56	0	2,8,10	0.42	0
1	ME0	D	634[A]	1	5,8,9	0.55	0	2,8,10	0.44	0
1	TY8	C	405[A]	1	13,16,17	4.91	9 (69%)	15,21,23	2.50	6 (40%)
1	TY8	A	405[A]	1	13,16,17	4.91	9 (69%)	15,21,23	2.51	6 (40%)
1	TY9	D	405[B]	-	13,16,17	4.61	8 (61%)	14,21,23	1.96	4 (28%)
1	ME0	F	634[A]	1	5,8,9	0.56	0	2,8,10	0.43	0
1	TY8	B	405[A]	1	13,16,17	4.91	9 (69%)	15,21,23	2.51	6 (40%)
1	TY8	D	405[A]	1	13,16,17	4.91	9 (69%)	15,21,23	2.50	6 (40%)
1	ME0	B	634[A]	1	5,8,9	0.57	0	2,8,10	0.42	0
1	TY8	E	405[A]	1	13,16,17	4.90	9 (69%)	15,21,23	2.51	6 (40%)
1	ME0	A	634[A]	1	5,8,9	0.56	0	2,8,10	0.42	0
1	TY8	F	405[A]	1	13,16,17	4.91	9 (69%)	15,21,23	2.51	6 (40%)
1	TY9	B	405[B]	-	13,16,17	4.61	8 (61%)	14,21,23	1.97	4 (28%)
1	ME0	C	634[A]	1	5,8,9	0.57	0	2,8,10	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TY9	F	405[B]	-	-	0/5/10/12	0/1/1/1
1	TY9	A	405[B]	-	-	0/5/10/12	0/1/1/1
1	TY9	C	405[B]	-	-	0/5/10/12	0/1/1/1
1	TY9	E	405[B]	-	-	0/5/10/12	0/1/1/1
1	ME0	E	634[A]	1	-	1/5/7/9	-
1	ME0	D	634[A]	1	-	1/5/7/9	-
1	TY8	C	405[A]	1	-	0/5/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TY8	A	405[A]	1	-	0/5/10/12	0/1/1/1
1	TY9	D	405[B]	-	-	0/5/10/12	0/1/1/1
1	ME0	F	634[A]	1	-	1/5/7/9	-
1	TY8	B	405[A]	1	-	0/5/10/12	0/1/1/1
1	TY8	D	405[A]	1	-	0/5/10/12	0/1/1/1
1	ME0	B	634[A]	1	-	1/5/7/9	-
1	TY8	E	405[A]	1	-	0/5/10/12	0/1/1/1
1	ME0	A	634[A]	1	-	1/5/7/9	-
1	TY8	F	405[A]	1	-	0/5/10/12	0/1/1/1
1	TY9	B	405[B]	-	-	0/5/10/12	0/1/1/1
1	ME0	C	634[A]	1	-	1/5/7/9	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405[A]	TY8	C6-C5	8.60	1.51	1.38
1	B	405[B]	TY9	C6-C5	8.60	1.51	1.38
1	A	405[A]	TY8	C6-C5	8.56	1.51	1.38
1	A	405[B]	TY9	C6-C5	8.56	1.51	1.38
1	E	405[A]	TY8	C6-C5	8.55	1.51	1.38
1	E	405[B]	TY9	C6-C5	8.55	1.51	1.38
1	F	405[A]	TY8	C6-C5	8.55	1.51	1.38
1	F	405[B]	TY9	C6-C5	8.55	1.51	1.38
1	D	405[A]	TY8	C6-C5	8.55	1.51	1.38
1	D	405[B]	TY9	C6-C5	8.55	1.51	1.38
1	C	405[A]	TY8	C6-C5	8.54	1.51	1.38
1	C	405[B]	TY9	C6-C5	8.54	1.51	1.38
1	D	405[A]	TY8	CB-C1	-7.66	1.41	1.51
1	F	405[A]	TY8	CB-C1	-7.66	1.41	1.51
1	A	405[A]	TY8	CB-C1	-7.65	1.41	1.51
1	C	405[A]	TY8	CB-C1	-7.65	1.41	1.51
