



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 06:12 am BST

PDB ID : 3NBJ  
Title : Crystal Structure of Y305F mutant of the copper amine oxidase from Hansenula polymorpha expressed in yeast  
Authors : Chen, Z.; Datta, S.; DuBois, J.L.; Klinman, J.P.; Mathews, F.S.  
Deposited on : 2010-06-03  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

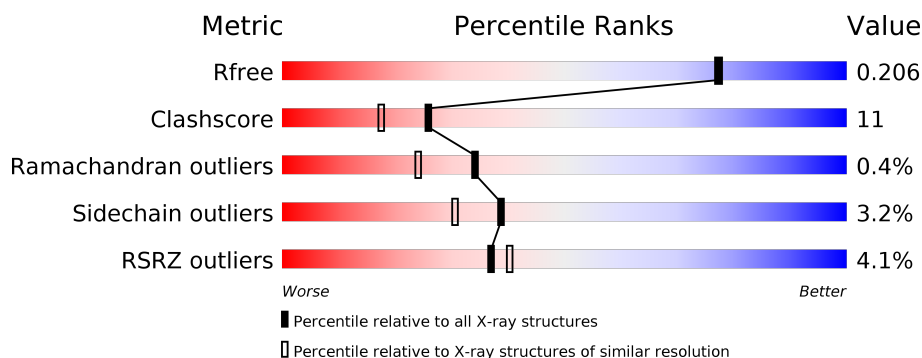
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	694	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	B	694	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	C	694	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	D	694	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	E	694	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	F	694	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 34140 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	655	Total	C	N	O	S	0	2	0
			5219	3319	894	982	24			
1	B	655	Total	C	N	O	S	0	2	0
			5219	3319	894	982	24			
1	C	655	Total	C	N	O	S	0	2	0
			5219	3319	894	982	24			
1	D	655	Total	C	N	O	S	0	2	0
			5219	3319	894	982	24			
1	E	655	Total	C	N	O	S	0	2	0
			5219	3319	894	982	24			
1	F	655	Total	C	N	O	S	0	2	0
			5219	3319	894	982	24			

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).

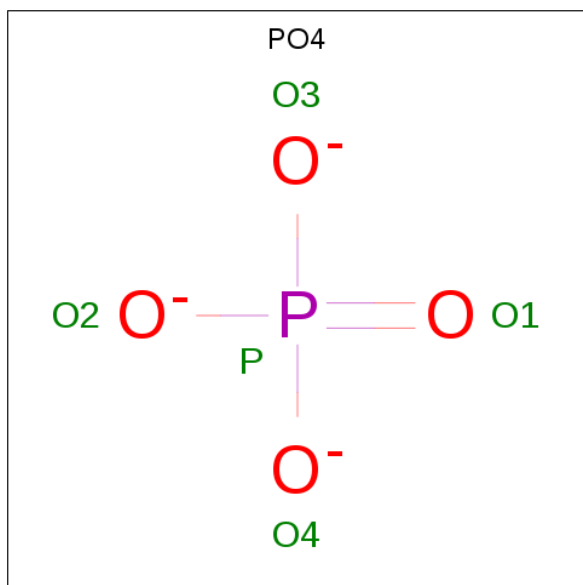
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cu	0	0
			1	1		
2	E	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

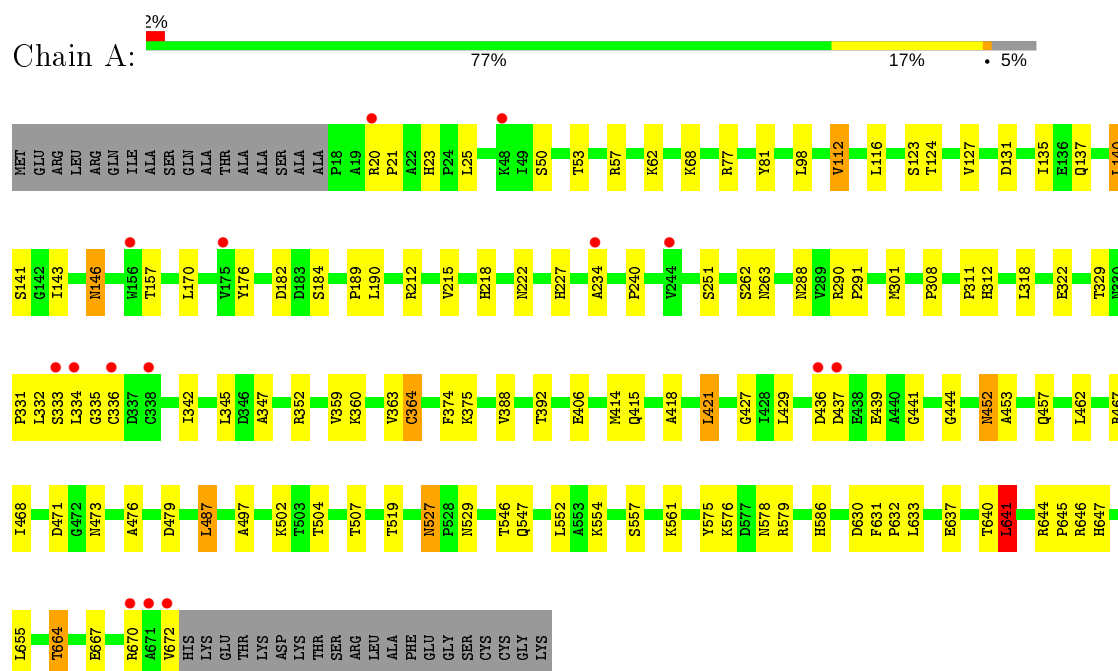
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	456	Total	O	0	0
			456	456		
4	B	456	Total	O	0	0
			456	456		
4	C	453	Total	O	0	0
			453	453		
4	D	455	Total	O	0	0
			455	455		
4	E	454	Total	O	0	0
			454	454		
4	F	456	Total	O	0	0
			456	456		

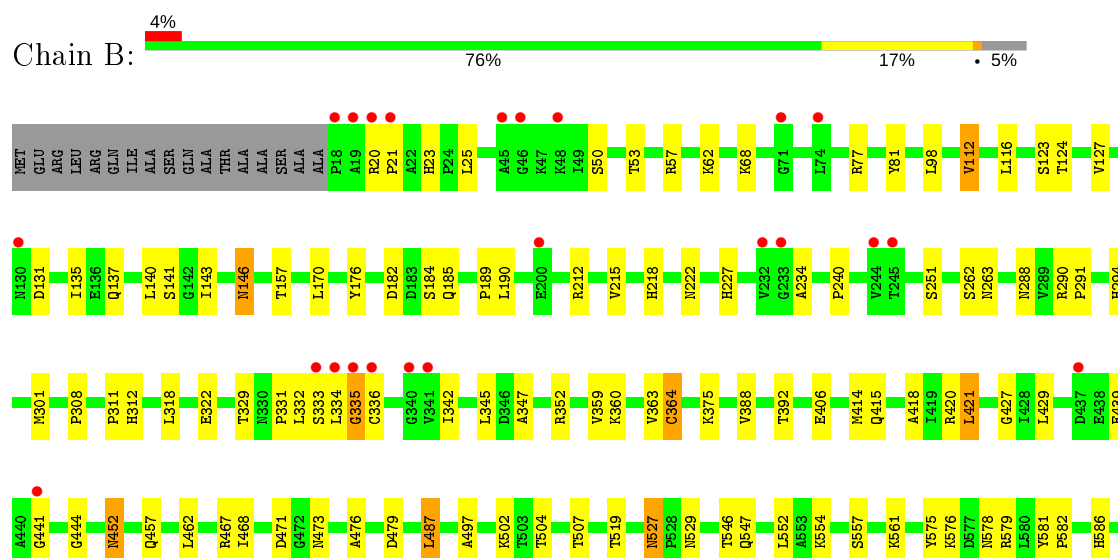
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

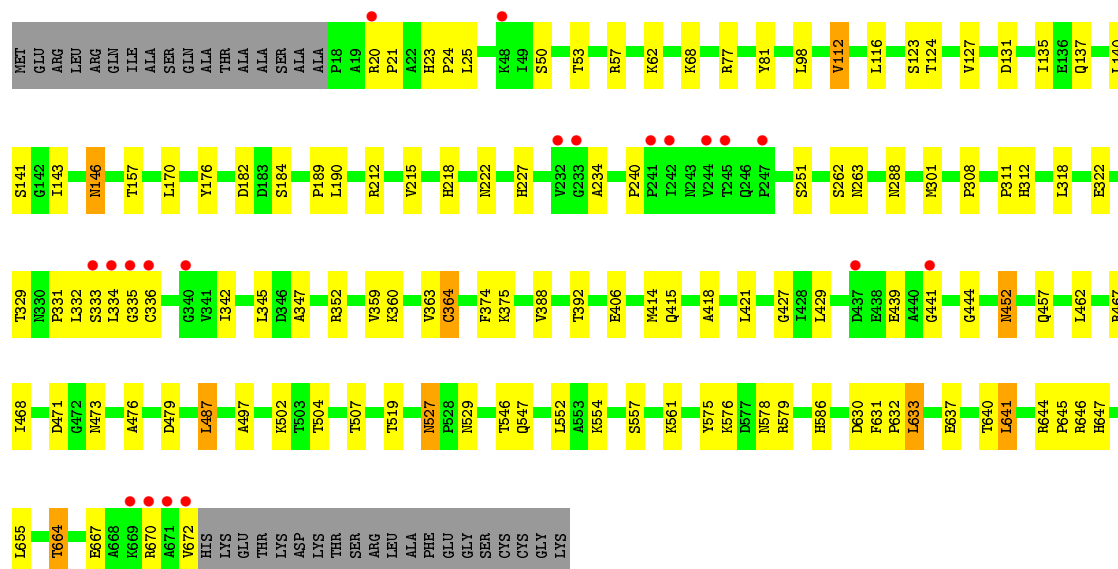
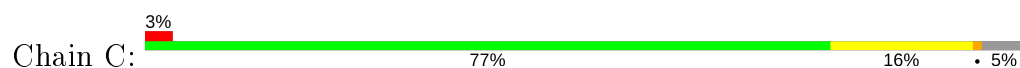


- Molecule 1: Peroxisomal primary amine oxidase

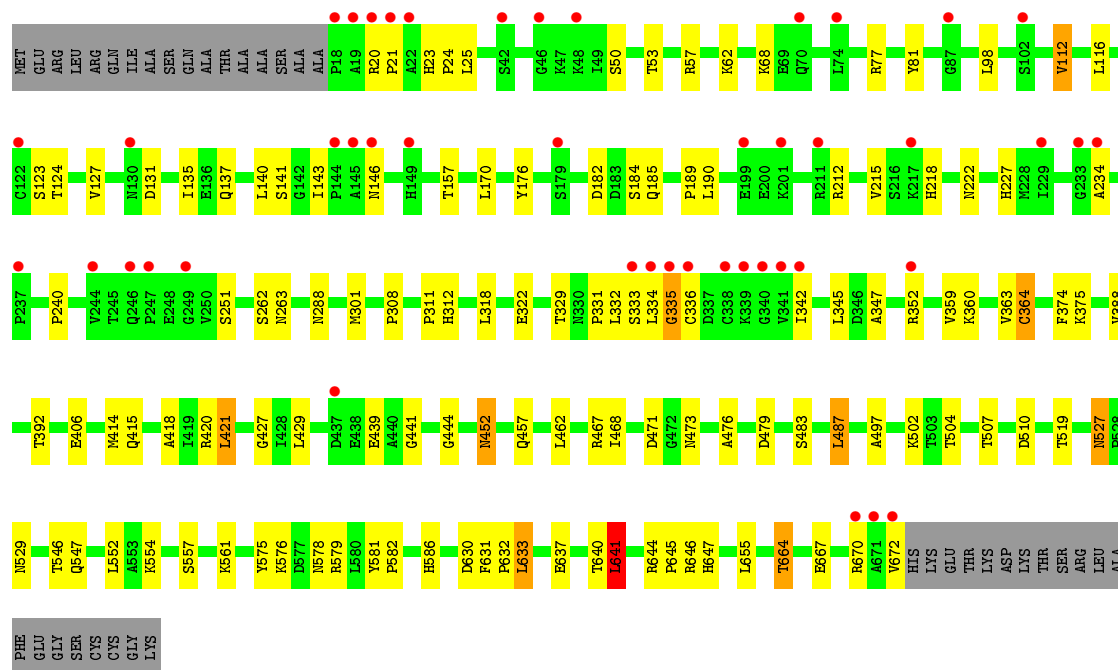
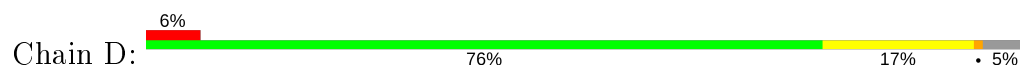





