



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:43 PM UTC

PDB ID : 2ZC0 / pdb_00002zc0
Title : Crystal structure of an archaeal alanine:glyoxylate aminotransferase
Authors : Sakuraba, H.; Yoneda, K.; Tsuge, H.; Ohshima, T.
Deposited on : 2007-10-31
Resolution : 2.30 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

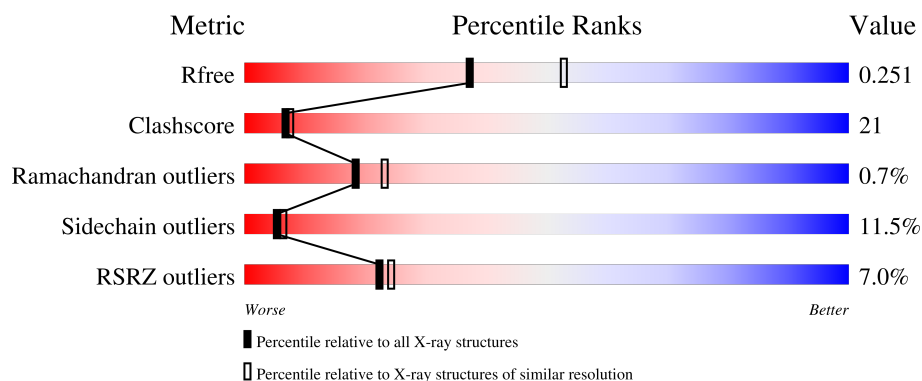
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	407	7% 57% 36% 5%
1	B	407	4% 60% 33% 7%
1	C	407	9% 53% 39% 8%
1	D	407	8% 58% 36% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12914 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.

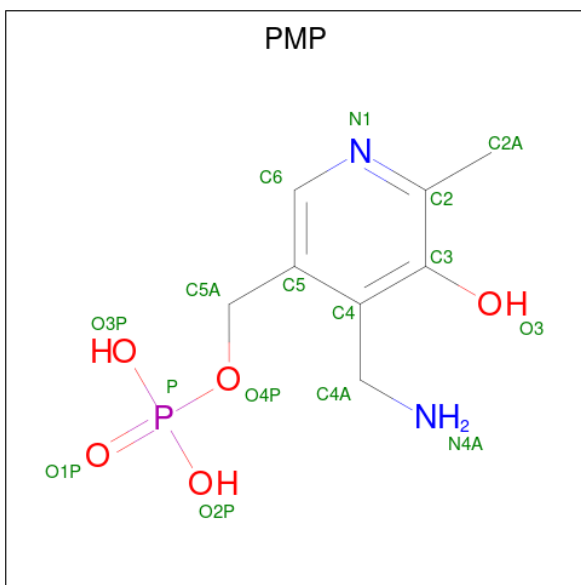
- Molecule 1 is a protein called Alanine glyoxylate transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3111	2007	513	578	13			
1	B	405	Total	C	N	O	S	0	0	0
			3111	2007	513	578	13			
1	C	405	Total	C	N	O	S	0	0	0
			3111	2007	513	578	13			
1	D	405	Total	C	N	O	S	0	0	0
			3111	2007	513	578	13			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

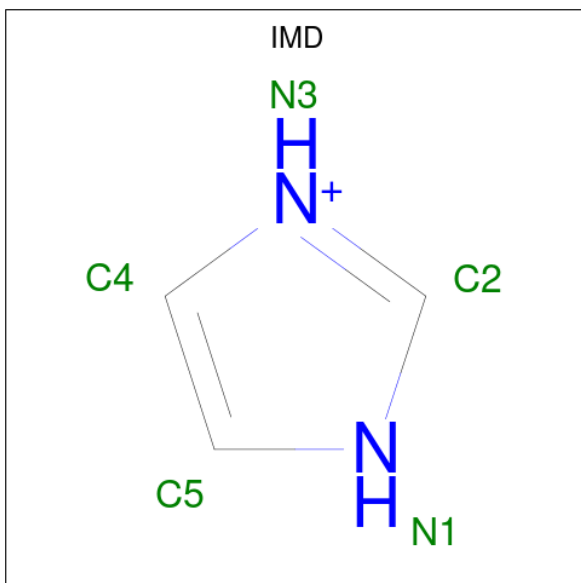
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C₈H₁₃N₂O₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 5 3 2	0	0
4	B	1	Total C N 5 3 2	0	0
4	C	1	Total C N 5 3 2	0	0
4	D	1	Total C N 5 3 2	0	0