1	B	405[A]	TY8	CB-C1	-7.63	1.41	1.51
1	E	405[A]	TY8	CB-C1	-7.62	1.41	1.51
1	D	405[A]	TY8	C3-C2	6.58	1.50	1.38
1	D	405[B]	TY9	C2-C3	6.58	1.50	1.38
1	E	405[A]	TY8	C3-C2	6.57	1.50	1.38
1	E	405[B]	TY9	C2-C3	6.57	1.50	1.38
1	C	405[A]	TY8	C3-C2	6.57	1.50	1.38
1	C	405[B]	TY9	C2-C3	6.57	1.50	1.38
1	A	405[A]	TY8	C3-C2	6.56	1.50	1.38
1	A	405[B]	TY9	C2-C3	6.56	1.50	1.38
1	B	405[A]	TY8	C3-C2	6.55	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405[B]	TY9	C2-C3	6.55	1.50	1.38
1	F	405[A]	TY8	C3-C2	6.55	1.50	1.38
1	F	405[B]	TY9	C2-C3	6.55	1.50	1.38
1	F	405[A]	TY8	C5-C4	6.26	1.51	1.40
1	D	405[A]	TY8	C5-C4	6.25	1.51	1.40
1	A	405[A]	TY8	C5-C4	6.24	1.51	1.40
1	C	405[A]	TY8	C5-C4	6.24	1.51	1.40
1	E	405[A]	TY8	C5-C4	6.23	1.51	1.40
1	B	405[A]	TY8	C5-C4	6.20	1.51	1.40
1	F	405[B]	TY9	C5-C4	5.52	1.51	1.40
1	D	405[B]	TY9	C5-C4	5.51	1.51	1.40
1	A	405[B]	TY9	C5-C4	5.51	1.51	1.40
1	C	405[B]	TY9	C5-C4	5.51	1.51	1.40
1	E	405[B]	TY9	C5-C4	5.49	1.51	1.40
1	B	405[B]	TY9	C5-C4	5.47	1.51	1.40
1	C	405[B]	TY9	C2-C1	5.43	1.48	1.39
1	A	405[B]	TY9	C2-C1	5.42	1.48	1.39
1	B	405[B]	TY9	C2-C1	5.42	1.48	1.39
1	E	405[B]	TY9	C2-C1	5.40	1.48	1.39
1	F	405[B]	TY9	C2-C1	5.40	1.48	1.39
1	D	405[B]	TY9	C2-C1	5.40	1.48	1.39
1	E	405[A]	TY8	O5-C5	-5.38	1.25	1.36
1	E	405[B]	TY9	O5-C5	-5.38	1.25	1.36
1	D	405[A]	TY8	O5-C5	-5.37	1.25	1.36
1	D	405[B]	TY9	O5-C5	-5.37	1.25	1.36
1	F	405[A]	TY8	O5-C5	-5.36	1.25	1.36
1	F	405[B]	TY9	O5-C5	-5.36	1.25	1.36
1	A	405[A]	TY8	O5-C5	-5.36	1.25	1.36
1	A	405[B]	TY9	O5-C5	-5.36	1.25	1.36
1	B	405[A]	TY8	O5-C5	-5.34	1.25	1.36
1	B	405[B]	TY9	O5-C5	-5.34	1.25	1.36
1	C	405[A]	TY8	O5-C5	-5.32	1.25	1.36
1	C	405[B]	TY9	O5-C5	-5.32	1.25	1.36
1	F	405[B]	TY9	O3A-O3	-5.29	1.31	1.46
1	C	405[B]	TY9	O3A-O3	-5.28	1.31	1.46
1	A	405[B]	TY9	O3A-O3	-5.27	1.31	1.46
1	D	405[B]	TY9	O3A-O3	-5.27	1.31	1.46
1	E	405[B]	TY9	O3A-O3	-5.26	1.31	1.46
1	B	405[B]	TY9	O3A-O3	-5.25	1.31	1.46
1	C	405[A]	TY8	C2-C1	5.25	1.48	1.40
1	A	405[A]	TY8	C2-C1	5.24	1.48	1.40
1	B	405[A]	TY8	C2-C1	5.23	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405[A]	TY8	C2-C1	5.22	1.48	1.40
1	F	405[A]	TY8	C2-C1	5.22	1.48	1.40