- Molecule 1: Peroxisomal primary amine oxidase

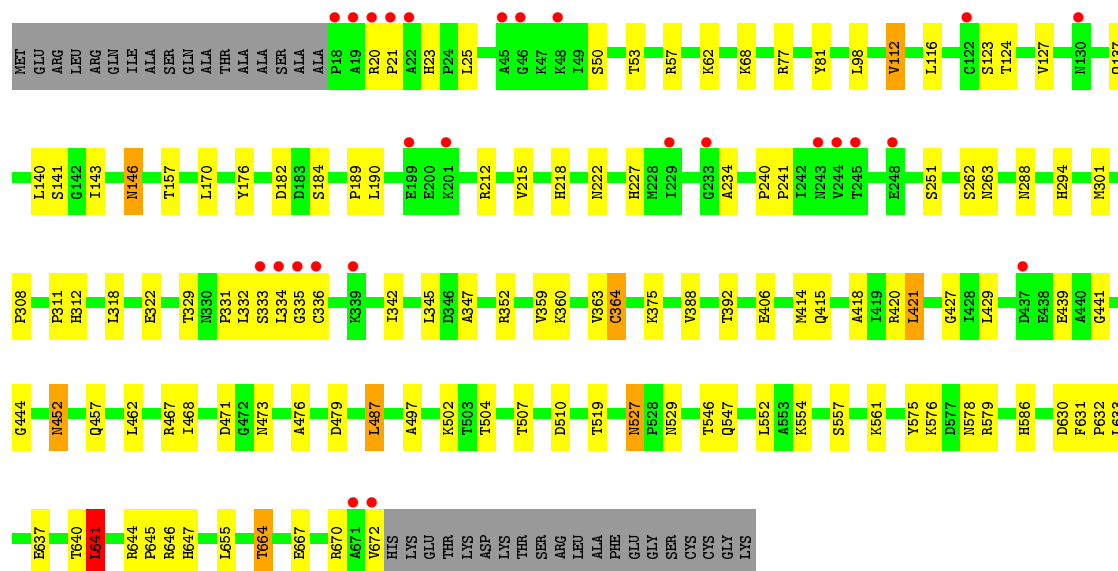


- Molecule 1: Peroxisomal primary amine oxidase




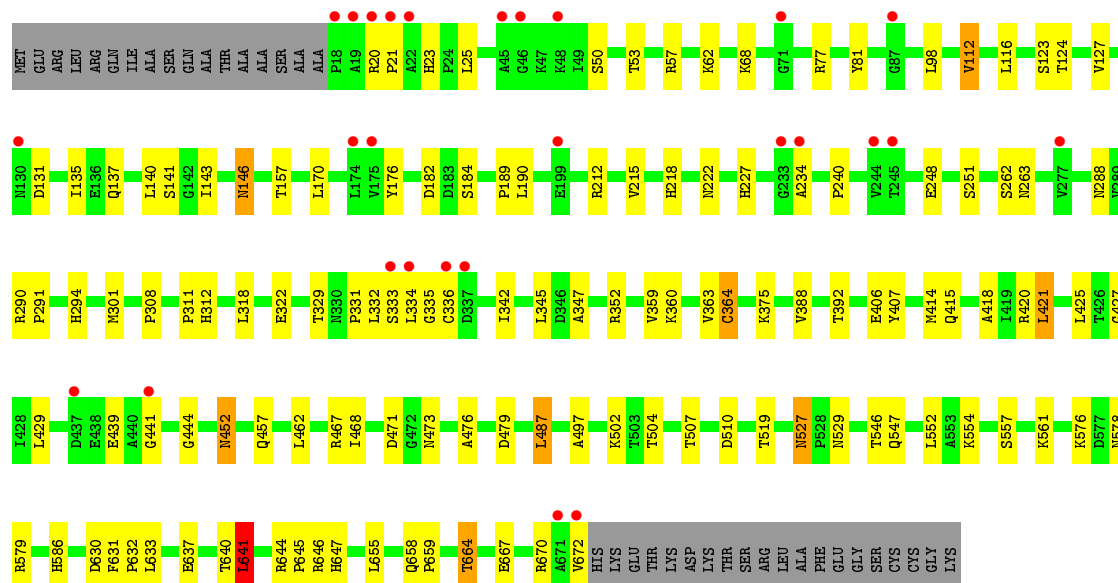
- Molecule 1: Peroxisomal primary amine oxidase

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, $\alpha$ , $\beta$ , $\gamma$	96.29Å 232.47Å 104.31Å 90.00° 93.68° 90.00°	Depositor
Resolution (Å)	29.88 – 1.90 29.88 – 1.85	Depositor EDS
% Data completeness (in resolution range)	76.1 (29.88-1.90) 72.3 (29.88-1.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 1.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.213 , 0.217 0.202 , 0.206	Depositor DCC
$R_{free}$ test set	13502 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.1	Xtriage
Anisotropy	0.899	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	34140	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, TY8, TY9, CU, ME0

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	0.33	0/5326	0.68	3/7246 (0.0%)
1	B	0.33	0/5326	0.68	3/7246 (0.0%)
1	C	0.33	0/5326	0.68	3/7246 (0.0%)
1	D	0.33	0/5326	0.68	3/7246 (0.0%)
1	E	0.33	0/5326	0.68	3/7246 (0.0%)
1	F	0.33	0/5326	0.68	3/7246 (0.0%)
All	All	0.33	0/31956	0.68	18/43476 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	641	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	641	LEU	CA-CB-CG	5.78	128.59	115.30
1	C	641	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	641	LEU	CA-CB-CG	5.77	128.57	115.30
1	D	641	LEU	CA-CB-CG	5.77	128.57	115.30
1	E	641	LEU	CA-CB-CG	5.74	128.51	115.30
1	E	184	SER	N-CA-C	-5.20	96.95	111.00
1	A	184	SER	N-CA-C	-5.19	96.98	111.00
1	C	184	SER	N-CA-C	-5.19	96.98	111.00
1	D	184	SER	N-CA-C	-5.19	96.98	111.00
1	F	487	LEU	CA-CB-CG	5.19	127.24	115.30
1	E	487	LEU	CA-CB-CG	5.19	127.23	115.30
1	B	184	SER	N-CA-C	-5.19	97.00	111.00
1	F	184	SER	N-CA-C	-5.18	97.00	111.00
1	D	487	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	487	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	487	LEU	CA-CB-CG	5.18	127.21	115.30
1	C	487	LEU	CA-CB-CG	5.16	127.16	115.30

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	5219	0	5044	118	2
1	B	5219	0	5044	121	0
1	C	5219	0	5044	116	0
1	D	5219	0	5044	121	0
1	E	5219	0	5044	117	0
1	F	5219	0	5044	120	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	15	0	0	1	0
3	B	15	0	0	1	0
3	C	15	0	0	1	0
3	D	15	0	0	1	0
3	E	15	0	0	1	0
3	F	15	0	0	1	0
4	A	456	0	0	11	0
4	B	456	0	0	11	0
4	C	453	0	0	10	0
4	D	455	0	0	10	0
4	E	454	0	0	11	2
4	F	456	0	0	11	0
All	All	34140	0	30264	648	2

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 11.