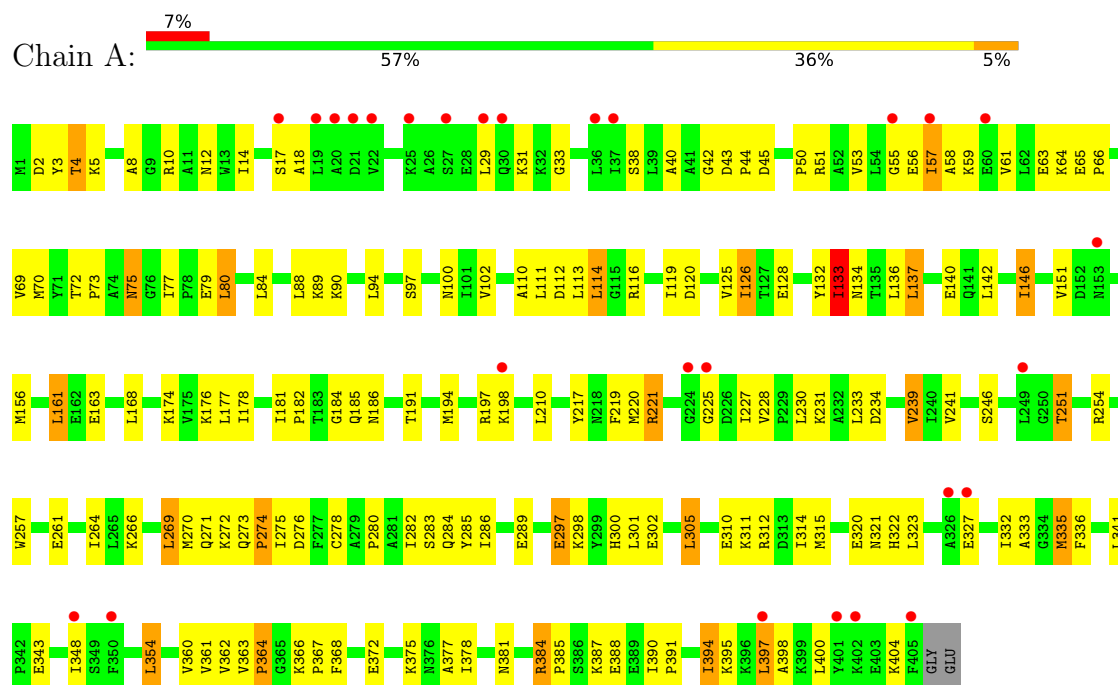
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	93	Total O 93 93	0	0
5	B	120	Total O 120 120	0	0
5	C	85	Total O 85 85	0	0
5	D	84	Total O 84 84	0	0

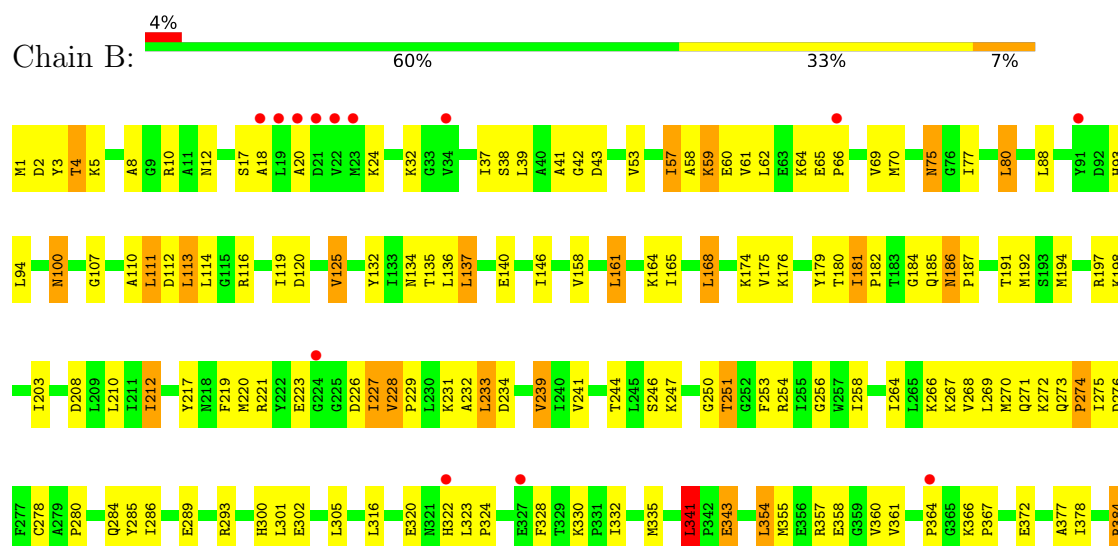
3 Residue-property plots

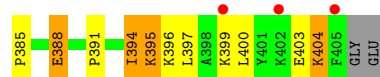
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Alanine glyoxylate transaminase