1	D	405[A]	TY8	C2-C1	5.21	1.48	1.40
1	B	405[A]	TY8	O4A-O4	-4.78	1.32	1.46
1	B	405[B]	TY9	O4A-O4	-4.78	1.32	1.46
1	C	405[A]	TY8	O4A-O4	-4.78	1.32	1.46
1	C	405[B]	TY9	O4A-O4	-4.78	1.32	1.46
1	D	405[A]	TY8	O4A-O4	-4.78	1.32	1.46
1	D	405[B]	TY9	O4A-O4	-4.78	1.32	1.46
1	A	405[A]	TY8	O4A-O4	-4.77	1.32	1.46
1	A	405[B]	TY9	O4A-O4	-4.77	1.32	1.46
1	F	405[A]	TY8	O4A-O4	-4.77	1.32	1.46
1	F	405[B]	TY9	O4A-O4	-4.77	1.32	1.46
1	E	405[A]	TY8	O4A-O4	-4.77	1.32	1.46
1	E	405[B]	TY9	O4A-O4	-4.77	1.32	1.46
1	D	405[B]	TY9	CB-C1	-4.11	1.41	1.51
1	F	405[B]	TY9	CB-C1	-4.10	1.41	1.51
1	A	405[B]	TY9	CB-C1	-4.10	1.41	1.51
1	C	405[B]	TY9	CB-C1	-4.10	1.41	1.51
1	B	405[B]	TY9	CB-C1	-4.09	1.41	1.51
1	E	405[B]	TY9	CB-C1	-4.08	1.41	1.51
1	C	405[A]	TY8	O2A-O2	-3.56	1.36	1.46
1	E	405[A]	TY8	O2A-O2	-3.54	1.36	1.46
1	A	405[A]	TY8	O2A-O2	-3.54	1.36	1.46
1	D	405[A]	TY8	O2A-O2	-3.53	1.36	1.46
1	B	405[A]	TY8	O2A-O2	-3.53	1.36	1.46
1	F	405[A]	TY8	O2A-O2	-3.50	1.36	1.46
1	F	405[A]	TY8	C3-C4	2.38	1.43	1.38
1	E	405[A]	TY8	C3-C4	2.35	1.43	1.38
1	A	405[A]	TY8	C3-C4	2.34	1.43	1.38
1	B	405[A]	TY8	C3-C4	2.32	1.43	1.38
1	C	405[A]	TY8	C3-C4	2.32	1.43	1.38
1	D	405[A]	TY8	C3-C4	2.32	1.43	1.38

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	405[A]	TY8	C1-CB-CA	6.78	125.00	114.53
1	E	405[A]	TY8	C1-CB-CA	6.75	124.97	114.53
1	A	405[A]	TY8	C1-CB-CA	6.75	124.96	114.53
1	B	405[A]	TY8	C1-CB-CA	6.74	124.94	114.53
1	C	405[A]	TY8	C1-CB-CA	6.73	124.94	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	405[A]	TY8	C1-CB-CA	6.73	124.92	114.53
1	F	405[B]	TY9	C1-CB-CA	5.39	125.00	114.10
1	E	405[B]	TY9	C1-CB-CA	5.37	124.97	114.10
1	A	405[B]	TY9	C1-CB-CA	5.37	124.96	114.10
1	B	405[B]	TY9	C1-CB-CA	5.36	124.94	114.10
1	C	405[B]	TY9	C1-CB-CA	5.35	124.94	114.10
1	D	405[B]	TY9	C1-CB-CA	5.35	124.92	114.10
1	B	405[A]	TY8	CB-C1-C2	4.11	124.95	120.89
1	A	405[A]	TY8	CB-C1-C2	4.10	124.94	120.89
1	D	405[A]	TY8	CB-C1-C2	4.09	124.93	120.89
1	F	405[A]	TY8	CB-C1-C2	4.09	124.93	120.89
1	C	405[A]	TY8	CB-C1-C2	4.08	124.92	120.89
1	E	405[A]	TY8	CB-C1-C2	4.06	124.90	120.89