All (648) 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:546:THR:HG21	1:B:546:THR:CG2	1.63	1.28
1:A:546:THR:CG2	1:B:546:THR:HG21	1.64	1.28
1:C:546:THR:CG2	1:D:546:THR:HG21	1.65	1.26
1:E:546:THR:HG21	1:F:546:THR:CG2	1.67	1.25
1:E:546:THR:CG2	1:F:546:THR:HG21	1.66	1.25
1:C:546:THR:HG21	1:D:546:THR:CG2	1.65	1.24
1:A:546:THR:HG21	1:B:546:THR:HG21	1.14	1.12
1:E:546:THR:HG21	1:F:546:THR:HG21	1.14	1.09
1:C:546:THR:HG21	1:D:546:THR:HG21	1.14	1.05
1:A:116:LEU:HD12	1:A:157:THR:HG22	1.40	1.04
1:D:116:LEU:HD12	1:D:157:THR:HG22	1.40	1.03
1:C:116:LEU:HD12	1:C:157:THR:HG22	1.40	1.02
1:B:116:LEU:HD12	1:B:157:THR:HG22	1.40	1.02
1:F:116:LEU:HD12	1:F:157:THR:HG22	1.40	1.01
1:E:116:LEU:HD12	1:E:157:THR:HG22	1.40	1.00
1:F:23:HIS:HD2	1:F:25:LEU:H	1.09	1.00
1:E:23:HIS:HD2	1:E:25:LEU:H	1.09	0.97
1:B:23:HIS:HD2	1:B:25:LEU:H	1.09	0.97
1:C:23:HIS:HD2	1:C:25:LEU:H	1.09	0.96
1:D:23:HIS:HD2	1:D:25:LEU:H	1.09	0.94
1:A:23:HIS:HD2	1:A:25:LEU:H	1.09	0.91
1:A:546:THR:HG21	1:B:546:THR:HG23	1.55	0.89
1:C:546:THR:HG23	1:D:546:THR:HG21	1.56	0.87
1:A:546:THR:HG23	1:B:546:THR:HG21	1.56	0.86
1:C:546:THR:HG21	1:D:546:THR:HG23	1.57	0.85
1:F:439:GLU:HG3	1:F:441:GLY:H	1.41	0.84
1:A:439:GLU:HG3	1:A:441:GLY:H	1.41	0.84
1:C:439:GLU:HG3	1:C:441:GLY:H	1.41	0.84
1:E:546:THR:HG23	1:F:546:THR:HG21	1.58	0.84
1:E:664:THR:HG22	1:E:667:GLU:H	1.43	0.84
1:C:664:THR:HG22	1:C:667:GLU:H	1.43	0.84
1:D:439:GLU:HG3	1:D:441:GLY:H	1.41	0.83
1:F:664:THR:HG22	1:F:667:GLU:H	1.43	0.83
1:E:439:GLU:HG3	1:E:441:GLY:H	1.41	0.83
1:B:664:THR:HG22	1:B:667:GLU:H	1.43	0.83
1:B:439:GLU:HG3	1:B:441:GLY:H	1.41	0.83
1:D:664:THR:HG22	1:D:667:GLU:H	1.43	0.83
1:E:546:THR:HG21	1:F:546:THR:HG23	1.59	0.82
1:D:137:GLN:OE1	1:D:212:ARG:NH2	2.11	0.81
1:A:664:THR:HG22	1:A:667:GLU:H	1.43	0.81
1:F:137:GLN:OE1	1:F:212:ARG:NH2	2.11	0.81
1:B:137:GLN:OE1	1:B:212:ARG:NH2	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLN:OE1	1:A:212:ARG:NH2	2.11	0.80
1:C:546:THR:CG2	1:D:546:THR:CG2	2.41	0.78
1:E:137:GLN:OE1	1:E:212:ARG:NH2	2.11	0.77
1:C:137:GLN:OE1	1:C:212:ARG:NH2	2.11	0.77
1:D:347:ALA:HB3	1:D:359:VAL:CG1	2.16	0.76
1:E:347:ALA:HB3	1:E:359:VAL:CG1	2.16	0.76
1:C:347:ALA:HB3	1:C:359:VAL:CG1	2.16	0.76
1:E:546:THR:CG2	1:F:546:THR:CG2	2.43	0.76
1:A:347:ALA:HB3	1:A:359:VAL:CG1	2.16	0.75
1:F:347:ALA:HB3	1:F:359:VAL:CG1	2.16	0.75
1:A:546:THR:CG2	1:B:546:THR:CG2	2.40	0.75
1:B:347:ALA:HB3	1:B:359:VAL:CG1	2.16	0.75
1:B:157:THR:HG21	1:B:322:GLU:HB3	1.69	0.75
1:D:157:THR:HG21	1:D:322:GLU:HB3	1.69	0.75
1:F:116:LEU:CD1	1:F:157:THR:HG22	2.17	0.75
1:C:116:LEU:CD1	1:C:157:THR:HG22	2.17	0.74
1:A:468:ILE:H	1:A:473:ASN:HD21	1.36	0.74
1:E:157:THR:HG21	1:E:322:GLU:HB3	1.69	0.74
1:A:157:THR:HG21	1:A:322:GLU:HB3	1.69	0.74
1:D:116:LEU:CD1	1:D:157:THR:HG22	2.17	0.74
1:E:116:LEU:CD1	1:E:157:THR:HG22	2.17	0.74
1:C:157:THR:HG21	1:C:322:GLU:HB3	1.69	0.74
1:E:468:ILE:H	1:E:473:ASN:HD21	1.36	0.73
1:F:157:THR:HG21	1:F:322:GLU:HB3	1.69	0.73
1:C:468:ILE:H	1:C:473:ASN:HD21	1.35	0.73
1:E:116:LEU:HD12	1:E:157:THR:CG2	2.18	0.73
1:B:116:LEU:CD1	1:B:157:THR:HG22	2.17	0.73
1:D:468:ILE:H	1:D:473:ASN:HD21	1.35	0.72
1:F:116:LEU:HD12	1:F:157:THR:CG2	2.18	0.72
1:B:468:ILE:H	1:B:473:ASN:HD21	1.36	0.71
1:D:23:HIS:CD2	1:D:25:LEU:H	2.02	0.71
1:A:116:LEU:HD12	1:A:157:THR:CG2	2.18	0.71
1:C:23:HIS:CD2	1:C:25:LEU:H	2.02	0.71
1:A:116:LEU:CD1	1:A:157:THR:HG22	2.17	0.71
1:F:527:ASN:HD22	1:F:529:ASN:H	1.39	0.71
1:B:116:LEU:HD12	1:B:157:THR:CG2	2.18	0.71
1:B:23:HIS:CD2	1:B:25:LEU:H	2.02	0.71
1:C:182:ASP:OD1	1:D:664:THR:HG23	1.91	0.71
1:D:116:LEU:HD12	1:D:157:THR:CG2	2.18	0.70
1:F:468:ILE:H	1:F:473:ASN:HD21	1.36	0.70
1:D:527:ASN:HD22	1:D:529:ASN:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ASN:HD22	1:A:529:ASN:H	1.39	0.70
1:C:116:LEU:HD12	1:C:157:THR:CG2	2.18	0.70
1:E:527:ASN:HD22	1:E:529:ASN:H	1.39	0.70
1:E:124:THR:O	1:E:127:VAL:HG22	1.92	0.69
1:A:124:THR:O	1:A:127:VAL:HG22	1.92	0.69
1:A:23:HIS:CD2	1:A:25:LEU:H	2.02	0.69
1:F:124:THR:O	1:F:127:VAL:HG22	1.92	0.69
1:B:527:ASN:HD22	1:B:529:ASN:H	1.39	0.69
1:C:527:ASN:HD22	1:C:529:ASN:H	1.39	0.69
1:D:124:THR:O	1:D:127:VAL:HG22	1.92	0.69
1:C:664:THR:HG23	1:D:182:ASP:OD1	1.93	0.69
1:B:124:THR:O	1:B:127:VAL:HG22	1.92	0.68
1:C:124:THR:O	1:C:127:VAL:HG22	1.92	0.68
1:D:21:PRO:HG3	1:D:77:ARG:CZ	2.25	0.67
1:E:439:GLU:HG3	1:E:441:GLY:N	2.10	0.67
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.25	0.67
1:A:439:GLU:HG3	1:A:441:GLY:N	2.10	0.67
1:A:664:THR:HG23	1:B:182:ASP:OD1	1.95	0.67
1:E:21:PRO:HG3	1:E:77:ARG:CZ	2.25	0.67
1:A:21:PRO:HG3	1:A:77:ARG:CZ	2.25	0.66
1:C:21:PRO:HG3	1:C:77:ARG:CZ	2.25	0.66
1:F:21:PRO:HG3	1:F:77:ARG:CZ	2.25	0.66
1:C:457:GLN:HE22	1:C:552:LEU:H	1.44	0.66
1:A:457:GLN:HE22	1:A:552:LEU:H	1.44	0.66
1:D:457:GLN:HE22	1:D:552:LEU:H	1.44	0.66
1:D:439:GLU:HG3	1:D:441:GLY:N	2.10	0.66
1:B:439:GLU:HG3	1:B:441:GLY:N	2.10	0.65
1:E:23:HIS:CD2	1:E:25:LEU:H	2.02	0.65
1:C:439:GLU:HG3	1:C:441:GLY:N	2.10	0.65
1:F:23:HIS:CD2	1:F:25:LEU:H	2.02	0.64
1:B:457:GLN:HE22	1:B:552:LEU:H	1.44	0.64
1:E:457:GLN:HE22	1:E:552:LEU:H	1.44	0.64
1:C:308:PRO:HB3	1:D:497:ALA:HB2	1.80	0.64
1:A:497:ALA:HB2	1:B:308:PRO:HB3	1.80	0.64
1:F:439:GLU:HG3	1:F:441:GLY:N	2.10	0.64
1:A:182:ASP:OD1	1:B:664:THR:HG23	1.98	0.63
1:F:457:GLN:HE22	1:F:552:LEU:H	1.44	0.63
1:A:439:GLU:C	1:A:441:GLY:H	2.03	0.62
1:E:182:ASP:OD1	1:F:664:THR:HG23	1.97	0.62
1:F:504:THR:HG21	4:F:1326:HOH:O	2.00	0.62
1:B:504:THR:HG21	4:B:1326:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:PRO:HB3	1:B:497:ALA:HB2	1.80	0.62
1:E:664:THR:HG23	1:F:182:ASP:OD1	1.99	0.62
1:D:439:GLU:C	1:D:441:GLY:H	2.03	0.62
1:B:439:GLU:C	1:B:441:GLY:H	2.03	0.62
1:E:504:THR:HG21	4:E:1326:HOH:O	2.00	0.61
1:E:439:GLU:C	1:E:441:GLY:H	2.03	0.61
1:F:439:GLU:C	1:F:441:GLY:H	2.03	0.61
1:A:504:THR:HG21	4:A:1326:HOH:O	2.00	0.61
1:A:112:VAL:HG21	1:A:586:HIS:HB2	1.83	0.61
1:D:504:THR:HG21	4:D:1326:HOH:O	2.00	0.61
1:E:308:PRO:HB3	1:F:497:ALA:HB2	1.83	0.61
1:C:504:THR:HG21	4:C:1326:HOH:O	2.00	0.60
1:C:112:VAL:HG21	1:C:586:HIS:HB2	1.83	0.60
1:B:57:ARG:CZ	1:B:578:ASN:HD21	2.14	0.60
1:B:112:VAL:HG21	1:B:586:HIS:HB2	1.83	0.60
1:F:141:SER:O	1:F:215:VAL:HG23	2.02	0.60
1:C:439:GLU:C	1:C:441:GLY:H	2.03	0.60
1:A:57:ARG:CZ	1:A:578:ASN:HD21	2.14	0.60
1:E:112:VAL:HG21	1:E:586:HIS:HB2	1.83	0.60
1:C:20:ARG:HH11	1:C:20:ARG:HG3	1.67	0.60
1:C:497:ALA:HB2	1:D:308:PRO:HB3	1.84	0.60
1:A:527:ASN:ND2	1:A:529:ASN:H	2.00	0.60
1:C:141:SER:O	1:C:215:VAL:HG23	2.02	0.60
1:F:112:VAL:HG21	1:F:586:HIS:HB2	1.83	0.60
1:A:141:SER:O	1:A:215:VAL:HG23	2.02	0.60
1:C:57:ARG:CZ	1:C:578:ASN:HD21	2.14	0.60
1:D:527:ASN:ND2	1:D:529:ASN:H	2.00	0.59
1:D:112:VAL:HG21	1:D:586:HIS:HB2	1.83	0.59
1:F:467:ARG:HD2	1:F:471:ASP:OD1	2.02	0.59
1:F:644:ARG:HD3	1:F:646:ARG:HD3	1.84	0.59
1:B:644:ARG:HD3	1:B:646:ARG:HD3	1.84	0.59
1:D:141:SER:O	1:D:215:VAL:HG23	2.02	0.59
1:C:507:THR:HG21	4:C:1196:HOH:O	2.02	0.59
1:E:141:SER:O	1:E:215:VAL:HG23	2.02	0.59
1:E:57:ARG:CZ	1:E:578:ASN:HD21	2.14	0.59
1:E:644:ARG:HD3	1:E:646:ARG:HD3	1.84	0.59
1:D:467:ARG:HD2	1:D:471:ASP:OD1	2.03	0.59
1:C:527:ASN:ND2	1:C:529:ASN:H	2.00	0.59
1:D:57:ARG:CZ	1:D:578:ASN:HD21	2.14	0.59
1:E:527:ASN:ND2	1:E:529:ASN:H	2.00	0.59
1:F:20:ARG:HH11	1:F:20:ARG:HG3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ARG:CZ	1:F:578:ASN:HD21	2.14	0.59
1:B:141:SER:O	1:B:215:VAL:HG23	2.02	0.59
1:B:527:ASN:ND2	1:B:529:ASN:H	2.00	0.59
1:A:644:ARG:HD3	1:A:646:ARG:HD3	1.84	0.59
1:D:507:THR:HG21	4:D:1196:HOH:O	2.03	0.59
1:A:20:ARG:HH11	1:A:20:ARG:HG3	1.67	0.59
1:A:507:THR:HG21	4:A:1196:HOH:O	2.02	0.59
1:C:467:ARG:HD2	1:C:471:ASP:OD1	2.02	0.59
1:D:644:ARG:HD3	1:D:646:ARG:HD3	1.84	0.59
1:B:467:ARG:HD2	1:B:471:ASP:OD1	2.02	0.58
1:E:20:ARG:HG3	1:E:20:ARG:HH11	1.67	0.58
1:F:507:THR:HG21	4:F:1196:HOH:O	2.02	0.58
1:F:527:ASN:ND2	1:F:529:ASN:H	2.00	0.58
1:E:467:ARG:HD2	1:E:471:ASP:OD1	2.03	0.58
1:B:507:THR:HG21	4:B:1196:HOH:O	2.02	0.58
1:D:20:ARG:HG3	1:D:20:ARG:HH11	1.67	0.58
1:E:190:LEU:HD22	1:E:215:VAL:HG22	1.86	0.58
1:B:20:ARG:HG3	1:B:20:ARG:HH11	1.67	0.58
1:E:507:THR:HG21	4:E:1196:HOH:O	2.02	0.58
1:A:467:ARG:HD2	1:A:471:ASP:OD1	2.02	0.58
1:B:190:LEU:HD22	1:B:215:VAL:HG22	1.86	0.58
1:C:664:THR:HG23	1:D:182:ASP:CG	2.24	0.58
1:D:190:LEU:HD22	1:D:215:VAL:HG22	1.86	0.58
1:F:190:LEU:HD22	1:F:215:VAL:HG22	1.86	0.57
1:C:644:ARG:HD3	1:C:646:ARG:HD3	1.84	0.57
1:C:190:LEU:HD22	1:C:215:VAL:HG22	1.86	0.57
1:E:497:ALA:HB2	1:F:308:PRO:HB3	1.86	0.57
1:B:527:ASN:HD21	1:B:529:ASN:HB2	1.70	0.57
1:A:527:ASN:HD21	1:A:529:ASN:HB2	1.70	0.56
1:E:527:ASN:HD21	1:E:529:ASN:HB2	1.70	0.56
1:B:112:VAL:CG2	1:B:586:HIS:HB2	2.35	0.56
1:B:527:ASN:C	1:B:527:ASN:HD22	2.09	0.56
1:A:190:LEU:HD22	1:A:215:VAL:HG22	1.86	0.56
1:A:527:ASN:HD22	1:A:527:ASN:C	2.09	0.56
1:C:527:ASN:HD22	1:C:527:ASN:C	2.09	0.56
1:C:527:ASN:HD21	1:C:529:ASN:HB2	1.70	0.56
1:A:112:VAL:CG2	1:A:586:HIS:HB2	2.35	0.56
1:D:112:VAL:CG2	1:D:586:HIS:HB2	2.36	0.56
1:F:112:VAL:CG2	1:F:586:HIS:HB2	2.36	0.56
1:E:112:VAL:CG2	1:E:586:HIS:HB2	2.35	0.56
1:C:112:VAL:CG2	1:C:586:HIS:HB2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:ASN:C	1:D:527:ASN:HD22	2.09	0.56
1:B:468:ILE:N	1:B:473:ASN:HD21	2.04	0.56
1:E:527:ASN:C	1:E:527:ASN:HD22	2.09	0.56
1:F:527:ASN:HD21	1:F:529:ASN:HB2	1.70	0.56
1:D:527:ASN:HD21	1:D:529:ASN:HB2	1.70	0.55
1:B:631:PHE:CG	1:B:632:PRO:HA	2.41	0.55
1:A:631:PHE:CG	1:A:632:PRO:HA	2.41	0.55
1:F:527:ASN:HD22	1:F:527:ASN:C	2.09	0.55
