



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:31 AM UTC

PDB ID : 3NBJ / pdb_00003nbj
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

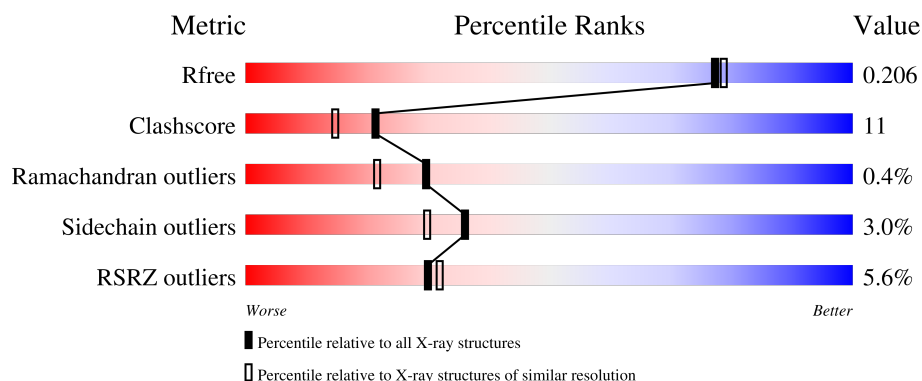
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	694	6% 73% 19% • 5%
1	B	694	5% 73% 19% • 5%
1	C	694	6% 74% 19% • 5%
1	D	694	5% 74% 19% • 5%
1	E	694	4% 74% 19% • 5%

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Mol	Chain	Length	Quality of chain
1	F	694	5% 73% 19% • 5%

2 Entry composition

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 (CCD ID: CU) (formula: Cu).

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

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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	F	1	Total	Cu	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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		

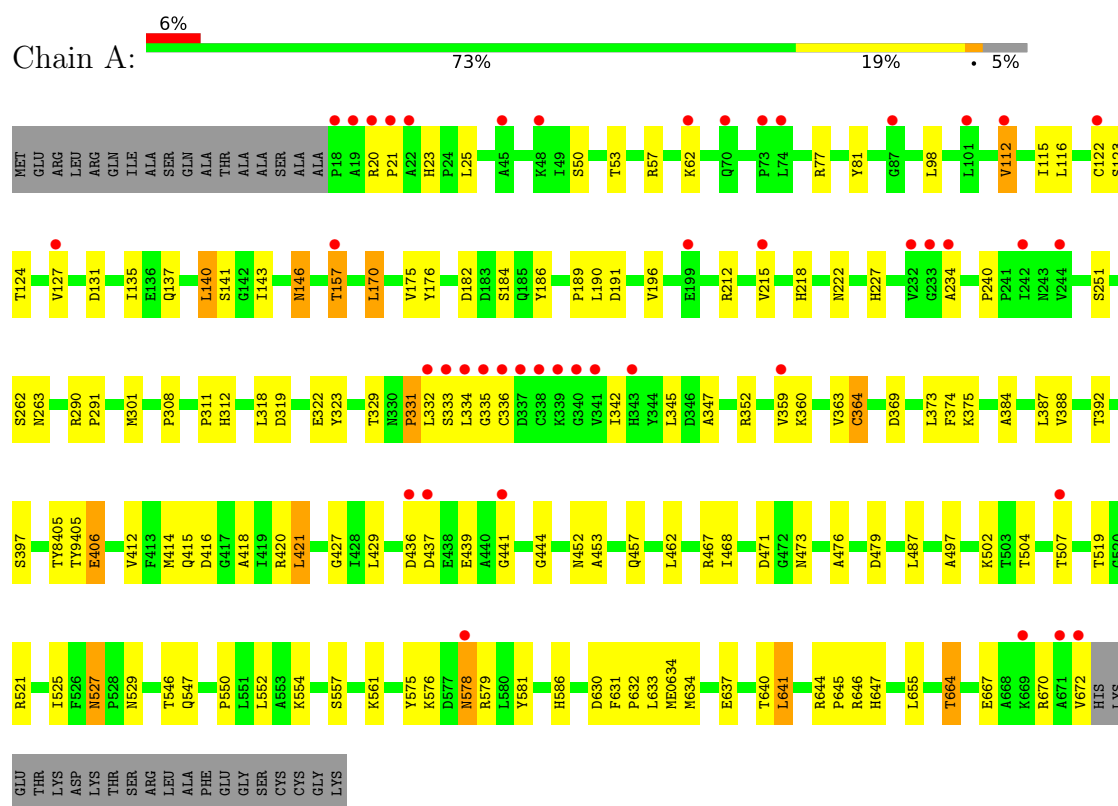
- Molecule 4 is water.

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		

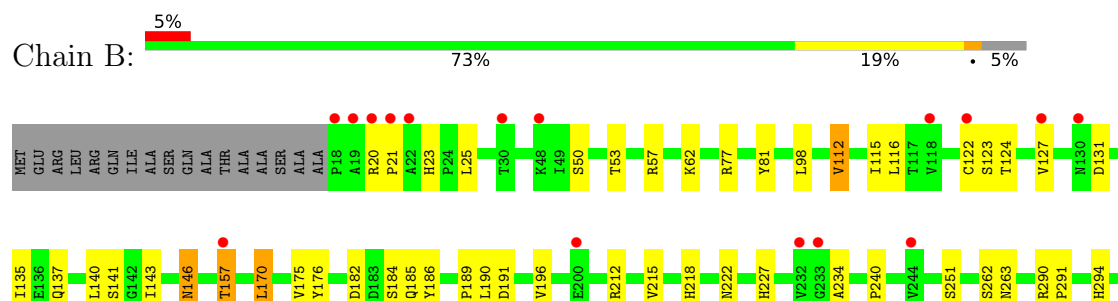
3 Residue-property plots [i](#)

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

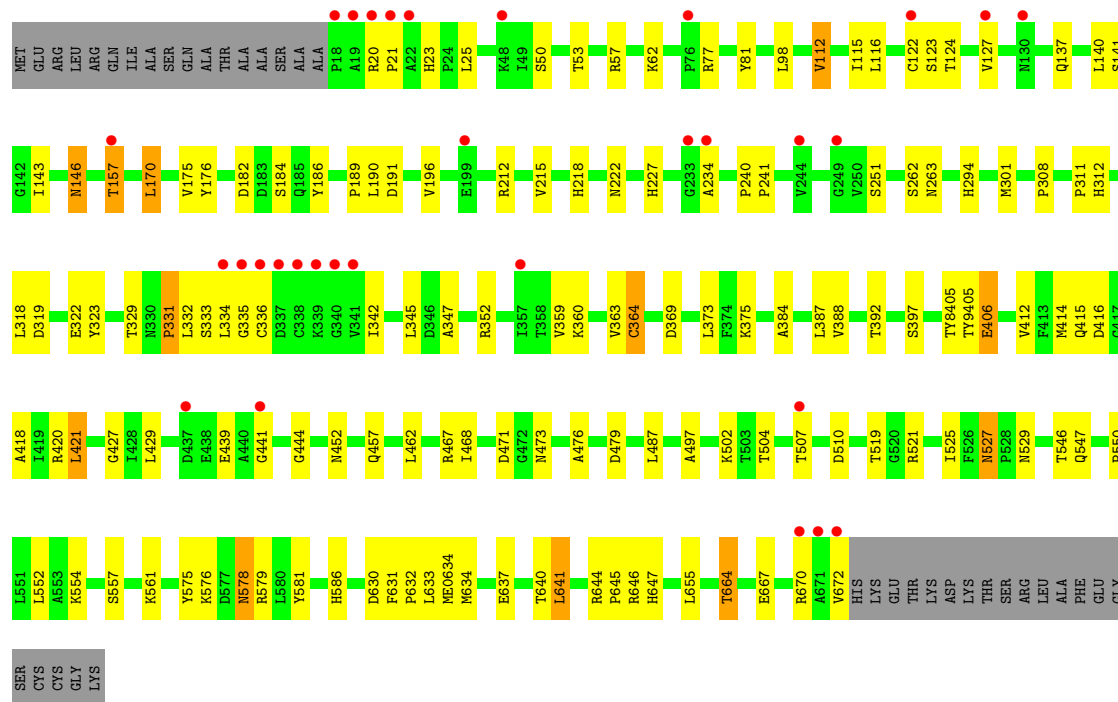
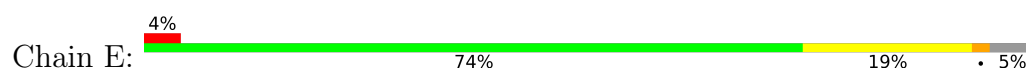