1	B	405[B]	TY9	CB-C1-C6	-3.30	114.77	120.44
1	F	405[B]	TY9	CB-C1-C6	-3.29	114.79	120.44
1	A	405[B]	TY9	CB-C1-C6	-3.28	114.81	120.44
1	D	405[B]	TY9	CB-C1-C6	-3.28	114.81	120.44
1	C	405[B]	TY9	CB-C1-C6	-3.28	114.81	120.44
1	E	405[B]	TY9	CB-C1-C6	-3.27	114.83	120.44
1	B	405[A]	TY8	CB-C1-C6	-2.82	114.77	119.77
1	D	405[A]	TY8	O2-C2-C1	2.82	121.00	116.04
1	F	405[A]	TY8	O2-C2-C1	2.81	120.99	116.04
1	F	405[A]	TY8	CB-C1-C6	-2.81	114.79	119.77
1	C	405[A]	TY8	O2-C2-C1	2.81	120.99	116.04
1	E	405[A]	TY8	O2-C2-C1	2.81	120.99	116.04
1	A	405[A]	TY8	CB-C1-C6	-2.80	114.81	119.77
1	D	405[A]	TY8	CB-C1-C6	-2.80	114.81	119.77
1	A	405[A]	TY8	O2-C2-C1	2.80	120.97	116.04
1	C	405[A]	TY8	CB-C1-C6	-2.79	114.81	119.77
1	B	405[A]	TY8	O2-C2-C1	2.79	120.96	116.04
1	E	405[A]	TY8	CB-C1-C6	-2.79	114.83	119.77
1	B	405[B]	TY9	CB-C1-C2	2.63	124.95	120.44
1	A	405[B]	TY9	CB-C1-C2	2.63	124.94	120.44
1	D	405[B]	TY9	CB-C1-C2	2.62	124.93	120.44
1	F	405[B]	TY9	CB-C1-C2	2.62	124.93	120.44
1	C	405[B]	TY9	CB-C1-C2	2.61	124.92	120.44
1	E	405[B]	TY9	CB-C1-C2	2.60	124.90	120.44
1	E	405[A]	TY8	O2-C2-C3	-2.18	118.87	123.78
1	F	405[A]	TY8	O2-C2-C3	-2.17	118.90	123.78
1	A	405[A]	TY8	O2-C2-C3	-2.16	118.91	123.78
1	D	405[A]	TY8	O2-C2-C3	-2.16	118.92	123.78
1	C	405[A]	TY8	O2-C2-C3	-2.15	118.92	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	405[A]	TY8	O2-C2-C3	-2.15	118.93	123.78
1	B	405[A]	TY8	CB-CA-C	-2.08	107.56	111.47
1	B	405[B]	TY9	CB-CA-C	-2.08	107.56	111.47
1	E	405[A]	TY8	CB-CA-C	-2.08	107.58	111.47
1	E	405[B]	TY9	CB-CA-C	-2.08	107.58	111.47
1	C	405[A]	TY8	CB-CA-C	-2.07	107.58	111.47
1	C	405[B]	TY9	CB-CA-C	-2.07	107.58	111.47
1	A	405[A]	TY8	CB-CA-C	-2.07	107.59	111.47
1	A	405[B]	TY9	CB-CA-C	-2.07	107.59	111.47
1	D	405[A]	TY8	CB-CA-C	-2.06	107.60	111.47
1	D	405[B]	TY9	CB-CA-C	-2.06	107.60	111.47
1	F	405[A]	TY8	CB-CA-C	-2.05	107.63	111.47
1	F	405[B]	TY9	CB-CA-C	-2.05	107.63	111.47

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	634[A]	ME0	CB-CG-SD-CE
1	B	634[A]	ME0	CB-CG-SD-CE
1	C	634[A]	ME0	CB-CG-SD-CE
1	D	634[A]	ME0	CB-CG-SD-CE
1	E	634[A]	ME0	CB-CG-SD-CE