1:C:468:ILE:N	1:C:473:ASN:HD21	2.04	0.55
1:E:468:ILE:N	1:E:473:ASN:HD21	2.04	0.55
1:F:631:PHE:CG	1:F:632:PRO:HA	2.41	0.55
1:E:631:PHE:CG	1:E:632:PRO:HA	2.41	0.55
1:C:631:PHE:CG	1:C:632:PRO:HA	2.41	0.55
1:A:347:ALA:HB3	1:A:359:VAL:HG13	1.90	0.54
1:C:670:ARG:C	1:C:672:VAL:H	2.11	0.54
1:D:631:PHE:CG	1:D:632:PRO:HA	2.41	0.54
1:F:670:ARG:C	1:F:672:VAL:H	2.10	0.54
1:B:670:ARG:C	1:B:672:VAL:H	2.10	0.54
1:E:670:ARG:C	1:E:672:VAL:H	2.11	0.54
1:A:190:LEU:CD2	1:A:215:VAL:HG22	2.38	0.54
1:A:554:LYS:HE3	4:B:1194:HOH:O	2.08	0.54
1:E:347:ALA:HB3	1:E:359:VAL:HG13	1.90	0.54
1:E:406:GLU:HG3	1:F:375:LYS:O	2.08	0.54
1:C:554:LYS:HE3	4:D:1194:HOH:O	2.08	0.54
1:E:190:LEU:CD2	1:E:215:VAL:HG22	2.38	0.54
1:F:347:ALA:HB3	1:F:359:VAL:HG13	1.90	0.54
1:D:468:ILE:N	1:D:473:ASN:HD21	2.04	0.53
1:F:439:GLU:C	1:F:441:GLY:N	2.62	0.53
1:C:439:GLU:C	1:C:441:GLY:N	2.62	0.53
4:C:1194:HOH:O	1:D:554:LYS:HE3	2.08	0.53
1:B:190:LEU:CD2	1:B:215:VAL:HG22	2.38	0.53
1:B:439:GLU:C	1:B:441:GLY:N	2.62	0.53
1:F:190:LEU:CD2	1:F:215:VAL:HG22	2.38	0.53
1:D:439:GLU:C	1:D:441:GLY:N	2.62	0.53
1:A:670:ARG:C	1:A:672:VAL:H	2.10	0.53
1:D:190:LEU:CD2	1:D:215:VAL:HG22	2.38	0.53
1:E:439:GLU:C	1:E:441:GLY:N	2.62	0.53
1:B:392:THR:HG22	4:B:1061:HOH:O	2.09	0.53
1:E:554:LYS:HE3	4:F:1194:HOH:O	2.08	0.53
1:C:190:LEU:CD2	1:C:215:VAL:HG22	2.38	0.53
1:D:670:ARG:C	1:D:672:VAL:H	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:392:THR:HG22	4:F:1061:HOH:O	2.09	0.53
1:F:468:ILE:N	1:F:473:ASN:HD21	2.04	0.53
1:B:347:ALA:HB3	1:B:359:VAL:HG13	1.89	0.52
4:A:1194:HOH:O	1:B:554:LYS:HE3	2.07	0.52
4:E:1194:HOH:O	1:F:554:LYS:HE3	2.08	0.52
1:A:439:GLU:C	1:A:441:GLY:N	2.62	0.52
1:C:632:PRO:HD2	1:D:655:LEU:HD11	1.91	0.52
1:A:468:ILE:N	1:A:473:ASN:HD21	2.04	0.52
1:D:301:MET:O	1:D:318:LEU:HA	2.10	0.52
1:D:392:THR:HG22	4:D:1061:HOH:O	2.09	0.52
1:C:392:THR:HG22	4:C:1061:HOH:O	2.09	0.51
1:F:57:ARG:NE	1:F:578:ASN:HD21	2.09	0.51
1:A:176:TYR:CE1	1:A:189:PRO:HB3	2.46	0.51
1:A:392:THR:HG22	4:A:1061:HOH:O	2.09	0.51
1:B:301:MET:O	1:B:318:LEU:HA	2.10	0.51
1:E:57:ARG:NE	1:E:578:ASN:HD21	2.08	0.51
1:B:57:ARG:NE	1:B:578:ASN:HD21	2.08	0.51
1:E:176:TYR:CE1	1:E:189:PRO:HB3	2.46	0.51
1:D:176:TYR:CE1	1:D:189:PRO:HB3	2.46	0.51
1:F:468:ILE:H	1:F:473:ASN:ND2	2.07	0.51
1:C:176:TYR:CE1	1:C:189:PRO:HB3	2.46	0.51
1:C:347:ALA:HB3	1:C:359:VAL:HG13	1.90	0.51
1:A:301:MET:O	1:A:318:LEU:HA	2.10	0.51
1:C:392:THR:HG22	1:C:415:GLN:OE1	2.11	0.51
1:C:57:ARG:NE	1:C:578:ASN:HD21	2.09	0.51
1:C:62:LYS:HE2	4:C:1309:HOH:O	2.11	0.51
1:A:62:LYS:HE2	4:A:1309:HOH:O	2.11	0.51
1:F:392:THR:HG22	1:F:415:GLN:OE1	2.10	0.51
1:B:176:TYR:CE1	1:B:189:PRO:HB3	2.46	0.51
1:E:392:THR:HG22	4:E:1061:HOH:O	2.09	0.51
1:E:62:LYS:HE2	4:E:1309:HOH:O	2.11	0.51
1:F:62:LYS:HE2	4:F:1309:HOH:O	2.11	0.51
1:A:392:THR:HG22	1:A:415:GLN:OE1	2.10	0.50
1:A:57:ARG:NE	1:A:578:ASN:HD21	2.08	0.50
1:F:176:TYR:CE1	1:F:189:PRO:HB3	2.46	0.50
1:B:392:THR:HG22	1:B:415:GLN:OE1	2.11	0.50
1:D:392:THR:HG22	1:D:415:GLN:OE1	2.10	0.50
1:F:301:MET:O	1:F:318:LEU:HA	2.10	0.50
1:C:406:GLU:HG3	1:D:375:LYS:O	2.12	0.50
1:E:301:MET:O	1:E:318:LEU:HA	2.10	0.50
1:D:375:LYS:HG3	1:D:388:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375:LYS:HG3	1:F:388:VAL:HG22	1.94	0.50
1:D:57:ARG:NE	1:D:578:ASN:HD21	2.09	0.50
1:E:392:THR:HG22	1:E:415:GLN:OE1	2.10	0.50
1:D:62:LYS:HE2	4:D:1309:HOH:O	2.11	0.50
1:E:251:SER:HB3	1:F:240:PRO:HD2	1.94	0.50
1:B:468:ILE:H	1:B:473:ASN:ND2	2.07	0.50
1:C:301:MET:O	1:C:318:LEU:HA	2.10	0.50
1:C:182:ASP:CG	1:D:664:THR:HG23	2.33	0.50
1:E:77:ARG:HG3	1:E:98:LEU:HD12	1.94	0.50
1:F:77:ARG:HG3	1:F:98:LEU:HD12	1.94	0.50
1:C:406:GLU:HG2	1:C:427:GLY:CA	2.43	0.49
1:B:62:LYS:HE2	4:B:1309:HOH:O	2.11	0.49
1:E:240:PRO:HD2	1:F:251:SER:HB3	1.93	0.49
1:B:375:LYS:HG3	1:B:388:VAL:HG22	1.94	0.49
1:E:375:LYS:HG3	1:E:388:VAL:HG22	1.94	0.49
1:F:406:GLU:HG2	1:F:427:GLY:CA	2.43	0.49
1:A:468:ILE:H	1:A:473:ASN:ND2	2.07	0.49
1:A:664:THR:HG23	1:B:182:ASP:CG	2.33	0.49
1:B:547:GLN:NE2	1:B:640:THR:H	2.11	0.49
1:D:347:ALA:HB3	1:D:359:VAL:HG13	1.90	0.49
1:C:375:LYS:HG3	1:C:388:VAL:HG22	1.94	0.49
1:F:429:LEU:HD11	1:F:630:ASP:HB2	1.95	0.49
1:E:637:GLU:HG3	1:F:644:ARG:HH22	1.78	0.49
1:A:429:LEU:HD11	1:A:630:ASP:HB2	1.95	0.49
1:B:429:LEU:HD11	1:B:630:ASP:HB2	1.95	0.49
1:C:77:ARG:HG3	1:C:98:LEU:HD12	1.94	0.49
1:A:77:ARG:HG3	1:A:98:LEU:HD12	1.94	0.49
1:C:655:LEU:HD11	1:D:632:PRO:HD2	1.94	0.49
1:E:406:GLU:HG2	1:E:427:GLY:CA	2.43	0.48
1:E:123:SER:O	1:E:127:VAL:HG13	2.14	0.48
1:B:414:MET:HE2	1:B:420:ARG:HB2	1.96	0.48
1:D:406:GLU:HG2	1:D:427:GLY:CA	2.43	0.48
1:D:429:LEU:HD11	1:D:630:ASP:HB2	1.95	0.48
1:D:77:ARG:HG3	1:D:98:LEU:HD12	1.94	0.48
1:F:547:GLN:NE2	1:F:640:THR:H	2.11	0.48
1:A:375:LYS:HG3	1:A:388:VAL:HG22	1.94	0.48
1:B:406:GLU:HG2	1:B:427:GLY:CA	2.42	0.48
1:B:457:GLN:NE2	1:B:552:LEU:H	2.11	0.48
1:C:429:LEU:HD11	1:C:630:ASP:HB2	1.95	0.48
1:C:547:GLN:NE2	1:C:640:THR:H	2.11	0.48
1:A:406:GLU:HG2	1:A:427:GLY:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:HG3	1:B:98:LEU:HD12	1.94	0.48
1:C:123:SER:O	1:C:127:VAL:HG13	2.14	0.48
1:B:262:SER:O	1:B:263:ASN:HB2	2.14	0.48
1:B:557:SER:O	1:B:561:LYS:HG3	2.14	0.48
1:A:655:LEU:HD11	1:B:632:PRO:HD2	1.95	0.48
1:C:557:SER:O	1:C:561:LYS:HG3	2.14	0.48
1:D:547:GLN:NE2	1:D:640:THR:H	2.11	0.48
1:F:123:SER:O	1:F:127:VAL:HG13	2.14	0.48
1:F:557:SER:O	1:F:561:LYS:HG3	2.14	0.48
1:E:429:LEU:HD11	1:E:630:ASP:HB2	1.95	0.48
1:B:123:SER:O	1:B:127:VAL:HG13	2.14	0.48
1:F:262:SER:O	1:F:263:ASN:HB2	2.14	0.48
1:B:439:GLU:HG3	1:B:441:GLY:CA	2.44	0.48
1:F:50:SER:HB2	1:F:352:ARG:CG	2.44	0.48
1:A:547:GLN:NE2	1:A:640:THR:H	2.11	0.47
1:C:50:SER:HB2	1:C:352:ARG:CG	2.44	0.47
1:D:123:SER:O	1:D:127:VAL:HG13	2.14	0.47
1:C:637:GLU:HG3	1:D:644:ARG:HH22	1.78	0.47
1:E:547:GLN:NE2	1:E:640:THR:H	2.11	0.47
1:A:222:ASN:HB3	1:A:227:HIS:ND1	2.29	0.47
1:A:262:SER:O	1:A:263:ASN:HB2	2.14	0.47
1:A:50:SER:HB2	1:A:352:ARG:CG	2.44	0.47
1:A:644:ARG:HH22	1:B:637:GLU:HG3	1.79	0.47
1:E:234:ALA:HB1	4:E:1259:HOH:O	2.14	0.47
1:E:262:SER:O	1:E:263:ASN:HB2	2.14	0.47
1:E:439:GLU:HG3	1:E:441:GLY:CA	2.44	0.47
1:E:468:ILE:H	1:E:473:ASN:ND2	2.07	0.47
1:F:439:GLU:HG3	1:F:441:GLY:CA	2.44	0.47
1:B:50:SER:HB2	1:B:352:ARG:CG	2.44	0.47
1:D:234:ALA:HB1	4:D:1259:HOH:O	2.15	0.47
1:C:414:MET:HE3	1:C:418:ALA:HB3	1.96	0.47
1:D:50:SER:HB2	1:D:352:ARG:CG	2.44	0.47
1:D:414:MET:HE2	1:D:420:ARG:HB2	1.96	0.47
1:E:457:GLN:NE2	1:E:552:LEU:H	2.11	0.47
1:F:23:HIS:HD2	1:F:25:LEU:N	1.94	0.47
4:E:1024:HOH:O	1:F:375:LYS:HE2	2.13	0.47
1:A:123:SER:O	1:A:127:VAL:HG13	2.14	0.47
1:D:439:GLU:HG3	1:D:441:GLY:CA	2.44	0.47
1:E:414:MET:HE2	1:E:420:ARG:HB2	1.97	0.47
1:A:557:SER:O	1:A:561:LYS:HG3	2.14	0.47
1:C:222:ASN:HB3	1:C:227:HIS:ND1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:SER:HB2	1:E:352:ARG:CG	2.44	0.47
1:F:222:ASN:HB3	1:F:227:HIS:ND1	2.30	0.47
1:A:439:GLU:HG3	1:A:441:GLY:CA	2.44	0.47
1:B:234:ALA:HB1	4:B:1259:HOH:O	2.15	0.47
1:C:262:SER:O	1:C:263:ASN:HB2	2.14	0.47
4:C:1024:HOH:O	1:D:375:LYS:HE2	2.14	0.47
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.50	0.47
1:A:414:MET:HE3	1:A:418:ALA:HB3	1.97	0.47
1:B:218:HIS:HD2	3:B:703:PO4:O4	1.98	0.47
1:D:557:SER:O	1:D:561:LYS:HG3	2.14	0.47
1:F:457:GLN:NE2	1:F:552:LEU:H	2.11	0.47
1:F:631:PHE:CD1	1:F:632:PRO:HA	2.50	0.47
1:A:406:GLU:HG3	1:B:375:LYS:O	2.15	0.47
1:C:143:ILE:HG13	1:C:215:VAL:HG21	1.97	0.47
1:D:222:ASN:HB3	1:D:227:HIS:ND1	2.29	0.47
1:E:222:ASN:HB3	1:E:227:HIS:ND1	2.29	0.47
1:A:218:HIS:HD2	3:A:703:PO4:O4	1.98	0.46
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.50	0.46
1:C:143:ILE:HD11	1:C:215:VAL:HG21	1.97	0.46
1:D:143:ILE:HD11	1:D:215:VAL:HG21	1.97	0.46
1:D:581:TYR:HA	1:D:582:PRO:HD2	1.82	0.46
1:E:557:SER:O	1:E:561:LYS:HG3	2.14	0.46
1:B:143:ILE:HG13	1:B:215:VAL:HG21	1.97	0.46
1:C:234:ALA:HB1	4:C:1259:HOH:O	2.15	0.46
1:D:527:ASN:HD21	1:D:529:ASN:HD22	1.63	0.46
1:D:631:PHE:CD1	1:D:632:PRO:HA	2.50	0.46
1:E:331:PRO:HD2	4:E:1345:HOH:O	2.16	0.46
1:E:631:PHE:CD1	1:E:632:PRO:HA	2.50	0.46
1:B:527:ASN:HD21	1:B:529:ASN:HD22	1.63	0.46
1:D:218:HIS:HD2	3:D:703:PO4:O4	1.98	0.46
1:D:444:GLY:HA3	1:D:452:ASN:HD21	1.81	0.46
1:E:218:HIS:HD2	3:E:703:PO4:O4	1.98	0.46
1:B:222:ASN:HB3	1:B:227:HIS:ND1	2.30	0.46
1:B:342:ILE:HG21	1:B:364:CYS:HB2	1.98	0.46
1:B:444:GLY:HA3	1:B:452:ASN:HD21	1.81	0.46
1:A:182:ASP:CG	1:B:664:THR:HG23	2.36	0.46
1:C:439:GLU:HG3	1:C:441:GLY:CA	2.44	0.46
1:E:444:GLY:HA3	1:E:452:ASN:HD21	1.81	0.46
1:E:527:ASN:HD21	1:E:529:ASN:HD22	1.63	0.46
1:A:234:ALA:HB1	4:A:1259:HOH:O	2.15	0.46
1:B:331:PRO:HD2	4:B:1345:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LYS:O	1:B:406:GLU:HG3	2.15	0.46
1:C:143:ILE:CG1	1:C:215:VAL:HG21	2.46	0.46
1:D:262:SER:O	1:D:263:ASN:HB2	2.14	0.46
1:E:375:LYS:O	1:F:406:GLU:HG3	2.16	0.46
1:A:143:ILE:CG1	1:A:215:VAL:HG21	2.46	0.46
1:A:143:ILE:HG13	1:A:215:VAL:HG21	1.97	0.46
1:A:444:GLY:HA3	1:A:452:ASN:HD21	1.81	0.46
1:A:527:ASN:HD21	1:A:529:ASN:HD22	1.63	0.46
1:E:143:ILE:CG1	1:E:215:VAL:HG21	2.46	0.46
1:F:143:ILE:HG13	1:F:215:VAL:HG21	1.97	0.46
1:F:527:ASN:HD21	1:F:529:ASN:HD22	1.63	0.46
1:C:331:PRO:HD2	4:C:1345:HOH:O	2.16	0.46
1:F:143:ILE:HD11	1:F:215:VAL:HG21	1.97	0.46
1:A:375:LYS:HE2	4:B:1024:HOH:O	2.16	0.46
1:A:637:GLU:HG3	1:B:644:ARG:HH22	1.80	0.46
1:A:632:PRO:HD2	1:B:655:LEU:HD11	1.98	0.46
1:C:444:GLY:HA3	1:C:452:ASN:HD21	1.81	0.46
1:C:631:PHE:CD1	1:C:632:PRO:HA	2.50	0.46
1:E:664:THR:HG23	1:F:182:ASP:CG	2.36	0.46