• Molecule 1: Peroxisomal primary amine oxidase

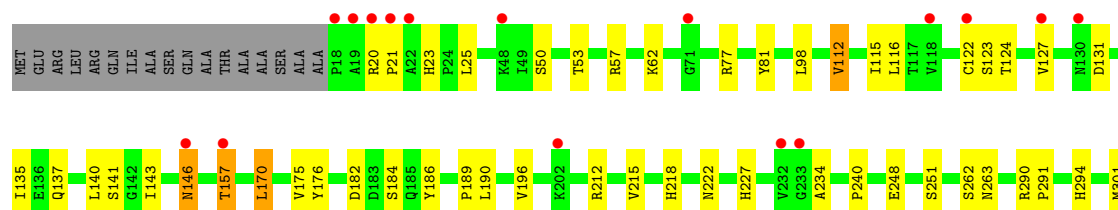
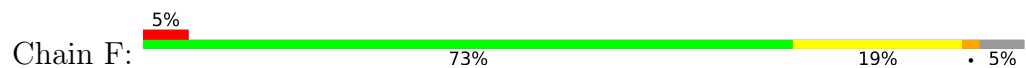


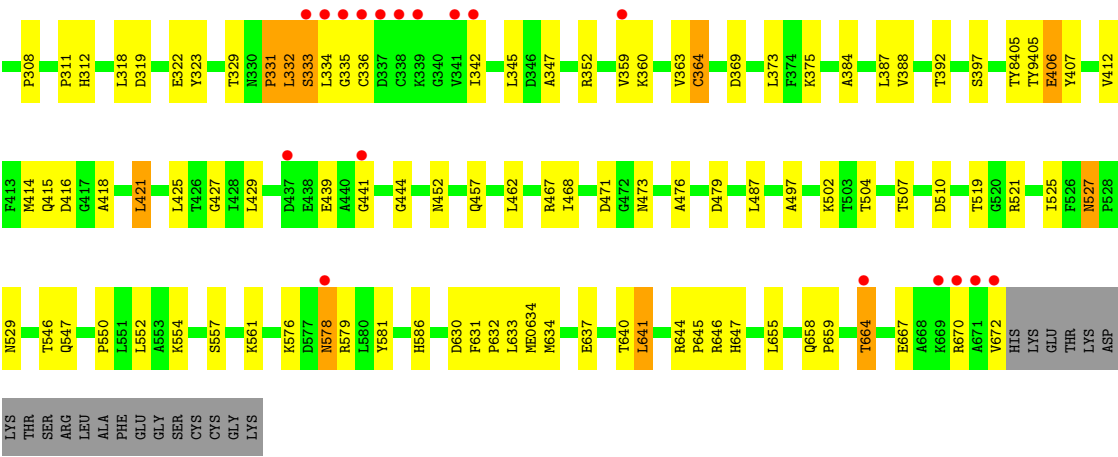


- Molecule 1: Peroxisomal primary amine oxidase



- Molecule 1: Peroxisomal primary amine oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.29Å 232.47Å 104.31Å 90.00° 93.68° 90.00°	Depositor
Resolution (Å)	29.88 – 1.90 29.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	76.1 (29.88-1.90) 76.1 (29.88-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	16.1	Xtriage
Anisotropy	0.899	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.36	0/5326	0.97	22/7246 (0.3%)
1	B	0.36	0/5326	0.97	22/7246 (0.3%)
1	C	0.36	0/5326	0.97	22/7246 (0.3%)
1	D	0.36	0/5326	0.97	22/7246 (0.3%)
1	E	0.36	0/5326	0.97	22/7246 (0.3%)
1	F	0.36	0/5326	0.97	21/7246 (0.3%)
All	All	0.36	0/31956	0.97	131/43476 (0.3%)

There are no bond length outliers.

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	THR	N-CA-C	-8.69	98.25	110.50
1	D	157	THR	N-CA-C	-8.68	98.27	110.50
1	A	157	THR	N-CA-C	-8.67	98.28	110.50
1	E	157	THR	N-CA-C	-8.67	98.27	110.50
1	C	157	THR	N-CA-C	-8.66	98.28	110.50
1	F	157	THR	N-CA-C	-8.66	98.29	110.50
1	F	581	TYR	CA-C-N	6.58	126.28	119.56
1	F	581	TYR	C-N-CA	6.58	126.28	119.56
1	E	184	SER	N-CA-C	-6.58	96.95	108.20
1	D	581	TYR	CA-C-N	6.58	126.27	119.56
1	D	581	TYR	C-N-CA	6.58	126.27	119.56
1	A	184	SER	N-CA-C	-6.56	96.98	108.20
1	C	184	SER	N-CA-C	-6.56	96.98	108.20
1	D	184	SER	N-CA-C	-6.56	96.98	108.20
1	A	581	TYR	CA-C-N	6.56	126.25	119.56
1	A	581	TYR	C-N-CA	6.56	126.25	119.56
1	B	184	SER	N-CA-C	-6.55	97.00	108.20
1	E	581	TYR	CA-C-N	6.55	126.24	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	581	TYR	C-N-CA	6.55	126.24	119.56
1	F	184	SER	N-CA-C	-6.55	97.00	108.20
1	C	581	TYR	CA-C-N	6.53	126.22	119.56
1	C	581	TYR	C-N-CA	6.53	126.22	119.56
1	B	581	TYR	CA-C-N	6.51	126.20	119.56
1	B	581	TYR	C-N-CA	6.51	126.20	119.56
1	B	196	VAL	N-CA-C	6.27	116.94	108.17
1	E	196	VAL	N-CA-C	6.25	116.92	108.17
1	D	196	VAL	N-CA-C	6.24	116.91	108.17
1	D	416	ASP	N-CA-C	-6.24	105.24	112.92
1	C	196	VAL	N-CA-C	6.24	116.91	108.17
1	A	196	VAL	N-CA-C	6.24	116.90	108.17
1	E	416	ASP	N-CA-C	-6.23	105.25	112.92
1	F	196	VAL	N-CA-C	6.23	116.89	108.17
1	B	416	ASP	N-CA-C	-6.21	105.28	112.92
1	A	416	ASP	N-CA-C	-6.21	105.28	112.92
1	C	416	ASP	N-CA-C	-6.21	105.28	112.92
1	F	416	ASP	N-CA-C	-6.21	105.28	112.92
1	E	331	PRO	N-CA-C	-6.09	101.60	110.80
1	C	331	PRO	N-CA-C	-6.09	101.60	110.80
1	B	331	PRO	N-CA-C	-6.09	101.61	110.80
1	A	331	PRO	N-CA-C	-6.08	101.62	110.80
1	C	550	PRO	N-CA-C	-6.05	102.38	111.57
1	D	331	PRO	N-CA-C	-6.05	101.67	110.80
1	D	550	PRO	N-CA-C	-6.04	102.39	111.57
1	F	331	PRO	N-CA-C	-6.04	101.68	110.80
1	A	550	PRO	N-CA-C	-6.02	102.43	111.57
1	B	550	PRO	N-CA-C	-6.01	102.43	111.57
1	F	550	PRO	N-CA-C	-6.01	102.43	111.57
1	B	186	TYR	N-CA-C	6.01	120.08	112.87
1	E	550	PRO	N-CA-C	-6.01	102.44	111.57
1	F	186	TYR	N-CA-C	5.98	120.05	112.87
1	C	373	LEU	N-CA-C	-5.97	104.15	112.45
1	D	373	LEU	N-CA-C	-5.97	104.14	112.45
1	A	373	LEU	N-CA-C	-5.97	104.15	112.45
1	A	186	TYR	N-CA-C	5.97	120.03	112.87
1	E	186	TYR	N-CA-C	5.96	120.03	112.87
1	E	373	LEU	N-CA-C	-5.96	104.16	112.45
1	B	373	LEU	N-CA-C	-5.96	104.17	112.45
1	C	186	TYR	N-CA-C	5.95	120.02	112.87
1	F	373	LEU	N-CA-C	-5.95	104.18	112.45
1	D	186	TYR	N-CA-C	5.94	120.00	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	397	SER	N-CA-C	5.78	118.48	109.52
1	C	521	ARG	N-CA-C	5.78	118.73	110.24
1	A	397	SER	N-CA-C	5.77	118.46	109.52
1	E	397	SER	N-CA-C	5.77	118.46	109.52
1	D	397	SER	N-CA-C	5.76	118.45	109.52
1	E	122	CYS	N-CA-C	5.76	119.41	112.38
1	A	521	ARG	N-CA-C	5.76	118.70	110.24
1	D	521	ARG	N-CA-C	5.76	118.70	110.24
1	E	521	ARG	N-CA-C	5.76	118.70	110.24
1	D	122	CYS	N-CA-C	5.75	119.40	112.38
1	F	122	CYS	N-CA-C	5.75	119.39	112.38
1	A	122	CYS	N-CA-C	5.75	119.39	112.38
1	B	521	ARG	N-CA-C	5.74	118.68	110.24
1	C	397	SER	N-CA-C	5.74	118.42	109.52
1	B	122	CYS	N-CA-C	5.74	119.38	112.38
1	B	397	SER	N-CA-C	5.74	118.41	109.52
1	C	122	CYS	N-CA-C	5.73	119.37	112.38
1	B	525	ILE	N-CA-C	-5.73	98.17	107.28
1	F	525	ILE	N-CA-C	-5.72	98.18	107.28
1	E	525	ILE	N-CA-C	-5.72	98.18	107.28
1	F	521	ARG	N-CA-C	5.72	118.65	110.24
1	C	525	ILE	N-CA-C	-5.71	98.19	107.28
1	A	525	ILE	N-CA-C	-5.71	98.20	107.28
1	D	525	ILE	N-CA-C	-5.71	98.21	107.28
1	E	412	VAL	N-CA-C	5.71	116.08	107.75
1	F	412	VAL	N-CA-C	5.67	116.04	107.75
1	A	412	VAL	N-CA-C	5.67	116.02	107.75
1	D	412	VAL	N-CA-C	5.66	116.01	107.75
1	C	412	VAL	N-CA-C	5.65	116.00	107.75
1	B	412	VAL	N-CA-C	5.64	115.98	107.75
1	B	319	ASP	N-CA-C	5.49	117.70	111.11
1	C	319	ASP	N-CA-C	5.47	117.67	111.11
1	F	319	ASP	N-CA-C	5.45	117.65	111.11
1	A	319	ASP	N-CA-C	5.45	117.65	111.11
1	D	319	ASP	N-CA-C	5.41	117.60	111.11
1	E	319	ASP	N-CA-C	5.41	117.60	111.11
1	C	170	LEU	N-CA-C	5.28	118.20	109.85
1	F	170	LEU	N-CA-C	5.25	118.15	109.85
1	A	170	LEU	N-CA-C	5.25	118.14	109.85
1	B	170	LEU	N-CA-C	5.24	118.14	109.85
1	D	170	LEU	N-CA-C	5.24	118.13	109.85
1	D	175	VAL	N-CA-C	5.23	116.82	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	170	LEU	N-CA-C	5.22	118.10	109.85
1	F	175	VAL	N-CA-C	5.21	116.80	108.87
1	B	175	VAL	N-CA-C	5.21	116.79	108.87
1	A	175	VAL	N-CA-C	5.20	116.78	108.87
1	C	175	VAL	N-CA-C	5.20	116.77	108.87
1	D	369	ASP	N-CA-C	-5.19	103.18	110.50
1	E	175	VAL	N-CA-C	5.18	116.75	108.87
1	A	369	ASP	N-CA-C	-5.15	103.23	110.50
1	B	369	ASP	N-CA-C	-5.15	103.23	110.50
1	E	369	ASP	N-CA-C	-5.15	103.24	110.50
1	C	369	ASP	N-CA-C	-5.14	103.26	110.50
1	F	369	ASP	N-CA-C	-5.11	103.29	110.50
1	E	384	ALA	N-CA-C	-5.10	105.80	111.36
1	F	384	ALA	N-CA-C	-5.08	105.83	111.36
1	B	384	ALA	N-CA-C	-5.07	105.83	111.36
1	D	634[B]	MET	N-CA-C	5.07	116.97	109.62
1	A	384	ALA	N-CA-C	-5.07	105.84	111.36
1	B	191	ASP	N-CA-C	5.06	119.45	113.28
1	E	634[B]	MET	N-CA-C	5.06	116.96	109.62
1	D	384	ALA	N-CA-C	-5.06	105.85	111.36
1	C	384	ALA	N-CA-C	-5.06	105.85	111.36
1	A	634[B]	MET	N-CA-C	5.05	116.95	109.62
1	D	191	ASP	N-CA-C	5.05	119.44	113.28
1	F	634[B]	MET	N-CA-C	5.04	116.93	109.62
1	C	191	ASP	N-CA-C	5.04	119.42	113.28
1	B	634[B]	MET	N-CA-C	5.02	116.90	109.62
1	A	191	ASP	N-CA-C	5.02	119.40	113.28
1	C	634[B]	MET	N-CA-C	5.01	116.89	109.62
1	E	191	ASP	N-CA-C	5.00	119.38	113.28