1	F	634[A]	ME0	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	634[A]	ME0	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	659/694 (94%)	0.06	25 (3%)	40	44	18, 26, 46, 99	0
1	B	659/694 (94%)	0.12	23 (3%)	44	48	18, 26, 46, 99	0
1	C	659/694 (94%)	-0.01	14 (2%)	63	67	18, 26, 46, 99	0
1	D	659/694 (94%)	0.20	36 (5%)	25	27	18, 26, 46, 99	0
1	E	659/694 (94%)	-0.08	14 (2%)	63	67	18, 26, 46, 99	0
1	F	659/694 (94%)	0.01	23 (3%)	44	48	18, 26, 46, 99	0
All	All	3954/4164 (94%)	0.05	135 (3%)	45	49	18, 26, 46, 99	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	675	GLU	16.2
1	B	672	VAL	15.9
1	E	674	LYS	14.4
1	C	672	VAL	13.7
1	E	673	HIS	12.5
1	A	672	VAL	12.1
1	D	15	SER	12.1
1	B	675	GLU	12.0
1	C	15	SER	12.0
1	C	675	GLU	11.8
1	D	17	ALA	11.1
1	C	673	HIS	10.9
1	E	672	VAL	10.9
1	D	674	LYS	10.0
1	F	674	LYS	10.0
1	B	674	LYS	10.0
1	F	675	GLU	9.4
1	F	15	SER	9.3
1	B	673	HIS	9.1

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Mol	Chain	Res	Type	RSRZ
1	C	674	LYS	8.0
1	F	672	VAL	7.4
1	A	673	HIS	7.3
1	E	15	SER	7.2
1	E	675	GLU	7.1
1	A	15	SER	6.7
1	B	15	SER	6.6
1	A	16	ALA	6.4
1	D	672	VAL	6.2
1	D	16	ALA	5.6
1	A	17	ALA	5.5
1	D	18	PRO	5.4
1	D	99	ALA	5.3
1	D	673	HIS	5.2
1	C	671	ALA	5.1
1	D	335	GLY	5.0
1	F	17	ALA	4.7
1	B	671	ALA	4.6
1	F	673	HIS	4.5
1	F	334	LEU	4.5
1	D	19	ALA	4.4
1	D	98	LEU	4.1
1	D	44	PHE	4.0
1	A	674	LYS	4.0
1	A	675	GLU	3.9
1	D	334	LEU	3.8
1	F	16	ALA	3.6
1	D	20	ARG	3.6
1	B	437	ASP	3.5
1	E	334	LEU	3.4
1	A	18	PRO	3.4
1	D	40	VAL	3.4
1	E	16	ALA	3.3
1	B	421	LEU	3.3
1	D	101	LEU	3.3
1	C	437	ASP	3.3
1	D	22	ALA	3.3
1	F	18	PRO	3.3
1	A	99	ALA	3.3
1	B	334	LEU	3.2
1	A	19	ALA	3.1
1	B	641	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	78	LEU	3.0
1	D	247	PRO	3.0
1	D	333	SER	3.0
1	A	334	LEU	2.9
1	D	103	VAL	2.9
1	B	20	ARG	2.9
1	D	102	SER	2.9
1	A	437	ASP	2.8
1	A	20	ARG	2.8
1	D	74	LEU	2.7
1	C	17	ALA	2.7
1	F	70	GLN	2.7
1	C	670	ARG	2.7
1	E	130	ASN	2.7
1	A	145	ALA	2.6
1	B	16	ALA	2.6
1	D	42	SER	2.6
1	F	437	ASP	2.6
1	D	96	VAL	2.5
1	A	67	TRP	2.5
1	B	73	PRO	2.5
1	C	334	LEU	2.5
1	A	72	GLY	2.5
1	B	233	GLY	2.5
1	F	19	ALA	2.5
1	F	73	PRO	2.5
1	C	16	ALA	2.5
1	E	671	ALA	2.5