1:A:143:ILE:HD11	1:A:215:VAL:HG21	1.97	0.46
1:D:476:ALA:HB2	1:D:504:THR:HA	1.98	0.46
1:E:143:ILE:HD11	1:E:215:VAL:HG21	1.97	0.46
1:E:664:THR:HB	1:E:667:GLU:HG3	1.98	0.46
1:F:234:ALA:HB1	4:F:1259:HOH:O	2.15	0.46
1:F:342:ILE:HG21	1:F:364:CYS:HB2	1.98	0.46
1:B:143:ILE:HD11	1:B:215:VAL:HG21	1.97	0.45
1:C:218:HIS:HD2	3:C:703:PO4:O4	1.98	0.45
1:D:143:ILE:CG1	1:D:215:VAL:HG21	2.46	0.45
1:E:359:VAL:HG13	1:E:359:VAL:O	2.16	0.45
1:F:143:ILE:CG1	1:F:215:VAL:HG21	2.46	0.45
1:A:359:VAL:O	1:A:359:VAL:HG13	2.16	0.45
1:A:476:ALA:HB2	1:A:504:THR:HA	1.98	0.45
1:D:342:ILE:HG21	1:D:364:CYS:HB2	1.98	0.45
1:D:664:THR:HB	1:D:667:GLU:HG3	1.98	0.45
1:E:439:GLU:HG3	1:E:441:GLY:HA2	1.98	0.45
1:F:444:GLY:HA3	1:F:452:ASN:HD21	1.81	0.45
1:A:331:PRO:HD2	4:A:1345:HOH:O	2.16	0.45
1:E:375:LYS:HE2	4:F:1024:HOH:O	2.16	0.45
1:F:664:THR:HB	1:F:667:GLU:HG3	1.98	0.45
1:B:581:TYR:HA	1:B:582:PRO:HD2	1.82	0.45
1:C:359:VAL:O	1:C:359:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:664:THR:HB	1:C:667:GLU:HG3	1.98	0.45
1:F:439:GLU:HG3	1:F:441:GLY:HA2	1.98	0.45
1:F:218:HIS:HD2	3:F:703:PO4:O4	1.98	0.45
1:B:143:ILE:CG1	1:B:215:VAL:HG21	2.46	0.45
1:B:359:VAL:HG13	1:B:359:VAL:O	2.16	0.45
1:D:335:GLY:O	1:D:336:CYS:HB2	2.17	0.45
1:A:457:GLN:NE2	1:A:552:LEU:H	2.11	0.45
1:C:527:ASN:HD21	1:C:529:ASN:HD22	1.63	0.45
1:D:359:VAL:O	1:D:359:VAL:HG13	2.16	0.45
1:F:331:PRO:HD2	4:F:1345:HOH:O	2.15	0.45
1:C:335:GLY:O	1:C:336:CYS:HB2	2.17	0.45
1:D:457:GLN:NE2	1:D:552:LEU:H	2.11	0.45
1:F:359:VAL:HG13	1:F:359:VAL:O	2.16	0.45
1:E:335:GLY:O	1:E:336:CYS:HB2	2.17	0.45
1:B:664:THR:HB	1:B:667:GLU:HG3	1.98	0.45
1:D:439:GLU:HG3	1:D:441:GLY:HA2	1.98	0.45
1:D:143:ILE:HG13	1:D:215:VAL:HG21	1.97	0.45
1:D:331:PRO:HD2	4:D:1345:HOH:O	2.16	0.45
1:B:439:GLU:HG3	1:B:441:GLY:HA2	1.98	0.44
1:C:457:GLN:NE2	1:C:552:LEU:H	2.11	0.44
1:F:476:ALA:HB2	1:F:504:THR:HA	1.98	0.44
1:A:312:HIS:HE1	4:A:1015:HOH:O	2.00	0.44
1:B:335:GLY:O	1:B:336:CYS:HB2	2.17	0.44
1:E:143:ILE:HG13	1:E:215:VAL:HG21	1.97	0.44
1:E:23:HIS:HD2	1:E:25:LEU:N	1.94	0.44
1:A:342:ILE:HG21	1:A:364:CYS:HB2	1.98	0.44
1:B:476:ALA:HB2	1:B:504:THR:HA	1.98	0.44
1:B:479:ASP:HB3	1:B:519:THR:HB	2.00	0.44
1:E:342:ILE:HG21	1:E:364:CYS:HB2	1.98	0.44
1:B:23:HIS:HD2	1:B:25:LEU:N	1.94	0.44
1:E:312:HIS:HE1	4:E:1015:HOH:O	2.00	0.44
1:F:414:MET:HE2	1:F:420:ARG:HB2	2.00	0.44
1:A:335:GLY:O	1:A:336:CYS:HB2	2.17	0.44
1:C:468:ILE:H	1:C:473:ASN:ND2	2.07	0.44
1:D:345:LEU:HB2	1:D:363:VAL:HB	2.00	0.44
1:C:633:LEU:HD13	1:D:374:PHE:CD1	2.53	0.44
1:F:312:HIS:HE1	4:F:1015:HOH:O	2.00	0.44
1:A:345:LEU:HB2	1:A:363:VAL:HB	2.00	0.44
1:A:439:GLU:HG3	1:A:441:GLY:HA2	1.98	0.44
1:C:375:LYS:HE2	4:D:1024:HOH:O	2.17	0.44
1:C:439:GLU:HG3	1:C:441:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:ALA:HB2	1:C:504:THR:HA	1.98	0.44
1:E:345:LEU:HB2	1:E:363:VAL:HB	2.00	0.44
1:E:632:PRO:HD2	1:F:655:LEU:HD11	2.00	0.44
1:A:646:ARG:O	1:A:647:HIS:HB2	2.18	0.44
1:C:342:ILE:HG21	1:C:364:CYS:HB2	1.98	0.44
1:D:576:LYS:HB2	1:D:579:ARG:HD2	2.00	0.44
1:E:476:ALA:HB2	1:E:504:THR:HA	1.98	0.44
1:F:335:GLY:O	1:F:336:CYS:HB2	2.17	0.44
1:A:479:ASP:HB3	1:A:519:THR:HB	2.00	0.44
1:D:312:HIS:HE1	4:D:1015:HOH:O	2.00	0.44
1:F:414:MET:HE3	1:F:418:ALA:HB3	2.00	0.44
1:F:479:ASP:HB3	1:F:519:THR:HB	2.00	0.44
1:E:644:ARG:HH22	1:F:637:GLU:HG3	1.83	0.44
1:F:646:ARG:O	1:F:647:HIS:HB2	2.18	0.44
1:A:290:ARG:HA	1:A:291:PRO:HD3	1.91	0.44
1:B:345:LEU:HB2	1:B:363:VAL:HB	2.00	0.44
1:C:646:ARG:O	1:C:647:HIS:HB2	2.18	0.44
1:E:646:ARG:O	1:E:647:HIS:HB2	2.18	0.44
1:A:664:THR:HB	1:A:667:GLU:HG3	1.98	0.43
1:B:576:LYS:HB2	1:B:579:ARG:HD2	2.00	0.43
1:C:20:ARG:NH1	1:C:20:ARG:HG3	2.33	0.43
1:D:20:ARG:HG3	1:D:20:ARG:NH1	2.33	0.43
1:E:576:LYS:HB2	1:E:579:ARG:HD2	2.00	0.43
1:F:345:LEU:HB2	1:F:363:VAL:HB	2.00	0.43
1:A:240:PRO:HD2	1:B:251:SER:HB3	1.98	0.43
1:D:468:ILE:H	1:D:473:ASN:ND2	2.07	0.43
1:B:20:ARG:NH1	1:B:20:ARG:HG3	2.33	0.43
1:F:672:VAL:HG12	1:F:672:VAL:O	2.19	0.43
1:C:479:ASP:HB3	1:C:519:THR:HB	2.00	0.43
1:D:646:ARG:O	1:D:647:HIS:HB2	2.18	0.43
4:A:1024:HOH:O	1:B:375:LYS:HE2	2.19	0.43
1:D:502:LYS:HE2	1:D:504:THR:HG22	2.00	0.43
1:A:50:SER:HB2	1:A:352:ARG:HG3	2.01	0.43
1:B:672:VAL:O	1:B:672:VAL:HG12	2.19	0.43
1:E:502:LYS:HE2	1:E:504:THR:HG22	2.00	0.43
1:E:50:SER:HB2	1:E:352:ARG:HG3	2.01	0.43
1:D:479:ASP:HB3	1:D:519:THR:HB	2.00	0.43
1:E:672:VAL:O	1:E:672:VAL:HG12	2.19	0.43
1:A:672:VAL:O	1:A:672:VAL:HG12	2.19	0.43
1:B:502:LYS:HE2	1:B:504:THR:HG22	2.00	0.43
1:C:312:HIS:HE1	4:C:1015:HOH:O	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:HIS:HD2	1:D:25:LEU:N	1.94	0.43
1:B:53:THR:O	1:B:81:TYR:HA	2.19	0.43
1:C:576:LYS:HB2	1:C:579:ARG:HD2	2.00	0.43
1:C:672:VAL:HG12	1:C:672:VAL:O	2.19	0.43
1:F:50:SER:HB2	1:F:352:ARG:HG3	2.01	0.43
1:A:576:LYS:HB2	1:A:579:ARG:HD2	2.00	0.43
1:F:53:THR:O	1:F:81:TYR:HA	2.19	0.43
1:A:502:LYS:HE2	1:A:504:THR:HG22	2.00	0.42
1:B:646:ARG:O	1:B:647:HIS:HB2	2.18	0.42
1:C:554:LYS:NZ	1:D:483:SER:O	2.49	0.42
1:C:644:ARG:HH22	1:D:637:GLU:HG3	1.84	0.42
1:F:290:ARG:HA	1:F:291:PRO:HD3	1.91	0.42
1:C:50:SER:HB2	1:C:352:ARG:HG3	2.01	0.42
1:C:312:HIS:HD2	4:C:1195:HOH:O	2.03	0.42
1:D:672:VAL:O	1:D:672:VAL:HG12	2.19	0.42
1:D:53:THR:O	1:D:81:TYR:HA	2.19	0.42
1:F:576:LYS:HB2	1:F:579:ARG:HD2	2.00	0.42
1:E:312:HIS:HD2	4:E:1195:HOH:O	2.03	0.42
1:A:23:HIS:HD2	1:A:25:LEU:N	1.94	0.42
1:B:312:HIS:HE1	4:B:1015:HOH:O	2.00	0.42
1:C:345:LEU:HB2	1:C:363:VAL:HB	2.00	0.42
1:F:502:LYS:HE2	1:F:504:THR:HG22	2.00	0.42
1:B:50:SER:HB2	1:B:352:ARG:HG3	2.01	0.42
1:E:479:ASP:HB3	1:E:519:THR:HB	2.00	0.42
1:A:452:ASN:C	1:A:452:ASN:HD22	2.23	0.42
1:C:502:LYS:HE2	1:C:504:THR:HG22	2.00	0.42
1:C:53:THR:O	1:C:81:TYR:HA	2.19	0.42
1:E:452:ASN:C	1:E:452:ASN:HD22	2.23	0.42
1:A:20:ARG:HG3	1:A:20:ARG:NH1	2.33	0.42
1:D:50:SER:HB2	1:D:352:ARG:HG3	2.01	0.42
1:F:20:ARG:HG3	1:F:20:ARG:NH1	2.33	0.42
1:F:312:HIS:HD2	4:F:1195:HOH:O	2.03	0.42
1:C:637:GLU:HG3	1:D:644:ARG:NH2	2.35	0.42
1:E:360:LYS:HB3	1:E:360:LYS:NZ	2.35	0.42
1:D:57:ARG:CZ	1:D:578:ASN:ND2	2.83	0.41
1:E:53:THR:O	1:E:81:TYR:HA	2.19	0.41
1:E:241:PRO:HD2	1:F:248:GLU:HB2	2.01	0.41
1:A:670:ARG:C	1:A:672:VAL:N	2.74	0.41
1:B:146:ASN:HD22	1:B:146:ASN:N	2.18	0.41
1:D:421:LEU:HB3	1:D:641:LEU:HD13	2.02	0.41
1:F:360:LYS:HB3	1:F:360:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:THR:O	1:A:81:TYR:HA	2.19	0.41
1:C:23:HIS:HA	1:C:24:PRO:HD3	1.94	0.41
1:C:57:ARG:CZ	1:C:578:ASN:ND2	2.83	0.41
1:D:312:HIS:HD2	4:D:1195:HOH:O	2.03	0.41
1:A:312:HIS:HD2	4:A:1195:HOH:O	2.03	0.41
1:A:374:PHE:CD1	1:B:633:LEU:HD13	2.56	0.41
1:C:360:LYS:NZ	1:C:360:LYS:HB3	2.35	0.41
1:D:360:LYS:NZ	1:D:360:LYS:HB3	2.35	0.41
1:A:575:TYR:O	1:A:576:LYS:HD2	2.21	0.41
1:D:23:HIS:HA	1:D:24:PRO:HD3	1.94	0.41
1:C:240:PRO:HD2	1:D:251:SER:HB3	2.01	0.41
1:F:146:ASN:N	1:F:146:ASN:HD22	2.18	0.41
1:C:645:PRO:O	1:C:646:ARG:HD2	2.21	0.41
1:E:20:ARG:HG3	1:E:20:ARG:NH1	2.33	0.41
1:F:452:ASN:C	1:F:452:ASN:HD22	2.23	0.41
1:E:655:LEU:HD11	1:F:632:PRO:HD2	2.02	0.41
1:F:421:LEU:HB3	1:F:641:LEU:HD13	2.02	0.41
1:A:251:SER:HB3	1:B:240:PRO:HD2	2.02	0.41
1:A:360:LYS:HB3	1:A:360:LYS:NZ	2.35	0.41
1:B:360:LYS:NZ	1:B:360:LYS:HB3	2.35	0.41
1:C:374:PHE:CD1	1:D:633:LEU:HD13	2.56	0.41
1:C:575:TYR:O	1:C:576:LYS:HD2	2.21	0.41
1:E:645:PRO:O	1:E:646:ARG:HD2	2.21	0.41
1:A:131:ASP:O	1:A:135:ILE:HG13	2.21	0.41
1:A:645:PRO:O	1:A:646:ARG:HD2	2.21	0.41
1:B:575:TYR:O	1:B:576:LYS:HD2	2.21	0.41
1:D:645:PRO:O	1:D:646:ARG:HD2	2.21	0.41
1:E:414:MET:HE3	1:E:418:ALA:HB3	2.02	0.41
1:E:507:THR:HG22	1:E:510:ASP:OD2	2.21	0.41
1:E:575:TYR:O	1:E:576:LYS:HD2	2.21	0.41
1:B:414:MET:HE3	1:B:418:ALA:HB3	2.03	0.41
1:C:406:GLU:HG2	1:C:427:GLY:HA3	2.03	0.41
1:D:406:GLU:HG2	1:D:427:GLY:HA3	2.03	0.41
1:A:140:LEU:HD13	4:A:1397:HOH:O	2.21	0.41
1:A:146:ASN:N	1:A:146:ASN:HD22	2.18	0.41
1:A:452:ASN:HD22	1:A:453:ALA:N	2.19	0.41
1:A:421:LEU:HB3	1:A:641:LEU:HD13	2.02	0.41
1:B:131:ASP:O	1:B:135:ILE:HG13	2.21	0.41
1:B:421:LEU:HB3	1:B:641:LEU:HD13	2.02	0.41
1:D:131:ASP:O	1:D:135:ILE:HG13	2.21	0.41
1:E:421:LEU:HB3	1:E:641:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:637:GLU:HG3	1:F:644:ARG:NH2	2.36	0.41
1:F:507:THR:HG22	1:F:510:ASP:OD2	2.21	0.41
1:F:645:PRO:O	1:F:646:ARG:HD2	2.21	0.41
1:B:176:TYR:HB3	1:B:185:GLN:HB2	2.03	0.41
1:B:312:HIS:HD2	4:B:1195:HOH:O	2.03	0.41
1:B:452:ASN:HD22	1:B:452:ASN:C	2.23	0.41
1:B:670:ARG:C	1:B:672:VAL:N	2.74	0.41
1:D:507:THR:HG22	1:D:510:ASP:OD2	2.21	0.41
1:D:575:TYR:O	1:D:576:LYS:HD2	2.21	0.41
1:B:645:PRO:O	1:B:646:ARG:HD2	2.21	0.40
1:D:176:TYR:HB3	1:D:185:GLN:HB2	2.03	0.40
1:D:421:LEU:HB3	1:D:641:LEU:CD1	2.51	0.40
1:D:414:MET:HE3	1:D:418:ALA:HB3	2.03	0.40
1:E:146:ASN:HD22	1:E:146:ASN:N	2.18	0.40
1:E:294:HIS:HD2	4:E:1182:HOH:O	2.05	0.40
1:F:670:ARG:C	1:F:672:VAL:N	2.74	0.40
1:B:290:ARG:HA	1:B:291:PRO:HD3	1.91	0.40
1:E:406:GLU:HG2	1:E:427:GLY:HA3	2.03	0.40
1:F:658:GLN:HA	1:F:659:PRO:HD3	1.93	0.40
1:B:406:GLU:HG2	1:B:427:GLY:HA3	2.03	0.40
1:B:57:ARG:CZ	1:B:578:ASN:ND2	2.83	0.40
1:C:131:ASP:O	1:C:135:ILE:HG13	2.21	0.40
1:F:131:ASP:O	1:F:135:ILE:HG13	2.21	0.40
1:F:407:TYR:CD2	1:F:425:LEU:HD22	2.57	0.40
1:A:421:LEU:HB3	1:A:641:LEU:CD1	2.51	0.40
1:B:294:HIS:HD2	4:B:1182:HOH:O	2.05	0.40
1:C:146:ASN:N	1:C:146:ASN:HD22	2.18	0.40
1:C:251:SER:HB3	1:D:240:PRO:HD2	2.04	0.40
1:C:670:ARG:C	1:C:672:VAL:N	2.74	0.40
1:E:421:LEU:HB3	1:E:641:LEU:CD1	2.51	0.40
1:F:294:HIS:HD2	4:F:1182:HOH:O	2.05	0.40
1:F:406:GLU:HG2	1:F:427:GLY:HA3	2.03	0.40