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	122	2
1	B	5219	0	5044	125	0
1	C	5219	0	5044	120	0
1	D	5219	0	5044	124	0
1	E	5219	0	5044	122	0
1	F	5219	0	5044	124	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	672	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 (672) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:HIS:CD2	1:B:25:LEU:H	2.02	0.71
1:B:116:LEU:HD12	1:B:157:THR:CG2	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:439:GLU:C	1:A:441:GLY:H	2.03	0.67
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:B:439:GLU:C	1:B:441:GLY:H	2.03	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:D:439:GLU:C	1:D:441:GLY:H	2.03	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:C:439:GLU:C	1:C:441:GLY:H	2.03	0.66
1:D:457:GLN:HE22	1:D:552:LEU:H	1.44	0.66
1:E:439:GLU:C	1:E:441:GLY:H	2.03	0.66
1:F:439:GLU:C	1:F:441:GLY:H	2.03	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: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
1:C:664:THR:HG23	1:D:182:ASP:CG	2.24	0.62
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:E:527:ASN:HD22	1:E:527:ASN:C	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ASN:HD22	1:B:527:ASN:C	2.09	0.61
1:E:504:THR:HG21	4:E:1326:HOH:O	2.00	0.61
1:A:527:ASN:HD22	1:A:527:ASN:C	2.09	0.61
1:C:527:ASN:HD22	1:C:527:ASN:C	2.09	0.61
1:A:112:VAL:HG21	1:A:586:HIS:HB2	1.83	0.61
1:A:504:THR:HG21	4:A:1326:HOH:O	2.00	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:D:527:ASN:HD22	1:D:527:ASN:C	2.09	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: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:HG3	1:C:20:ARG:HH11	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:F:527:ASN:HD22	1:F:527:ASN:C	2.09	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:112:VAL:HG21	1:D:586:HIS:HB2	1.83	0.59
1:D:527:ASN:ND2	1:D:529:ASN:H	2.00	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:670:ARG:C	1:C:672:VAL:H	2.11	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:HG3	1:F:20:ARG:HH11	1.67	0.59
1:F:57:ARG:CZ	1:F:578:ASN:HD21	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:670:ARG:C	1:E:672:VAL:H	2.11	0.59
1:F:670:ARG:C	1:F:672:VAL:H	2.10	0.59
1:A:644:ARG:HD3	1:A:646:ARG:HD3	1.84	0.59
1:B:670:ARG:C	1:B:672:VAL:H	2.10	0.59
1:D:507:THR:HG21	4:D:1196:HOH:O	2.03	0.59
1:A:20:ARG:HG3	1:A:20:ARG:HH11	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:A:670:ARG:C	1:A:672:VAL:H	2.10	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: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:D:670:ARG:C	1:D:672:VAL:H	2.10	0.57
1:E:497:ALA:HB2	1:F:308:PRO:HB3	1.86	0.57
1:A:439:GLU:C	1:A:441:GLY:N	2.62	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:A:190:LEU:HD22	1:A:215:VAL:HG22	1.86	0.56
1:D:439:GLU:C	1:D:441:GLY:N	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:468:ILE:N	1:B:473:ASN:HD21	2.04	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:439:GLU:C	1:B:441:GLY:N	2.62	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:E:439:GLU:C	1:E:441:GLY:N	2.62	0.55
1:C:439:GLU:C	1:C:441:GLY:N	2.62	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:182:ASP:CG	1:D:664:THR:HG23	2.33	0.54
1:D:631:PHE:CG	1:D:632:PRO:HA	2.41	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:F:439:GLU:C	1:F:441:GLY:N	2.62	0.54
1:A:664:THR:HG23	1:B:182:ASP:CG	2.33	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
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:F:190:LEU:CD2	1:F:215:VAL:HG22	2.38	0.53
1:D:190:LEU:CD2	1:D:215:VAL:HG22	2.38	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: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
4:A:1194:HOH:O	1:B:554:LYS:HE3	2.07	0.52
1:B:347:ALA:HB3	1:B:359:VAL:HG13	1.89	0.52
4:E:1194:HOH:O	1:F:554:LYS:HE3	2.08	0.52
1:C:632:PRO:HD2	1:D:655:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:392:THR:HG22	1:C:415:GLN:OE1	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:A:182:ASP:CG	1:B:664:THR:HG23	2.36	0.51
1:B:176:TYR:CE1	1:B:189:PRO:HB3	2.46	0.51
1:E:62:LYS:HE2	4:E:1309:HOH:O	2.11	0.51
1:E:392:THR:HG22	4:E:1061:HOH:O	2.09	0.51
1:F:62:LYS:HE2	4:F:1309:HOH:O	2.11	0.51
1:A:57:ARG:NE	1:A:578:ASN:HD21	2.08	0.50
1:A:392:THR:HG22	1:A:415:GLN:OE1	2.10	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:E:664:THR:HG23	1:F:182:ASP:CG	2.36	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:637:GLU:HG3	1:F:644:ARG:HH22	1.78	0.49
1:F:429:LEU:HD11	1:F:630:ASP:HB2	1.95	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:D:77:ARG:HG3	1:D:98:LEU:HD12	1.94	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: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
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:A:655:LEU:HD11	1:B:632:PRO:HD2	1.95	0.48
1:B:557:SER:O	1:B:561:LYS:HG3	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:637:GLU:HG3	1:D:644:ARG:HH22	1.78	0.47
1:D:123:SER:O	1:D:127:VAL:HG13	2.14	0.47
1:E:547:GLN:NE2	1:E:640:THR:H	2.11	0.47
1:A:50:SER:HB2	1:A:352:ARG:CG	2.44	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: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: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:D:50:SER:HB2	1:D:352:ARG:CG	2.44	0.47
1:E:262:SER:O	1:E:263:ASN:HB2	2.14	0.47
1:E:457:GLN:NE2	1:E:552:LEU:H	2.11	0.47
4:E:1024:HOH:O	1:F:375:LYS:HE2	2.13	0.47
1:F:23:HIS:HD2	1:F:25:LEU:N	1.94	0.47
1:A:123:SER:O	1:A:127:VAL:HG13	2.14	0.47
1:B:262:SER:O	1:B:263:ASN:HB2	2.14	0.47
1:D:439:GLU:HG3	1:D:441:GLY:CA	2.44	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
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:B:452:ASN:C	1:B:452:ASN:HD22	2.23	0.47
1:E:452:ASN:C	1:E:452:ASN:HD22	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:452:ASN:C	1:A:452:ASN:HD22	2.23	0.47
1:B:414:MET:HE3	1:B:418:ALA:HB3	1.97	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:F:414:MET:HE3	1:F:418:ALA:HB3	1.98	0.46
1:A:670:ARG:C	1:A:672:VAL:N	2.74	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:A:414:MET:HE3	1:A:418:ALA:HB3	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: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:A:375:LYS:O	1:B:406:GLU:HG3	2.15	0.46
1:B:331:PRO:HD2	4:B:1345:HOH:O	2.16	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:F:452:ASN:C	1:F:452:ASN:HD22	2.23	0.46