1	D	38	ASN	2.4
1	D	97	ASP	2.4
1	E	248	GLU	2.4
1	D	357	ILE	2.4
1	A	22	ALA	2.4
1	E	670	ARG	2.4
1	A	73	PRO	2.4
1	A	48	LYS	2.4
1	D	21	PRO	2.3
1	F	99	ALA	2.3
1	B	640	THR	2.3
1	B	74	LEU	2.3
1	F	130	ASN	2.3
1	D	45	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	210	ASN	2.3
1	A	21	PRO	2.3
1	F	247	PRO	2.3
1	A	98	LEU	2.3
1	B	234	ALA	2.3
1	F	45	ALA	2.3
1	B	211	ARG	2.2
1	C	669	LYS	2.2
1	D	46	GLY	2.2
1	B	423	ILE	2.2
1	E	17	ALA	2.2
1	F	245	THR	2.2
1	D	39	THR	2.2
1	F	63	ALA	2.2
1	E	233	GLY	2.2
1	F	20	ARG	2.2
1	A	671	ALA	2.2
1	D	670	ARG	2.2
1	D	104	ILE	2.1
1	A	101	LEU	2.1
1	F	21	PRO	2.1
1	C	199	GLU	2.1
1	A	74	LEU	2.1
1	A	335	GLY	2.1
1	B	360	LYS	2.1
1	F	87	GLY	2.1
1	B	642	MET	2.1
1	B	232	VAL	2.1
1	B	418	ALA	2.0
1	E	360	LYS	2.0
1	F	48	LYS	2.0
1	D	100	SER	2.0

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

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
1	TY8	B	405[A]	16/17	0.84	0.23	25,38,49,53	16

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
1	TY9	B	405[B]	16/17	0.84	0.23	25,38,49,53	16
1	TY8	F	405[A]	16/17	0.84	0.17	25,38,49,53	16
1	TY9	F	405[B]	16/17	0.84	0.19	25,38,49,53	16
1	TY8	D	405[A]	16/17	0.85	0.17	25,38,49,53	16
1	TY8	E	405[A]	16/17	0.87	0.21	25,38,49,53	16
1	TY9	E	405[B]	16/17	0.87	0.22	25,38,49,53	16
1	TY9	C	405[B]	16/17	0.87	0.22	25,38,49,53	16
1	TY9	D	405[B]	16/17	0.87	0.17	25,38,49,53	16
1	TY8	C	405[A]	16/17	0.88	0.22	25,38,49,53	16
1	TY9	A	405[B]	16/17	0.88	0.19	25,38,49,53	16
1	TY8	A	405[A]	16/17	0.89	0.19	25,38,49,53	16
1	ME0	C	634[A]	9/10	0.92	0.16	24,26,42,47	9
1	ME0	B	634[A]	9/10	0.94	0.13	24,26,42,47	9
1	ME0	A	634[A]	9/10	0.94	0.18	24,26,42,47	9
1	ME0	E	634[A]	9/10	0.95	0.15	24,26,42,47	9
1	ME0	F	634[A]	9/10	0.96	0.10	24,26,42,47	9
1	ME0	D	634[A]	9/10	0.97	0.10	24,26,42,47	9

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	CU	C	701	1/1	0.99	0.09	26,26,26,26	0
2	CU	B	701	1/1	1.00	0.12	26,26,26,26	0
2	CU	A	701	1/1	1.00	0.12	26,26,26,26	0
2	CU	D	701	1/1	1.00	0.11	26,26,26,26	0
2	CU	E	701	1/1	1.00	0.12	26,26,26,26	0
2	CU	F	701	1/1	1.00	0.08	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.