All (2) 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:A:437:ASP:CA	4:E:1439:HOH:O[1_655]	2.07	0.13
1:A:436:ASP:O	4:E:1439:HOH:O[1_655]	2.16	0.04

## 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	651/694 (94%)	619 (95%)	30 (5%)	2 (0%)	41	31
1	B	651/694 (94%)	619 (95%)	29 (4%)	3 (0%)	29	18
1	C	651/694 (94%)	619 (95%)	30 (5%)	2 (0%)	41	31
1	D	651/694 (94%)	619 (95%)	29 (4%)	3 (0%)	29	18
1	E	651/694 (94%)	619 (95%)	30 (5%)	2 (0%)	41	31
1	F	651/694 (94%)	619 (95%)	30 (5%)	2 (0%)	41	31
All	All	3906/4164 (94%)	3714 (95%)	178 (5%)	14 (0%)	34	24

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	SER
1	B	333	SER
1	C	333	SER
1	D	333	SER
1	E	333	SER
1	F	333	SER
1	A	334	LEU
1	B	334	LEU
1	C	334	LEU
1	D	334	LEU
1	E	334	LEU
1	F	334	LEU
1	B	335	GLY
1	D	335	GLY

### 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	565/593 (95%)	547 (97%)	18 (3%)	39	30
1	B	565/593 (95%)	547 (97%)	18 (3%)	39	30
1	C	565/593 (95%)	547 (97%)	18 (3%)	39	30
1	D	565/593 (95%)	547 (97%)	18 (3%)	39	30
1	E	565/593 (95%)	547 (97%)	18 (3%)	39	30
1	F	565/593 (95%)	547 (97%)	18 (3%)	39	30
All	All	3390/3558 (95%)	3282 (97%)	108 (3%)	39	30

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	112	VAL
1	A	140	LEU
1	A	146	ASN
1	A	170	LEU
1	A	288	ASN
1	A	311	PRO
1	A	329	THR
1	A	332	LEU
1	A	364	CYS
1	A	421	LEU
1	A	452	ASN
1	A	462	LEU
1	A	487	LEU
1	A	527	ASN
1	A	633	LEU
1	A	641	LEU
1	A	664	THR
1	B	68	LYS
1	B	112	VAL
1	B	140	LEU
1	B	146	ASN
1	B	170	LEU
1	B	288	ASN
1	B	311	PRO
1	B	329	THR
1	B	332	LEU

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Mol	Chain	Res	Type
1	B	364	CYS
1	B	421	LEU
1	B	452	ASN
1	B	462	LEU
1	B	487	LEU
1	B	527	ASN
1	B	633	LEU
1	B	641	LEU
1	B	664	THR
1	C	68	LYS
1	C	112	VAL
1	C	140	LEU
1	C	146	ASN
1	C	170	LEU
1	C	288	ASN
1	C	311	PRO
1	C	329	THR
1	C	332	LEU
1	C	364	CYS
1	C	421	LEU
1	C	452	ASN
1	C	462	LEU
1	C	487	LEU
1	C	527	ASN
1	C	633	LEU
1	C	641	LEU
1	C	664	THR
1	D	68	LYS
1	D	112	VAL
1	D	140	LEU
1	D	146	ASN
1	D	170	LEU
1	D	288	ASN
1	D	311	PRO
1	D	329	THR
1	D	332	LEU
1	D	364	CYS
1	D	421	LEU
1	D	452	ASN
1	D	462	LEU
1	D	487	LEU
1	D	527	ASN

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Mol	Chain	Res	Type
1	D	633	LEU
1	D	641	LEU
1	D	664	THR
1	E	68	LYS
1	E	112	VAL
1	E	140	LEU
1	E	146	ASN
1	E	170	LEU
1	E	288	ASN
1	E	311	PRO
1	E	329	THR
1	E	332	LEU
1	E	364	CYS
1	E	421	LEU
1	E	452	ASN
1	E	462	LEU
1	E	487	LEU
1	E	527	ASN
1	E	633	LEU
1	E	641	LEU
1	E	664	THR
1	F	68	LYS
1	F	112	VAL
1	F	140	LEU
1	F	146	ASN
1	F	170	LEU
1	F	288	ASN
1	F	311	PRO
1	F	329	THR
1	F	332	LEU
1	F	364	CYS
1	F	421	LEU
1	F	452	ASN
1	F	462	LEU
1	F	487	LEU
1	F	527	ASN
1	F	633	LEU
1	F	641	LEU
1	F	664	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	66	GLN
1	A	70	GLN
1	A	146	ASN
1	A	218	HIS
1	A	263	ASN
1	A	288	ASN
1	A	294	HIS
1	A	312	HIS
1	A	330	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	A	578	ASN
1	B	23	HIS
1	B	66	GLN
1	B	70	GLN
1	B	146	ASN
1	B	218	HIS
1	B	288	ASN
1	B	294	HIS
1	B	312	HIS
1	B	330	ASN
1	B	382	ASN
1	B	450	ASN
1	B	452	ASN
1	B	457	GLN
1	B	473	ASN
1	B	527	ASN
1	B	547	GLN
1	B	578	ASN
1	C	23	HIS
1	C	66	GLN
1	C	70	GLN
1	C	146	ASN
1	C	218	HIS
1	C	263	ASN
1	C	288	ASN
1	C	294	HIS

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Mol	Chain	Res	Type
1	C	312	HIS
1	C	330	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	C	578	ASN
1	C	658	GLN
1	D	23	HIS
1	D	66	GLN
1	D	70	GLN
1	D	146	ASN
1	D	218	HIS
1	D	288	ASN
1	D	294	HIS
1	D	312	HIS
1	D	330	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	D	578	ASN
1	D	658	GLN
1	E	23	HIS
1	E	66	GLN
1	E	70	GLN
1	E	146	ASN
1	E	218	HIS
1	E	243	ASN
1	E	263	ASN
1	E	288	ASN
1	E	294	HIS
1	E	312	HIS
1	E	330	ASN
1	E	382	ASN
1	E	450	ASN

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Mol	Chain	Res	Type
1	E	452	ASN
1	E	457	GLN
1	E	473	ASN
1	E	527	ASN
1	E	547	GLN
1	E	578	ASN
1	F	23	HIS
1	F	66	GLN
1	F	70	GLN
1	F	146	ASN
1	F	218	HIS
1	F	243	ASN
1	F	288	ASN
1	F	294	HIS
1	F	312	HIS
1	F	330	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
1	F	578	ASN