1:A:143:ILE:CG1	1:A:215:VAL:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:414:MET:HE3	1:C:418:ALA:HB3	1.98	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:D:670:ARG:C	1:D:672:VAL:N	2.74	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:632:PRO:HD2	1:B:655:LEU:HD11	1.98	0.46
1:A:637:GLU:HG3	1:B:644:ARG:HH22	1.80	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: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:HG13	1:A:359:VAL:O	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:C:452:ASN:C	1:C:452:ASN:HD22	2.23	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:HG13	1:C:359:VAL:O	2.16	0.45
1:C:664:THR:HB	1:C:667:GLU:HG3	1.98	0.45
1:F:218:HIS:HD2	3:F:703:PO4:O4	1.98	0.45
1:F:439:GLU:HG3	1:F:441:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:414:MET:HE3	1:D:418:ALA:HB3	1.98	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:HG13	1:D:359:VAL:O	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:452:ASN:HD22	1:D:452:ASN:C	2.23	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:C:670:ARG:C	1:C:672:VAL:N	2.74	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:E:414:MET:HE3	1:E:418:ALA:HB3	1.97	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:23:HIS:HD2	1:E:25:LEU:N	1.94	0.44
1:E:143:ILE:HG13	1:E:215:VAL:HG21	1.97	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: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:C:633:LEU:HD13	1:D:374:PHE:CD1	2.53	0.44
1:D:345:LEU:HB2	1:D:363:VAL:HB	2.00	0.44
1:E:182:ASP:CG	1:F:664:THR:HG23	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:GLU:HG3	1:C:441:GLY:HA2	1.99	0.44
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:F:670:ARG:C	1:F:672:VAL:N	2.74	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:E:644:ARG:HH22	1:F:637:GLU:HG3	1.83	0.44
1:F:479:ASP:HB3	1:F:519:THR:HB	2.00	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:HG3	1:C:20:ARG:NH1	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:HG3	1:B:20:ARG:NH1	2.33	0.43
1:F:672:VAL:O	1:F:672:VAL:HG12	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:HG12	1:B:672:VAL:O	2.19	0.43
1:E:50:SER:HB2	1:E:352:ARG:HG3	2.01	0.43
1:E:502:LYS:HE2	1:E:504:THR:HG22	2.00	0.43
1:B:670:ARG:C	1:B:672:VAL:N	2.74	0.43
1:D:479:ASP:HB3	1:D:519:THR:HB	2.00	0.43
1:E:672:VAL:HG12	1:E:672:VAL:O	2.19	0.43
1:A:672:VAL:O	1:A:672:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:387:LEU:C	1:C:387:LEU:HD23	2.44	0.43
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:E:115:ILE:HD11	1:E:323:TYR:C	2.44	0.43
1:E:387:LEU:C	1:E:387:LEU:HD23	2.44	0.43
1:F:50:SER:HB2	1:F:352:ARG:HG3	2.01	0.43
1:A:387:LEU:C	1:A:387:LEU:HD23	2.44	0.43
1:A:576:LYS:HB2	1:A:579:ARG:HD2	2.00	0.43
1:A:641:LEU:C	1:A:641:LEU:HD22	2.44	0.43
1:B:387:LEU:C	1:B:387:LEU:HD23	2.44	0.43
1:C:641:LEU:C	1:C:641:LEU:HD22	2.44	0.43
1:D:115:ILE:HD11	1:D:323:TYR:C	2.44	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: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:E:641:LEU:C	1:E:641:LEU:HD22	2.44	0.42
1:C:312:HIS:HD2	4:C:1195:HOH:O	2.03	0.42
1:D:53:THR:O	1:D:81:TYR:HA	2.19	0.42
1:D:672:VAL:HG12	1:D:672:VAL:O	2.19	0.42
1:F:576:LYS:HB2	1:F:579:ARG:HD2	2.00	0.42
1:D:387:LEU:HD23	1:D:387:LEU:C	2.44	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:387:LEU:C	1:F:387:LEU:HD23	2.44	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:C:53:THR:O	1:C:81:TYR:HA	2.19	0.42
1:C:502:LYS:HE2	1:C:504:THR:HG22	2.00	0.42
1:F:641:LEU:C	1:F:641:LEU:HD22	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NZ	1:E:360:LYS:HB3	2.35	0.42
1:C:115:ILE:HD11	1:C:323:TYR:C	2.44	0.41
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:B:115:ILE:HD11	1:B:323:TYR:C	2.44	0.41
1:B:146:ASN:N	1:B:146:ASN:HD22	2.18	0.41
1:D:421:LEU:HB3	1:D:641:LEU:HD13	2.02	0.41
1:F:360:LYS:NZ	1:F:360:LYS:HB3	2.35	0.41
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:D:641:LEU:C	1:D:641:LEU:HD22	2.44	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:C:240:PRO:HD2	1:D:251:SER:HB3	2.01	0.41
1:D:23:HIS:HA	1:D:24:PRO:HD3	1.94	0.41
1:F:146:ASN:N	1:F:146:ASN:HD22	2.18	0.41
1:A:115:ILE:HD11	1:A:323:TYR:C	2.44	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: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:NZ	1:A:360:LYS:HB3	2.35	0.41
1:B:360:LYS:NZ	1:B:360:LYS:HB3	2.35	0.41
1:B:641:LEU:C	1:B:641:LEU:HD22	2.44	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:F:115:ILE:HD11	1:F:323:TYR:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:645:PRO:O	1:D:646:ARG:HD2	2.21	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: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:421:LEU:HB3	1:A:641:LEU:HD13	2.02	0.41
1:A:452:ASN:HD22	1:A:453:ALA:N	2.19	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:C:332:LEU:O	1:C:333:SER:C	2.64	0.41
1:C:406:GLU:HG2	1:C:427:GLY:HA3	2.03	0.41
1:D:131:ASP:O	1:D:135:ILE:HG13	2.21	0.41
1:D:406:GLU:HG2	1:D:427:GLY:HA3	2.03	0.41
1:E:421:LEU:HB3	1:E:641:LEU:HD13	2.02	0.41
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: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:E:146:ASN:N	1:E:146:ASN:HD22	2.18	0.40
1:E:294:HIS:HD2	4:E:1182:HOH:O	2.05	0.40
1:B:290:ARG:HA	1:B:291:PRO:HD3	1.91	0.40
1:B:414:MET:HE2	1:B:420:ARG:HB2	2.04	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:A:414:MET:HE2	1:A:420:ARG:HB2	2.04	0.40
1:B:57:ARG:CZ	1:B:578:ASN:ND2	2.83	0.40
1:B:406:GLU:HG2	1:B:427:GLY:HA3	2.03	0.40
1:C:131:ASP:O	1:C:135:ILE:HG13	2.21	0.40
1:E:670:ARG:C	1:E:672:VAL:N	2.74	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:146:ASN:HD22	1:B:146:ASN:C	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:SER:HB3	1:D:240:PRO:HD2	2.04	0.40
1:E:414:MET:HE2	1:E:420:ARG:HB2	2.04	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:332:LEU:O	1:F:333:SER:C	2.64	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%)	36	29
1	B	651/694 (94%)	619 (95%)	29 (4%)	3 (0%)	24	16
1	C	651/694 (94%)	619 (95%)	30 (5%)	2 (0%)	36	29
1	D	651/694 (94%)	619 (95%)	29 (4%)	3 (0%)	24	16
1	E	651/694 (94%)	619 (95%)	30 (5%)	2 (0%)	36	29
1	F	651/694 (94%)	619 (95%)	30 (5%)	2 (0%)	36	29
All	All	3906/4164 (94%)	3714 (95%)	178 (5%)	14 (0%)	30	22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	SER