### 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	TY8	F	405[A]	1	13,16,17	4.95	9 (69%)	15,21,23	2.61	6 (40%)
1	ME0	C	634[A]	1	5,8,9	0.55	0	2,8,10	0.19	0
1	TY9	A	405[B]	-	13,16,17	4.68	8 (61%)	14,21,23	2.04	4 (28%)
1	ME0	D	634[A]	1	5,8,9	0.55	0	2,8,10	0.19	0
1	TY8	C	405[A]	1	13,16,17	4.96	9 (69%)	15,21,23	2.61	6 (40%)
1	TY9	D	405[B]	-	13,16,17	4.67	8 (61%)	14,21,23	2.04	4 (28%)
1	TY8	A	405[A]	1	13,16,17	4.95	9 (69%)	15,21,23	2.61	6 (40%)
1	TY9	F	405[B]	-	13,16,17	4.67	8 (61%)	14,21,23	2.04	4 (28%)
1	ME0	B	634[A]	1	5,8,9	0.58	0	2,8,10	0.18	0
1	TY8	E	405[A]	1	13,16,17	4.95	9 (69%)	15,21,23	2.60	6 (40%)
1	TY8	B	405[A]	1	13,16,17	4.95	9 (69%)	15,21,23	2.60	6 (40%)
1	ME0	F	634[A]	1	5,8,9	0.57	0	2,8,10	0.19	0
1	ME0	E	634[A]	1	5,8,9	0.55	0	2,8,10	0.18	0
1	TY9	E	405[B]	-	13,16,17	4.69	8 (61%)	14,21,23	2.04	4 (28%)
1	TY9	C	405[B]	-	13,16,17	4.69	8 (61%)	14,21,23	2.04	4 (28%)
1	TY8	D	405[A]	1	13,16,17	4.94	9 (69%)	15,21,23	2.61	6 (40%)
1	TY9	B	405[B]	-	13,16,17	4.68	8 (61%)	14,21,23	2.04	4 (28%)
1	ME0	A	634[A]	1	5,8,9	0.56	0	2,8,10	0.19	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	TY8	F	405[A]	1	-	0/5/10/12	0/1/1/1
1	ME0	C	634[A]	1	-	1/5/7/9	-
1	TY9	A	405[B]	-	-	0/5/10/12	0/1/1/1
1	ME0	D	634[A]	1	-	1/5/7/9	-
1	TY8	C	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	TY8	A	405[A]	1	-	0/5/10/12	0/1/1/1
1	TY9	F	405[B]	-	-	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	TY8	B	405[A]	1	-	0/5/10/12	0/1/1/1
1	ME0	F	634[A]	1	-	1/5/7/9	-
1	ME0	E	634[A]	1	-	1/5/7/9	-
1	TY9	E	405[B]	-	-	0/5/10/12	0/1/1/1
1	TY9	C	405[B]	-	-	0/5/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TY8	D	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	A	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	C	405[A]	TY8	C6-C5	8.87	1.51	1.38
1	C	405[B]	TY9	C6-C5	8.87	1.51	1.38
1	E	405[A]	TY8	C6-C5	8.85	1.51	1.38
1	E	405[B]	TY9	C6-C5	8.85	1.51	1.38
1	A	405[B]	TY9	C6-C5	8.82	1.51	1.38
1	A	405[A]	TY8	C6-C5	8.82	1.51	1.38
1	D	405[B]	TY9	C6-C5	8.81	1.51	1.38
1	D	405[A]	TY8	C6-C5	8.81	1.51	1.38
1	B	405[A]	TY8	C6-C5	8.79	1.51	1.38
1	B	405[B]	TY9	C6-C5	8.79	1.51	1.38
1	F	405[A]	TY8	C6-C5	8.77	1.51	1.38
1	F	405[B]	TY9	C6-C5	8.77	1.51	1.38
1	F	405[A]	TY8	CB-C1	-7.42	1.41	1.51
1	B	405[A]	TY8	CB-C1	-7.40	1.41	1.51
1	D	405[A]	TY8	CB-C1	-7.39	1.41	1.51
1	A	405[A]	TY8	CB-C1	-7.38	1.41	1.51
1	C	405[A]	TY8	CB-C1	-7.37	1.41	1.51
1	E	405[A]	TY8	CB-C1	-7.35	1.41	1.51
1	B	405[A]	TY8	C5-C4	6.61	1.52	1.40
1	C	405[A]	TY8	C3-C2	6.61	1.50	1.38
1	C	405[B]	TY9	C2-C3	6.61	1.50	1.38
1	F	405[A]	TY8	C5-C4	6.60	1.52	1.40
1	E	405[A]	TY8	C3-C2	6.60	1.50	1.38
1	E	405[B]	TY9	C2-C3	6.60	1.50	1.38
1	D	405[B]	TY9	C2-C3	6.59	1.50	1.38
1	D	405[A]	TY8	C3-C2	6.59	1.50	1.38
1	B	405[A]	TY8	C3-C2	6.59	1.50	1.38
1	B	405[B]	TY9	C2-C3	6.59	1.50	1.38
1	C	405[A]	TY8	C5-C4	6.59	1.52	1.40
1	D	405[A]	TY8	C5-C4	6.58	1.52	1.40
1	A	405[A]	TY8	C5-C4	6.58	1.52	1.40
1	A	405[B]	TY9	C2-C3	6.57	1.50	1.38
1	A	405[A]	TY8	C3-C2	6.57	1.50	1.38
1	F	405[A]	TY8	C3-C2	6.57	1.50	1.38
1	F	405[B]	TY9	C2-C3	6.57	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405[A]	TY8	C5-C4	6.56	1.52	1.40
1	B	405[B]	TY9	C5-C4	5.83	1.52	1.40
1	F	405[B]	TY9	C5-C4	5.82	1.52	1.40
1	C	405[B]	TY9	C5-C4	5.81	1.52	1.40
1	D	405[B]	TY9	C5-C4	5.80	1.52	1.40
1	A	405[B]	TY9	C5-C4	5.80	1.52	1.40
1	E	405[B]	TY9	C5-C4	5.79	1.52	1.40
1	E	405[B]	TY9	C2-C1	5.60	1.48	1.39
1	B	405[B]	TY9	C2-C1	5.58	1.48	1.39
1	A	405[B]	TY9	C2-C1	5.57	1.48	1.39
1	F	405[B]	TY9	C2-C1	5.56	1.48	1.39
1	C	405[B]	TY9	C2-C1	5.56	1.48	1.39
1	D	405[B]	TY9	C2-C1	5.54	1.48	1.39
1	E	405[A]	TY8	C2-C1	5.42	1.48	1.40
1	C	405[B]	TY9	O3A-O3	-5.41	1.30	1.46
1	B	405[A]	TY8	C2-C1	5.40	1.48	1.40
1	A	405[A]	TY8	C2-C1	5.39	1.48	1.40
1	A	405[B]	TY9	O3A-O3	-5.39	1.30	1.46
1	F	405[B]	TY9	O3A-O3	-5.39	1.30	1.46
1	E	405[B]	TY9	O3A-O3	-5.39	1.30	1.46
1	B	405[B]	TY9	O3A-O3	-5.39	1.30	1.46
1	D	405[B]	TY9	O3A-O3	-5.39	1.30	1.46
1	F	405[A]	TY8	C2-C1	5.38	1.48	1.40
1	C	405[A]	TY8	C2-C1	5.38	1.48	1.40
1	D	405[A]	TY8	C2-C1	5.36	1.48	1.40
1	D	405[B]	TY9	O5-C5	-5.09	1.26	1.36
1	D	405[A]	TY8	O5-C5	-5.09	1.26	1.36
1	E	405[A]	TY8	O5-C5	-5.09	1.26	1.36
1	E	405[B]	TY9	O5-C5	-5.09	1.26	1.36
1	C	405[A]	TY8	O5-C5	-5.08	1.26	1.36
1	C	405[B]	TY9	O5-C5	-5.08	1.26	1.36
1	A	405[B]	TY9	O5-C5	-5.06	1.26	1.36
1	A	405[A]	TY8	O5-C5	-5.06	1.26	1.36
1	B	405[A]	TY8	O5-C5	-5.06	1.26	1.36
1	B	405[B]	TY9	O5-C5	-5.06	1.26	1.36
1	F	405[A]	TY8	O5-C5	-5.05	1.26	1.36
1	F	405[B]	TY9	O5-C5	-5.05	1.26	1.36
1	C	405[A]	TY8	O4A-O4	-4.96	1.32	1.46
1	C	405[B]	TY9	O4A-O4	-4.96	1.32	1.46
1	F	405[A]	TY8	O4A-O4	-4.96	1.32	1.46
1	F	405[B]	TY9	O4A-O4	-4.96	1.32	1.46
1	E	405[A]	TY8	O4A-O4	-4.95	1.32	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405[B]	TY9	O4A-O4	-4.95	1.32	1.46
1	B	405[A]	TY8	O4A-O4	-4.94	1.32	1.46
1	B	405[B]	TY9	O4A-O4	-4.94	1.32	1.46
1	A	405[B]	TY9	O4A-O4	-4.94	1.32	1.46
1	A	405[A]	TY8	O4A-O4	-4.94	1.32	1.46
1	D	405[B]	TY9	O4A-O4	-4.91	1.32	1.46
1	D	405[A]	TY8	O4A-O4	-4.91	1.32	1.46
1	F	405[B]	TY9	CB-C1	-3.97	1.41	1.51
1	B	405[B]	TY9	CB-C1	-3.96	1.41	1.51
1	D	405[B]	TY9	CB-C1	-3.95	1.41	1.51
1	A	405[B]	TY9	CB-C1	-3.95	1.41	1.51
1	C	405[B]	TY9	CB-C1	-3.95	1.41	1.51
1	E	405[B]	TY9	CB-C1	-3.93	1.41	1.51
1	C	405[A]	TY8	O2A-O2	-3.54	1.36	1.46
1	F	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	E	405[A]	TY8	O2A-O2	-3.53	1.36	1.46
1	D	405[A]	TY8	O2A-O2	-3.53	1.36	1.46
1	B	405[A]	TY8	O2A-O2	-3.52	1.36	1.46
1	B	405[A]	TY8	C3-C4	2.28	1.42	1.38
1	F	405[A]	TY8	C3-C4	2.26	1.42	1.38
1	E	405[A]	TY8	C3-C4	2.26	1.42	1.38
1	A	405[A]	TY8	C3-C4	2.25	1.42	1.38
1	C	405[A]	TY8	C3-C4	2.23	1.42	1.38
1	D	405[A]	TY8	C3-C4	2.22	1.42	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	7.12	125.53	114.53
1	B	405[A]	TY8	C1-CB-CA	7.11	125.53	114.53
1	A	405[A]	TY8	C1-CB-CA	7.09	125.49	114.53
1	D	405[A]	TY8	C1-CB-CA	7.08	125.48	114.53
1	C	405[A]	TY8	C1-CB-CA	7.07	125.46	114.53
1	E	405[A]	TY8	C1-CB-CA	7.07	125.46	114.53
1	F	405[B]	TY9	C1-CB-CA	5.65	125.53	114.10
1	B	405[B]	TY9	C1-CB-CA	5.64	125.53	114.10
1	A	405[B]	TY9	C1-CB-CA	5.63	125.49	114.10
1	D	405[B]	TY9	C1-CB-CA	5.62	125.48	114.10
1	C	405[B]	TY9	C1-CB-CA	5.61	125.46	114.10
1	E	405[B]	TY9	C1-CB-CA	5.61	125.46	114.10
1	F	405[A]	TY8	CB-C1-C2	4.26	125.10	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	405[A]	TY8	CB-C1-C2	4.26	125.09	120.89
1	C	405[A]	TY8	CB-C1-C2	4.24	125.08	120.89
1	A	405[A]	TY8	CB-C1-C2	4.24	125.08	120.89
1	E	405[A]	TY8	CB-C1-C2	4.23	125.07	120.89
1	B	405[A]	TY8	CB-C1-C2	4.21	125.04	120.89
1	C	405[B]	TY9	CB-C1-C6	-3.39	114.61	120.44
1	D	405[B]	TY9	CB-C1-C6	-3.39	114.62	120.44
1	E	405[B]	TY9	CB-C1-C6	-3.38	114.63	120.44
1	F	405[B]	TY9	CB-C1-C6	-3.38	114.64	120.44
1	A	405[B]	TY9	CB-C1-C6	-3.38	114.64	120.44
1	B	405[B]	TY9	CB-C1-C6	-3.36	114.67	120.44
1	C	405[A]	TY8	CB-C1-C6	-2.91	114.61	119.77
1	D	405[A]	TY8	CB-C1-C6	-2.90	114.62	119.77
1	E	405[A]	TY8	CB-C1-C6	-2.90	114.63	119.77
1	F	405[A]	TY8	CB-C1-C6	-2.89	114.64	119.77
1	A	405[A]	TY8	CB-C1-C6	-2.89	114.64	119.77
1	B	405[A]	TY8	CB-C1-C6	-2.87	114.67	119.77
1	E	405[A]	TY8	O2-C2-C1	2.85	121.06	116.04
1	C	405[A]	TY8	O2-C2-C1	2.85	121.06	116.04
1	B	405[A]	TY8	O2-C2-C1	2.85	121.06	116.04
1	A	405[A]	TY8	O2-C2-C1	2.84	121.05	116.04
1	F	405[A]	TY8	O2-C2-C1	2.83	121.03	116.04
1	D	405[A]	TY8	O2-C2-C1	2.83	121.03	116.04
1	F	405[B]	TY9	CB-C1-C2	2.72	125.10	120.44
1	D	405[B]	TY9	CB-C1-C2	2.72	125.09	120.44
1	C	405[B]	TY9	CB-C1-C2	2.71	125.08	120.44
1	A	405[B]	TY9	CB-C1-C2	2.71	125.08	120.44
1	E	405[B]	TY9	CB-C1-C2	2.70	125.07	120.44
1	B	405[B]	TY9	CB-C1-C2	2.69	125.04	120.44
1	C	405[A]	TY8	O2-C2-C3	-2.25	118.71	123.78
1	B	405[A]	TY8	O2-C2-C3	-2.25	118.72	123.78
1	D	405[A]	TY8	O2-C2-C3	-2.24	118.72	123.78
1	A	405[A]	TY8	O2-C2-C3	-2.24	118.72	123.78
1	F	405[A]	TY8	O2-C2-C3	-2.24	118.73	123.78
1	E	405[A]	TY8	O2-C2-C3	-2.24	118.73	123.78
1	C	405[A]	TY8	CB-CA-C	-2.09	107.55	111.47
1	C	405[B]	TY9	CB-CA-C	-2.09	107.55	111.47
1	E	405[A]	TY8	CB-CA-C	-2.09	107.56	111.47
1	E	405[B]	TY9	CB-CA-C	-2.09	107.56	111.47
1	A	405[B]	TY9	CB-CA-C	-2.08	107.57	111.47
1	A	405[A]	TY8	CB-CA-C	-2.08	107.57	111.47
1	D	405[B]	TY9	CB-CA-C	-2.08	107.57	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405[A]	TY8	CB-CA-C	-2.08	107.57	111.47
1	D	405[A]	TY8	CB-CA-C	-2.08	107.57	111.47
1	B	405[B]	TY9	CB-CA-C	-2.08	107.57	111.47
1	F	405[A]	TY8	CB-CA-C	-2.07	107.59	111.47
1	F	405[B]	TY9	CB-CA-C	-2.07	107.59	111.47