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Mol	Chain	Res	Type
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%)	548 (97%)	17 (3%)	36	30
1	B	565/593 (95%)	548 (97%)	17 (3%)	36	30
1	C	565/593 (95%)	548 (97%)	17 (3%)	36	30
1	D	565/593 (95%)	548 (97%)	17 (3%)	36	30
1	E	565/593 (95%)	548 (97%)	17 (3%)	36	30
1	F	565/593 (95%)	548 (97%)	17 (3%)	36	30
All	All	3390/3558 (95%)	3288 (97%)	102 (3%)	36	30

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	VAL
1	A	140	LEU
1	A	146	ASN
1	A	170	LEU
1	A	311	PRO

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Mol	Chain	Res	Type
1	A	329	THR
1	A	332	LEU
1	A	364	CYS
1	A	406	GLU
1	A	421	LEU
1	A	462	LEU
1	A	487	LEU
1	A	527	ASN
1	A	578	ASN
1	A	633	LEU
1	A	641	LEU
1	A	664	THR
1	B	112	VAL
1	B	140	LEU
1	B	146	ASN
1	B	170	LEU
1	B	311	PRO
1	B	329	THR
1	B	332	LEU
1	B	364	CYS
1	B	406	GLU
1	B	421	LEU
1	B	462	LEU
1	B	487	LEU
1	B	527	ASN
1	B	578	ASN
1	B	633	LEU
1	B	641	LEU
1	B	664	THR
1	C	112	VAL
1	C	140	LEU
1	C	146	ASN
1	C	170	LEU
1	C	311	PRO
1	C	329	THR
1	C	332	LEU
1	C	364	CYS
1	C	406	GLU
1	C	421	LEU
1	C	462	LEU
1	C	487	LEU
1	C	527	ASN

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Mol	Chain	Res	Type
1	C	578	ASN
1	C	633	LEU
1	C	641	LEU
1	C	664	THR
1	D	112	VAL
1	D	140	LEU
1	D	146	ASN
1	D	170	LEU
1	D	311	PRO
1	D	329	THR
1	D	332	LEU
1	D	364	CYS
1	D	406	GLU
1	D	421	LEU
1	D	462	LEU
1	D	487	LEU
1	D	527	ASN
1	D	578	ASN
1	D	633	LEU
1	D	641	LEU
1	D	664	THR
1	E	112	VAL
1	E	140	LEU
1	E	146	ASN
1	E	170	LEU
1	E	311	PRO
1	E	329	THR
1	E	332	LEU
1	E	364	CYS
1	E	406	GLU
1	E	421	LEU
1	E	462	LEU
1	E	487	LEU
1	E	527	ASN
1	E	578	ASN
1	E	633	LEU
1	E	641	LEU
1	E	664	THR
1	F	112	VAL
1	F	140	LEU
1	F	146	ASN
1	F	170	LEU

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Mol	Chain	Res	Type
1	F	311	PRO
1	F	329	THR
1	F	332	LEU
1	F	364	CYS
1	F	406	GLU
1	F	421	LEU
1	F	462	LEU
1	F	487	LEU
1	F	527	ASN
1	F	578	ASN
1	F	633	LEU
1	F	641	LEU
1	F	664	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) 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	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	529	ASN
1	A	547	GLN
1	A	578	ASN
1	A	611	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

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Mol	Chain	Res	Type
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	529	ASN
1	B	547	GLN
1	B	578	ASN
1	B	611	ASN
1	C	23	HIS
1	C	66	GLN
1	C	70	GLN
1	C	146	ASN
1	C	218	HIS
1	C	288	ASN
1	C	294	HIS
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	529	ASN
1	C	547	GLN
1	C	578	ASN
1	C	611	ASN
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

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Mol	Chain	Res	Type
1	D	450	ASN
1	D	452	ASN
1	D	457	GLN
1	D	473	ASN
1	D	527	ASN
1	D	529	ASN
1	D	547	GLN
1	D	578	ASN
1	D	611	ASN
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	246	GLN
1	E	288	ASN
1	E	294	HIS
1	E	312	HIS
1	E	330	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	529	ASN
1	E	547	GLN
1	E	578	ASN
1	E	611	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	246	GLN
1	F	288	ASN
1	F	294	HIS
1	F	312	HIS
1	F	330	ASN
1	F	382	ASN

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Mol	Chain	Res	Type
1	F	450	ASN
1	F	452	ASN
1	F	457	GLN
1	F	473	ASN
1	F	527	ASN
1	F	529	ASN
1	F	547	GLN
1	F	578	ASN
1	F	611	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	ME0	C	634[A]	1	6,8,9	1.43	1 (16%)	2,8,10	0.23	0
1	ME0	D	634[A]	1	6,8,9	1.43	1 (16%)	2,8,10	0.23	0
1	ME0	E	634[A]	1	6,8,9	1.44	1 (16%)	2,8,10	0.22	0
1	TY9	A	405[B]	-	15,16,17	4.81	9 (60%)	13,21,23	1.33	2 (15%)
1	TY8	F	405[A]	1	15,16,17	4.90	10 (66%)	13,21,23	1.84	4 (30%)
1	TY9	E	405[B]	-	15,16,17	4.81	9 (60%)	13,21,23	1.34	2 (15%)
1	TY9	B	405[B]	-	15,16,17	4.81	9 (60%)	13,21,23	1.33	2 (15%)
1	ME0	B	634[A]	1	6,8,9	1.44	1 (16%)	2,8,10	0.23	0
1	ME0	A	634[A]	1	6,8,9	1.44	1 (16%)	2,8,10	0.23	0
1	TY8	D	405[A]	1	15,16,17	4.89	10 (66%)	13,21,23	1.85	4 (30%)
1	ME0	F	634[A]	1	6,8,9	1.44	1 (16%)	2,8,10	0.24	0
1	TY8	A	405[A]	1	15,16,17	4.90	10 (66%)	13,21,23	1.84	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TY8	E	405[A]	1	15,16,17	4.90	10 (66%)	13,21,23	1.85	4 (30%)
1	TY9	F	405[B]	-	15,16,17	4.80	9 (60%)	13,21,23	1.33	2 (15%)
1	TY8	C	405[A]	1	15,16,17	4.91	10 (66%)	13,21,23	1.85	4 (30%)
1	TY9	C	405[B]	-	15,16,17	4.82	9 (60%)	13,21,23	1.34	2 (15%)
1	TY8	B	405[A]	1	15,16,17	4.90	10 (66%)	13,21,23	1.84	4 (30%)
1	TY9	D	405[B]	-	15,16,17	4.80	9 (60%)	13,21,23	1.34	2 (15%)

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	ME0	C	634[A]	1	-	1/5/7/9	-
1	ME0	D	634[A]	1	-	1/5/7/9	-
1	ME0	E	634[A]	1	-	1/5/7/9	-
1	TY9	A	405[B]	-	-	0/5/10/12	0/1/1/1
1	TY8	F	405[A]	1	-	0/5/10/12	0/1/1/1
1	TY9	E	405[B]	-	-	0/5/10/12	0/1/1/1
1	TY9	B	405[B]	-	-	0/5/10/12	0/1/1/1
1	ME0	B	634[A]	1	-	1/5/7/9	-
1	ME0	A	634[A]	1	-	1/5/7/9	-
1	TY8	D	405[A]	1	-	0/5/10/12	0/1/1/1
1	ME0	F	634[A]	1	-	1/5/7/9	-
1	TY8	A	405[A]	1	-	0/5/10/12	0/1/1/1
1	TY8	E	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	TY8	C	405[A]	1	-	0/5/10/12	0/1/1/1
1	TY9	C	405[B]	-	-	0/5/10/12	0/1/1/1
1	TY8	B	405[A]	1	-	0/5/10/12	0/1/1/1
1	TY9	D	405[B]	-	-	0/5/10/12	0/1/1/1

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	405[A]	TY8	C6-C5	8.84	1.51	1.38
1	C	405[B]	TY9	C6-C5	8.84	1.51	1.38
1	E	405[A]	TY8	C6-C5	8.82	1.51	1.38
1	E	405[B]	TY9	C6-C5	8.82	1.51	1.38
1	A	405[A]	TY8	C6-C5	8.79	1.51	1.38
1	A	405[B]	TY9	C6-C5	8.79	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	405[A]	TY8	C6-C5	8.78	1.51	1.38
1	D	405[B]	TY9	C6-C5	8.78	1.51	1.38
1	B	405[A]	TY8	C6-C5	8.76	1.51	1.38
1	B	405[B]	TY9	C6-C5	8.76	1.51	1.38
1	F	405[A]	TY8	C6-C5	8.74	1.51	1.38
1	F	405[B]	TY9	C6-C5	8.74	1.51	1.38
1	C	405[A]	TY8	C3-C2	7.06	1.50	1.38
1	C	405[B]	TY9	C2-C3	7.06	1.50	1.38
1	E	405[A]	TY8	C3-C2	7.05	1.50	1.38
1	E	405[B]	TY9	C2-C3	7.05	1.50	1.38
1	D	405[A]	TY8	C3-C2	7.04	1.50	1.38
1	D	405[B]	TY9	C2-C3	7.04	1.50	1.38
1	B	405[A]	TY8	C3-C2	7.04	1.50	1.38
1	B	405[B]	TY9	C2-C3	7.04	1.50	1.38
1	A	405[A]	TY8	C3-C2	7.03	1.50	1.38
1	A	405[B]	TY9	C2-C3	7.03	1.50	1.38
1	F	405[A]	TY8	C3-C2	7.02	1.50	1.38
1	F	405[B]	TY9	C2-C3	7.02	1.50	1.38
1	B	405[A]	TY8	C5-C4	6.78	1.52	1.40
1	F	405[A]	TY8	C5-C4	6.77	1.52	1.40
1	C	405[A]	TY8	C5-C4	6.75	1.52	1.40
1	D	405[A]	TY8	C5-C4	6.75	1.52	1.40
1	A	405[A]	TY8	C5-C4	6.74	1.52	1.40
1	E	405[A]	TY8	C5-C4	6.73	1.52	1.40
1	F	405[A]	TY8	O4-C4	-6.33	1.26	1.38
1	F	405[B]	TY9	O4-C4	-6.33	1.26	1.38
1	B	405[A]	TY8	O4-C4	-6.31	1.26	1.38
1	B	405[B]	TY9	O4-C4	-6.31	1.26	1.38
1	A	405[A]	TY8	O4-C4	-6.30	1.26	1.38
1	A	405[B]	TY9	O4-C4	-6.30	1.26	1.38
1	C	405[A]	TY8	O4-C4	-6.30	1.26	1.38
1	C	405[B]	TY9	O4-C4	-6.30	1.26	1.38
1	E	405[A]	TY8	O4-C4	-6.29	1.26	1.38
1	E	405[B]	TY9	O4-C4	-6.29	1.26	1.38
1	D	405[A]	TY8	O4-C4	-6.28	1.26	1.38
1	D	405[B]	TY9	O4-C4	-6.28	1.26	1.38
1	F	405[A]	TY8	CB-C1	-6.19	1.41	1.51
1	B	405[A]	TY8	CB-C1	-6.18	1.41	1.51
1	D	405[A]	TY8	CB-C1	-6.17	1.41	1.51
1	A	405[A]	TY8	CB-C1	-6.17	1.41	1.51
1	C	405[A]	TY8	CB-C1	-6.16	1.41	1.51
1	E	405[A]	TY8	CB-C1	-6.14	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	405[B]	TY9	O3A-O3	-5.99	1.30	1.46
1	A	405[B]	TY9	O3A-O3	-5.97	1.30	1.46
1	F	405[B]	TY9	O3A-O3	-5.97	1.30	1.46
1	E	405[B]	TY9	O3A-O3	-5.97	1.30	1.46
1	B	405[B]	TY9	O3A-O3	-5.97	1.30	1.46
1	D	405[B]	TY9	O3A-O3	-5.97	1.30	1.46
1	B	405[B]	TY9	C5-C4	5.92	1.52	1.40
1	F	405[B]	TY9	C5-C4	5.91	1.52	1.40
1	C	405[B]	TY9	C5-C4	5.89	1.52	1.40
1	D	405[B]	TY9	C5-C4	5.89	1.52	1.40
1	A	405[B]	TY9	C5-C4	5.88	1.52	1.40
1	E	405[B]	TY9	C5-C4	5.87	1.52	1.40
1	E	405[B]	TY9	C2-C1	5.65	1.48	1.39
1	B	405[B]	TY9	C2-C1	5.63	1.48	1.39
1	A	405[B]	TY9	C2-C1	5.62	1.48	1.39
1	F	405[B]	TY9	C2-C1	5.61	1.48	1.39
1	C	405[B]	TY9	C2-C1	5.60	1.48	1.39
1	D	405[B]	TY9	C2-C1	5.59	1.48	1.39
1	E	405[A]	TY8	C2-C1	5.50	1.48	1.39
1	C	405[A]	TY8	O4A-O4	-5.49	1.32	1.46
1	C	405[B]	TY9	O4A-O4	-5.49	1.32	1.46
1	F	405[A]	TY8	O4A-O4	-5.49	1.32	1.46
1	F	405[B]	TY9	O4A-O4	-5.49	1.32	1.46
1	B	405[A]	TY8	C2-C1	5.48	1.48	1.39
1	E	405[A]	TY8	O4A-O4	-5.48	1.32	1.46
1	E	405[B]	TY9	O4A-O4	-5.48	1.32	1.46
1	A	405[A]	TY8	C2-C1	5.47	1.48	1.39
1	B	405[A]	TY8	O4A-O4	-5.47	1.32	1.46
1	B	405[B]	TY9	O4A-O4	-5.47	1.32	1.46
1	A	405[A]	TY8	O4A-O4	-5.47	1.32	1.46
1	A	405[B]	TY9	O4A-O4	-5.47	1.32	1.46
1	F	405[A]	TY8	C2-C1	5.46	1.48	1.39
1	C	405[A]	TY8	C2-C1	5.46	1.48	1.39
1	D	405[A]	TY8	C2-C1	5.45	1.48	1.39
1	D	405[A]	TY8	O4A-O4	-5.44	1.32	1.46
1	D	405[B]	TY9	O4A-O4	-5.44	1.32	1.46
1	D	405[A]	TY8	O5-C5	-5.13	1.26	1.36
1	D	405[B]	TY9	O5-C5	-5.13	1.26	1.36
1	E	405[A]	TY8	O5-C5	-5.12	1.26	1.36
1	E	405[B]	TY9	O5-C5	-5.12	1.26	1.36
1	C	405[A]	TY8	O5-C5	-5.12	1.26	1.36
1	C	405[B]	TY9	O5-C5	-5.12	1.26	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405[A]	TY8	O5-C5	-5.10	1.26	1.36
1	A	405[B]	TY9	O5-C5	-5.10	1.26	1.36
1	B	405[A]	TY8	O5-C5	-5.10	1.26	1.36
1	B	405[B]	TY9	O5-C5	-5.10	1.26	1.36
1	F	405[A]	TY8	O5-C5	-5.09	1.26	1.36
1	F	405[B]	TY9	O5-C5	-5.09	1.26	1.36
1	F	405[B]	TY9	CB-C1	-4.05	1.41	1.51
1	B	405[B]	TY9	CB-C1	-4.05	1.41	1.51
1	D	405[B]	TY9	CB-C1	-4.04	1.41	1.51
1	A	405[B]	TY9	CB-C1	-4.04	1.41	1.51
1	C	405[B]	TY9	CB-C1	-4.03	1.41	1.51
1	E	405[B]	TY9	CB-C1	-4.02	1.41	1.51
1	C	405[A]	TY8	O2A-O2	-3.92	1.36	1.46
1	F	405[A]	TY8	O2A-O2	-3.91	1.36	1.46
1	A	405[A]	TY8	O2A-O2	-3.90	1.36	1.46
1	E	405[A]	TY8	O2A-O2	-3.90	1.36	1.46
1	D	405[A]	TY8	O2A-O2	-3.89	1.36	1.46
1	B	405[A]	TY8	O2A-O2	-3.89	1.36	1.46
1	E	634[A]	ME0	OF-CE	-3.29	1.24	1.41
1	F	634[A]	ME0	OF-CE	-3.29	1.24	1.41
1	A	634[A]	ME0	OF-CE	-3.29	1.24	1.41
1	C	634[A]	ME0	OF-CE	-3.28	1.24	1.41
1	B	634[A]	ME0	OF-CE	-3.28	1.24	1.41
1	D	634[A]	ME0	OF-CE	-3.28	1.24	1.41
1	B	405[A]	TY8	C3-C4	2.41	1.42	1.38
1	F	405[A]	TY8	C3-C4	2.38	1.42	1.38
1	E	405[A]	TY8	C3-C4	2.38	1.42	1.38
1	A	405[A]	TY8	C3-C4	2.37	1.42	1.38
1	C	405[A]	TY8	C3-C4	2.35	1.42	1.38
1	D	405[A]	TY8	C3-C4	2.34	1.42	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	405[A]	TY8	CB-C1-C2	3.90	125.10	120.88
1	D	405[A]	TY8	CB-C1-C2	3.90	125.09	120.88
1	C	405[A]	TY8	CB-C1-C2	3.88	125.08	120.88
1	A	405[A]	TY8	CB-C1-C2	3.88	125.08	120.88
1	E	405[A]	TY8	CB-C1-C2	3.88	125.07	120.88
1	B	405[A]	TY8	CB-C1-C2	3.85	125.04	120.88
1	C	405[B]	TY9	CB-C1-C6	-3.39	114.61	120.43
1	D	405[B]	TY9	CB-C1-C6	-3.38	114.62	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	405[B]	TY9	CB-C1-C6	-3.38	114.63	120.43
1	F	405[B]	TY9	CB-C1-C6	-3.37	114.64	120.43
1	A	405[B]	TY9	CB-C1-C6	-3.37	114.64	120.43
1	B	405[B]	TY9	CB-C1-C6	-3.35	114.67	120.43
1	B	405[A]	TY8	O2-C2-C1	2.92	121.06	115.99
1	C	405[A]	TY8	O2-C2-C1	2.92	121.06	115.99
1	E	405[A]	TY8	O2-C2-C1	2.92	121.06	115.99
1	A	405[A]	TY8	O2-C2-C1	2.91	121.05	115.99
1	F	405[A]	TY8	O2-C2-C1	2.90	121.03	115.99
1	D	405[A]	TY8	O2-C2-C1	2.90	121.03	115.99
1	C	405[A]	TY8	CB-C1-C6	-2.79	114.61	119.78
1	D	405[A]	TY8	CB-C1-C6	-2.78	114.62	119.78
1	E	405[A]	TY8	CB-C1-C6	-2.78	114.63	119.78
1	F	405[A]	TY8	CB-C1-C6	-2.77	114.64	119.78
1	A	405[A]	TY8	CB-C1-C6	-2.77	114.64	119.78
1	B	405[A]	TY8	CB-C1-C6	-2.76	114.67	119.78
1	F	405[B]	TY9	CB-C1-C2	2.72	125.10	120.43
1	D	405[B]	TY9	CB-C1-C2	2.72	125.09	120.43
1	C	405[B]	TY9	CB-C1-C2	2.71	125.08	120.43
1	A	405[B]	TY9	CB-C1-C2	2.71	125.08	120.43
1	E	405[B]	TY9	CB-C1-C2	2.70	125.07	120.43
1	B	405[B]	TY9	CB-C1-C2	2.69	125.04	120.43
1	C	405[A]	TY8	O2-C2-C3	-2.30	118.71	123.87
1	B	405[A]	TY8	O2-C2-C3	-2.30	118.72	123.87
1	D	405[A]	TY8	O2-C2-C3	-2.30	118.72	123.87
1	A	405[A]	TY8	O2-C2-C3	-2.30	118.72	123.87
1	F	405[A]	TY8	O2-C2-C3	-2.30	118.73	123.87
1	E	405[A]	TY8	O2-C2-C3	-2.29	118.73	123.87