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	E	703	-	4,4,4	1.71	0	6,6,6	0.43	0
3	PO4	F	703	-	4,4,4	1.71	0	6,6,6	0.44	0
3	PO4	C	703	-	4,4,4	1.71	0	6,6,6	0.43	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	D	703	-	4,4,4	1.72	0	6,6,6	0.43	0
3	PO4	F	704	-	4,4,4	1.68	0	6,6,6	0.42	0
3	PO4	C	702	-	4,4,4	1.59	0	6,6,6	0.43	0
3	PO4	A	702	-	4,4,4	1.59	0	6,6,6	0.42	0
3	PO4	B	704	-	4,4,4	1.66	0	6,6,6	0.41	0
3	PO4	D	704	-	4,4,4	1.66	0	6,6,6	0.42	0
3	PO4	E	702	-	4,4,4	1.58	0	6,6,6	0.43	0
3	PO4	F	702	-	4,4,4	1.58	0	6,6,6	0.43	0
3	PO4	E	704	-	4,4,4	1.68	0	6,6,6	0.41	0
3	PO4	D	702	-	4,4,4	1.58	0	6,6,6	0.42	0
3	PO4	A	704	-	4,4,4	1.67	0	6,6,6	0.42	0
3	PO4	B	702	-	4,4,4	1.59	0	6,6,6	0.43	0
3	PO4	C	704	-	4,4,4	1.67	0	6,6,6	0.41	0
3	PO4	A	703	-	4,4,4	1.71	0	6,6,6	0.43	0
3	PO4	B	703	-	4,4,4	1.71	0	6,6,6	0.43	0

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.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	703	PO4	1	0
3	F	703	PO4	1	0
3	C	703	PO4	1	0
3	D	703	PO4	1	0
3	A	703	PO4	1	0
3	B	703	PO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	653/694 (94%)	0.08	15 (2%)	60	63	14, 25, 46, 80	0
1	B	653/694 (94%)	0.07	27 (4%)	37	40	14, 25, 46, 80	0
1	C	653/694 (94%)	0.09	20 (3%)	49	51	14, 25, 46, 80	0
1	D	653/694 (94%)	0.29	45 (6%)	16	19	14, 25, 46, 80	0
1	E	653/694 (94%)	0.05	26 (3%)	38	41	14, 25, 46, 80	0
1	F	653/694 (94%)	0.12	27 (4%)	37	40	14, 25, 46, 80	0
All	All	3918/4164 (94%)	0.12	160 (4%)	37	40	14, 25, 46, 80	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	672	VAL	11.4
1	B	672	VAL	10.5
1	F	19	ALA	9.7
1	E	672	VAL	8.5
1	D	672	VAL	8.4
1	F	18	PRO	8.2
1	F	672	VAL	7.6
1	D	18	PRO	7.2
1	B	334	LEU	6.9
1	C	334	LEU	6.7
1	E	18	PRO	6.7
1	D	336	CYS	6.6
1	C	672	VAL	6.3
1	B	18	PRO	6.3
1	F	21	PRO	6.0
1	E	19	ALA	5.9
1	B	336	CYS	5.9
1	F	334	LEU	5.7
1	D	19	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
1	F	22	ALA	5.6
1	A	334	LEU	5.5
1	D	333	SER	5.4
1	D	341	VAL	5.4
1	D	20	ARG	5.3
1	B	19	ALA	5.3
1	F	20	ARG	5.2
1	F	336	CYS	5.2
1	D	244	VAL	5.1
1	C	336	CYS	5.0
1	A	671	ALA	4.6
1	F	333	SER	4.5
1	D	22	ALA	4.4
1	E	336	CYS	4.4
1	D	334	LEU	4.4
1	E	334	LEU	4.3
1	C	670	ARG	4.2
1	E	22	ALA	4.2
1	E	46	GLY	4.2
1	C	333	SER	4.1
1	B	20	ARG	4.1
1	E	20	ARG	3.9
1	B	671	ALA	3.8
1	F	48	LYS	3.8
1	D	21	PRO	3.7
1	B	335	GLY	3.7
1	D	342	ILE	3.5
1	B	48	LYS	3.4
1	D	233	GLY	3.4
1	F	130	ASN	3.4
1	D	247	PRO	3.4
1	E	244	VAL	3.4
1	C	233	GLY	3.3
1	D	340	GLY	3.3
1	E	437	ASP	3.3
1	A	20	ARG	3.3
1	B	46	GLY	3.3
1	B	333	SER	3.3
1	F	437	ASP	3.3
1	C	335	GLY	3.3
1	B	437	ASP	3.2
1	B	130	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	339	LYS	3.2
1	D	234	ALA	3.2
1	E	130	ASN	3.2
1	D	437	ASP	3.1
1	F	46	GLY	3.1
1	D	130	ASN	3.1
1	D	70	GLN	3.1
1	F	87	GLY	3.0
1	D	199	GLU	3.0
1	E	48	LYS	3.0
1	C	242	ILE	2.9
1	D	146	ASN	2.9
1	D	339	LYS	2.9
1	E	245	THR	2.9
1	D	671	ALA	2.8
1	D	229	ILE	2.8
1	D	87	GLY	2.8
1	A	234	ALA	2.7
1	C	437	ASP	2.7
1	B	341	VAL	2.6
1	C	48	LYS	2.6
1	D	338	CYS	2.6
1	D	102	SER	2.6
1	E	229	ILE	2.6
1	A	48	LYS	2.6
1	C	671	ALA	2.6
1	C	245	THR	2.6
1	E	199	GLU	2.6
1	D	48	LYS	2.6
1	F	441	GLY	2.6
1	B	45	ALA	2.5
1	B	340	GLY	2.5
1	D	249	GLY	2.5
1	D	670	ARG	2.5
1	D	42	SER	2.5
1	F	671	ALA	2.5
1	A	670	ARG	2.5
1	C	232	VAL	2.5
1	D	74	LEU	2.5
1	E	333	SER	2.5
1	B	633	LEU	2.5
1	D	246	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	199	GLU	2.4
1	B	21	PRO	2.4
1	E	671	ALA	2.4
1	D	217	LYS	2.4
1	D	335	GLY	2.4
1	E	248	GLU	2.4
1	B	74	LEU	2.4
1	A	436	ASP	2.4
1	A	244	VAL	2.4
1	F	175	VAL	2.4
1	E	21	PRO	2.4
1	C	20	ARG	2.3
1	D	211	ARG	2.3
1	C	244	VAL	2.3
1	D	149	HIS	2.3
1	D	201	LYS	2.3
1	F	71	GLY	2.3
1	C	441	GLY	2.3
1	E	233	GLY	2.3
1	F	233	GLY	2.3
1	D	122	CYS	2.3
1	D	46	GLY	2.2
1	B	245	THR	2.2
1	E	201	LYS	2.2
1	F	174	LEU	2.2
1	C	669	LYS	2.2
1	D	145	ALA	2.2
1	B	244	VAL	2.2
1	A	336	CYS	2.2
1	E	122	CYS	2.2
1	B	233	GLY	2.2
1	B	71	GLY	2.2
1	D	352	ARG	2.2
1	F	277	VAL	2.2
1	B	200	GLU	2.1
1	E	243	ASN	2.1
1	D	237	PRO	2.1
1	F	234	ALA	2.1
1	A	156	TRP	2.1
1	B	232	VAL	2.1
1	F	337	ASP	2.1
1	A	338	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	45	ALA	2.1
1	A	333	SER	2.1
1	A	437	ASP	2.1
1	E	335	GLY	2.1
1	A	175	VAL	2.1
1	C	340	GLY	2.1
1	F	245	THR	2.1
1	C	247	PRO	2.1
1	B	670	ARG	2.0
1	E	45	ALA	2.0
1	C	241	PRO	2.0
1	D	144	PRO	2.0
1	B	441	GLY	2.0
1	F	244	VAL	2.0
1	D	179	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	TY9	A	405[B]	16/17	0.83	0.18	24,38,48,51	16
1	TY8	E	405[A]	16/17	0.84	0.22	24,38,48,51	16
1	TY9	D	405[B]	16/17	0.84	0.20	24,38,48,51	16
1	TY9	E	405[B]	16/17	0.84	0.22	24,38,48,51	16
1	TY8	D	405[A]	16/17	0.84	0.20	24,38,48,51	16
1	TY8	A	405[A]	16/17	0.86	0.16	24,38,48,51	16
1	TY9	F	405[B]	16/17	0.88	0.17	24,38,48,51	16
1	TY8	B	405[A]	16/17	0.88	0.19	24,38,48,51	16
1	TY9	C	405[B]	16/17	0.89	0.19	24,38,48,51	16
1	TY9	B	405[B]	16/17	0.89	0.18	24,38,48,51	16
1	TY8	F	405[A]	16/17	0.90	0.17	24,38,48,51	16
1	TY8	C	405[A]	16/17	0.90	0.18	24,38,48,51	16
1	ME0	C	634[A]	9/10	0.92	0.15	21,25,41,42	9
1	ME0	D	634[A]	9/10	0.93	0.15	21,25,41,42	9
1	ME0	F	634[A]	9/10	0.93	0.15	21,25,41,42	9
1	ME0	A	634[A]	9/10	0.95	0.15	21,25,41,42	9
1	ME0	B	634[A]	9/10	0.96	0.14	21,25,41,42	9
1	ME0	E	634[A]	9/10	0.96	0.11	21,25,41,42	9

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PO4	D	704	5/5	0.85	0.20	86,87,87,88	0
3	PO4	B	704	5/5	0.88	0.18	86,87,87,88	0
3	PO4	C	704	5/5	0.91	0.17	86,87,87,88	0
3	PO4	A	704	5/5	0.92	0.14	86,87,87,88	0
3	PO4	D	702	5/5	0.92	0.23	34,36,38,39	0
3	PO4	E	704	5/5	0.93	0.22	86,87,87,88	0
3	PO4	E	703	5/5	0.94	0.13	46,49,49,50	0
3	PO4	F	704	5/5	0.94	0.17	86,87,87,88	0
3	PO4	C	702	5/5	0.95	0.10	34,36,38,39	0
3	PO4	D	703	5/5	0.95	0.18	46,49,49,50	0
3	PO4	F	703	5/5	0.95	0.12	46,49,49,50	0
3	PO4	B	702	5/5	0.97	0.11	34,36,38,39	0
3	PO4	C	703	5/5	0.97	0.19	46,49,49,50	0
3	PO4	B	703	5/5	0.97	0.08	46,49,49,50	0
3	PO4	E	702	5/5	0.98	0.11	34,36,38,39	0
3	PO4	F	702	5/5	0.98	0.09	34,36,38,39	0
3	PO4	A	702	5/5	0.98	0.08	34,36,38,39	0
2	CU	C	701	1/1	0.99	0.04	22,22,22,22	0
2	CU	D	701	1/1	0.99	0.03	22,22,22,22	0
2	CU	F	701	1/1	0.99	0.04	22,22,22,22	0
2	CU	E	701	1/1	0.99	0.08	22,22,22,22	0
3	PO4	A	703	5/5	0.99	0.08	46,49,49,50	0
2	CU	B	701	1/1	1.00	0.07	22,22,22,22	0
2	CU	A	701	1/1	1.00	0.07	22,22,22,22	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.