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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	704	-	4,4,4	1.72	0	6,6,6	0.45	0
3	PO4	E	702	-	4,4,4	1.64	0	6,6,6	0.46	0
3	PO4	C	702	-	4,4,4	1.64	0	6,6,6	0.46	0
3	PO4	D	704	-	4,4,4	1.72	0	6,6,6	0.45	0
3	PO4	F	703	-	4,4,4	1.77	2 (50%)	6,6,6	0.47	0
3	PO4	E	704	-	4,4,4	1.73	0	6,6,6	0.44	0
3	PO4	F	702	-	4,4,4	1.63	0	6,6,6	0.46	0
3	PO4	D	702	-	4,4,4	1.64	0	6,6,6	0.45	0
3	PO4	E	703	-	4,4,4	1.77	2 (50%)	6,6,6	0.46	0
3	PO4	C	703	-	4,4,4	1.77	2 (50%)	6,6,6	0.46	0
3	PO4	C	704	-	4,4,4	1.73	0	6,6,6	0.44	0
3	PO4	A	702	-	4,4,4	1.64	0	6,6,6	0.46	0
3	PO4	D	703	-	4,4,4	1.77	2 (50%)	6,6,6	0.46	0
3	PO4	F	704	-	4,4,4	1.73	1 (25%)	6,6,6	0.45	0
3	PO4	B	702	-	4,4,4	1.64	0	6,6,6	0.46	0
3	PO4	A	704	-	4,4,4	1.72	0	6,6,6	0.45	0
3	PO4	A	703	-	4,4,4	1.77	2 (50%)	6,6,6	0.46	0
3	PO4	B	703	-	4,4,4	1.76	2 (50%)	6,6,6	0.46	0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	703	PO4	P-O4	-2.05	1.48	1.54
3	F	703	PO4	P-O4	-2.05	1.48	1.54
3	A	703	PO4	P-O4	-2.04	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	PO4	P-O4	-2.04	1.48	1.54
3	F	703	PO4	P-O2	-2.04	1.48	1.54
3	E	703	PO4	P-O4	-2.04	1.48	1.54
3	D	703	PO4	P-O2	-2.04	1.48	1.54
3	A	703	PO4	P-O2	-2.03	1.48	1.54
3	C	703	PO4	P-O2	-2.03	1.48	1.54
3	B	703	PO4	P-O2	-2.02	1.48	1.54
3	E	703	PO4	P-O2	-2.02	1.48	1.54
3	C	703	PO4	P-O4	-2.01	1.48	1.54
3	F	704	PO4	P-O3	-2.00	1.48	1.54

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	F	703	PO4	1	0
3	E	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, 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	653/694 (94%)	0.49	44 (6%)	24	25	14, 24, 46, 80	0
1	B	653/694 (94%)	0.41	35 (5%)	31	33	14, 24, 46, 80	0
1	C	653/694 (94%)	0.49	41 (6%)	26	27	14, 24, 46, 80	0
1	D	653/694 (94%)	0.55	36 (5%)	30	32	14, 24, 46, 80	0
1	E	653/694 (94%)	0.43	31 (4%)	36	39	14, 24, 46, 80	0
1	F	653/694 (94%)	0.44	34 (5%)	33	35	14, 24, 46, 80	0
All	All	3918/4164 (94%)	0.47	221 (5%)	30	32	14, 25, 46, 80	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	672	VAL	8.8
1	B	672	VAL	7.2
1	A	672	VAL	6.7
1	F	672	VAL	6.5
1	D	672	VAL	6.2
1	F	19	ALA	6.0
1	F	21	PRO	6.0
1	F	18	PRO	5.9
1	C	672	VAL	5.6
1	E	18	PRO	5.6
1	C	335	GLY	5.2
1	A	334	LEU	5.1
1	A	18	PRO	5.0
1	B	18	PRO	5.0
1	A	437	ASP	4.8
1	C	233	GLY	4.8
1	E	22	ALA	4.8
1	C	334	LEU	4.8
1	C	18	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	19	ALA	4.6
1	F	441	GLY	4.6
1	F	22	ALA	4.6
1	A	436	ASP	4.5
1	C	19	ALA	4.5
1	D	18	PRO	4.4
1	E	334	LEU	4.4
1	C	20	ARG	4.3
1	F	437	ASP	4.3
1	D	334	LEU	4.2
1	A	20	ARG	4.2
1	B	19	ALA	4.2
1	D	671	ALA	4.2
1	B	130	ASN	4.2
1	B	336	CYS	4.2
1	B	441	GLY	4.2
1	D	335	GLY	4.2
1	B	335	GLY	4.1
1	F	130	ASN	4.0
1	A	441	GLY	4.0
1	E	441	GLY	3.9
1	E	130	ASN	3.9
1	C	333	SER	3.9
1	B	334	LEU	3.9
1	C	437	ASP	3.9
1	A	671	ALA	3.9
1	A	233	GLY	3.8
1	B	233	GLY	3.8
1	C	21	PRO	3.8
1	D	19	ALA	3.8
1	F	20	ARG	3.7
1	C	234	ALA	3.7
1	B	20	ARG	3.7
1	A	335	GLY	3.7
1	A	338	CYS	3.6
1	F	333	SER	3.6
1	A	333	SER	3.6
1	E	336	CYS	3.6
1	E	21	PRO	3.5
1	C	122	CYS	3.5
1	B	232	VAL	3.5
1	D	336	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	199	GLU	3.5
1	E	122	CYS	3.4
1	A	234	ALA	3.4
1	E	19	ALA	3.4
1	D	70	GLN	3.4
1	A	21	PRO	3.4
1	F	336	CYS	3.4
1	D	437	ASP	3.4
1	F	337	ASP	3.4
1	B	671	ALA	3.3
1	C	48	LYS	3.3
1	D	21	PRO	3.3
1	F	338	CYS	3.3
1	F	334	LEU	3.3
1	B	437	ASP	3.3
1	D	232	VAL	3.2
1	E	671	ALA	3.2
1	C	671	ALA	3.1
1	F	671	ALA	3.1
1	D	341	VAL	3.1
1	C	232	VAL	3.1
1	A	122	CYS	3.1
1	B	359	VAL	3.1
1	F	669	LYS	3.1
1	A	336	CYS	3.1
1	C	336	CYS	3.1
1	D	338	CYS	3.1
1	A	507	THR	3.1
1	F	157	THR	3.1
1	C	441	GLY	3.1
1	E	234	ALA	3.1
1	C	337	ASP	3.0
1	C	342	ILE	3.0
1	A	127	VAL	3.0
1	D	244	VAL	3.0
1	E	157	THR	3.0
1	F	578	ASN	3.0
1	F	359	VAL	2.9
1	E	335	GLY	2.9
1	F	122	CYS	2.9
1	B	337	ASP	2.9
1	A	157	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	340	GLY	2.9
1	E	339	LYS	2.9
1	A	244	VAL	2.9
1	A	48	LYS	2.9
1	D	130	ASN	2.8
1	F	127	VAL	2.8
1	F	342	ILE	2.8
1	D	441	GLY	2.8
1	B	342	ILE	2.8
1	B	341	VAL	2.8
1	B	122	CYS	2.8
1	E	437	ASP	2.8
1	A	62	LYS	2.7
1	E	357	ILE	2.7
1	A	232	VAL	2.7
1	C	338	CYS	2.7
1	C	74	LEU	2.7
1	E	233	GLY	2.7
1	A	337	ASP	2.7
1	C	106	THR	2.7
1	E	20	ARG	2.7
1	C	242	ILE	2.7
1	D	22	ALA	2.6
1	D	233	GLY	2.6
1	C	157	THR	2.6
1	F	48	LYS	2.6
1	F	202	LYS	2.6
1	E	338	CYS	2.6
1	B	578	ASN	2.6
1	F	335	GLY	2.6
1	A	340	GLY	2.6
1	A	215	VAL	2.6
1	B	670	ARG	2.5
1	C	84	LEU	2.5
1	A	242	ILE	2.5
1	A	578	ASN	2.5
1	B	22	ALA	2.5
1	D	234	ALA	2.5
1	A	341	VAL	2.5
1	A	359	VAL	2.5
1	C	352	ARG	2.5
1	D	20	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	127	VAL	2.5
1	C	103	VAL	2.5
1	A	339	LYS	2.5
1	C	339	LYS	2.5
1	D	122	CYS	2.5
1	D	342	ILE	2.5
1	A	22	ALA	2.4
1	B	339	LYS	2.4
1	C	578	ASN	2.4
1	F	146	ASN	2.4
1	D	333	SER	2.4
1	D	668	ALA	2.4
1	E	341	VAL	2.4
1	D	425	LEU	2.4
1	C	104	ILE	2.4
1	C	359	VAL	2.4
1	F	118	VAL	2.4
1	F	233	GLY	2.4
1	E	670	ARG	2.3
1	D	246	GLN	2.3
1	D	157	THR	2.3
1	A	73	PRO	2.3
1	B	244	VAL	2.3
1	F	232	VAL	2.3
1	C	199	GLU	2.3
1	B	338	CYS	2.3
1	A	343	HIS	2.3
1	C	379	PHE	2.3
1	D	179	SER	2.3
1	A	70	GLN	2.3
1	B	21	PRO	2.2
1	C	241	PRO	2.2
1	B	333	SER	2.2
1	D	339	LYS	2.2
1	E	48	LYS	2.2
1	B	157	THR	2.2
1	B	664	THR	2.2
1	A	101	LEU	2.2
1	E	199	GLU	2.2
1	B	384	ALA	2.2
1	A	669	LYS	2.2
1	B	30	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	74	LEU	2.2
1	F	339	LYS	2.2
1	B	118	VAL	2.2
1	F	341	VAL	2.2
1	E	337	ASP	2.2
1	E	249	GLY	2.2
1	C	240	PRO	2.2
1	A	45	ALA	2.2
1	F	71	GLY	2.1
1	C	341	VAL	2.1
1	D	103	VAL	2.1
1	D	670	ARG	2.1
1	C	109	LEU	2.1
1	C	45	ALA	2.1
1	C	202	LYS	2.1
1	C	546	THR	2.1
1	E	507	THR	2.1
1	D	40	VAL	2.1
1	E	127	VAL	2.1
1	E	244	VAL	2.1
1	A	332	LEU	2.1
1	C	46	GLY	2.0
1	A	112	VAL	2.0
1	D	359	VAL	2.0
1	D	84	LEU	2.0
1	D	86	ALA	2.0
1	B	200	GLU	2.0
1	B	48	LYS	2.0
1	A	87	GLY	2.0
1	B	340	GLY	2.0
1	D	340	GLY	2.0
1	F	664	THR	2.0
1	E	76	PRO	2.0
1	F	670	ARG	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($\text{\AA}^2$)	Q<0.9
1	TY8	B	405[A]	16/17	0.77	0.17	24,38,48,51	16
1	TY9	A	405[B]	16/17	-	-	24,38,48,51	16
1	TY8	D	405[A]	16/17	0.79	0.17	24,38,48,51	16
1	TY8	A	405[A]	16/17	0.81	0.18	24,38,48,51	16
1	TY9	B	405[B]	16/17	-	-	24,38,48,51	16
1	TY8	E	405[A]	16/17	0.81	0.20	24,38,48,51	16
1	TY8	F	405[A]	16/17	0.82	0.17	24,38,48,51	16
1	TY9	C	405[B]	16/17	-	-	24,38,48,51	16
1	TY8	C	405[A]	16/17	0.84	0.16	24,38,48,51	16
1	ME0	C	634[A]	9/10	0.86	0.13	21,25,41,42	9
1	TY9	D	405[B]	16/17	-	-	24,38,48,51	16
1	ME0	D	634[A]	9/10	0.89	0.12	21,25,41,42	9
1	ME0	A	634[A]	9/10	0.90	0.11	21,25,41,42	9
1	TY9	E	405[B]	16/17	-	-	24,38,48,51	16
1	ME0	F	634[A]	9/10	0.91	0.12	21,25,41,42	9
1	ME0	E	634[A]	9/10	0.93	0.12	21,25,41,42	9
1	TY9	F	405[B]	16/17	-	-	24,38,48,51	16
1	ME0	B	634[A]	9/10	0.94	0.10	21,25,41,42	9

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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($\text{\AA}^2$)	Q<0.9
3	PO4	D	704	5/5	0.80	0.15	86,87,87,88	0
3	PO4	C	704	5/5	0.82	0.16	86,87,87,88	0
3	PO4	F	704	5/5	0.84	0.14	86,87,87,88	0
3	PO4	A	704	5/5	0.85	0.17	86,87,87,88	0
3	PO4	E	704	5/5	0.85	0.12	86,87,87,88	0
3	PO4	D	702	5/5	0.85	0.18	34,36,38,39	0
3	PO4	B	704	5/5	0.87	0.14	86,87,87,88	0
3	PO4	D	703	5/5	0.89	0.12	46,49,49,50	0
3	PO4	F	703	5/5	0.89	0.10	46,49,49,50	0
3	PO4	E	703	5/5	0.89	0.12	46,49,49,50	0
3	PO4	C	702	5/5	0.90	0.11	34,36,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	C	703	5/5	0.91	0.13	46,49,49,50	0
3	PO4	B	702	5/5	0.92	0.10	34,36,38,39	0
3	PO4	B	703	5/5	0.93	0.08	46,49,49,50	0
3	PO4	A	703	5/5	0.94	0.09	46,49,49,50	0
3	PO4	A	702	5/5	0.95	0.09	34,36,38,39	0
3	PO4	E	702	5/5	0.95	0.07	34,36,38,39	0
3	PO4	F	702	5/5	0.96	0.09	34,36,38,39	0
2	CU	A	701	1/1	0.99	0.04	22,22,22,22	0
2	CU	B	701	1/1	0.99	0.03	22,22,22,22	0
2	CU	C	701	1/1	0.99	0.02	22,22,22,22	0
2	CU	D	701	1/1	0.99	0.03	22,22,22,22	0
2	CU	E	701	1/1	0.99	0.04	22,22,22,22	0
2	CU	F	701	1/1	0.99	0.02	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.