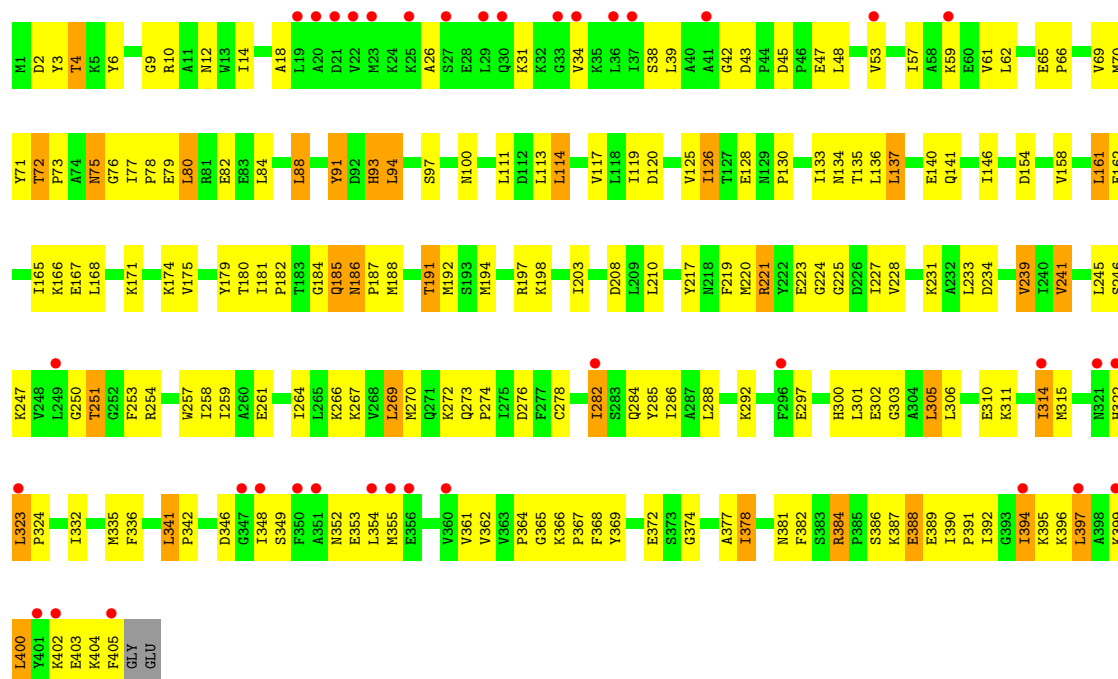


• Molecule 1: Alanine glyoxylate transaminase

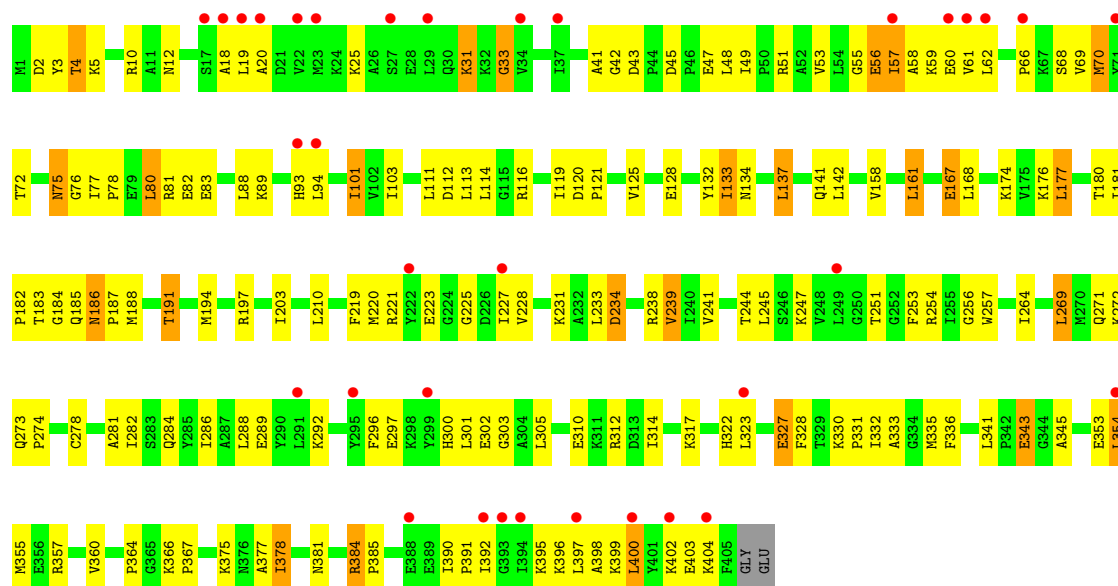




• Molecule 1: Alanine glyoxylate transaminase



• Molecule 1: Alanine glyoxylate transaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.69Å 112.52Å 207.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 2.30 49.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.40-2.30) 98.0 (49.40-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	58.13 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.261 0.238 , 0.251	Depositor DCC
R_{free} test set	4011 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12914	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: PMP, IMD, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	1/3169 (0.0%)	1.02	16/4279 (0.4%)
1	B	0.51	0/3169	1.06	16/4279 (0.4%)
1	C	0.46	0/3169	1.00	13/4279 (0.3%)
1	D	0.61	2/3169 (0.1%)	1.01	12/4279 (0.3%)
All	All	0.52	3/12676 (0.0%)	1.02	57/17116 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	225	GLY	C-N	18.23	1.57	1.33
1	D	220	MET	C-N	10.77	1.48	1.33
1	A	335	MET	SD-CE	-5.06	1.66	1.79

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	LYS	N-CA-C	10.34	122.14	111.07
1	B	272	LYS	N-CA-C	10.01	121.78	111.07
1	C	272	LYS	N-CA-C	9.04	120.91	111.14
1	D	332	ILE	N-CA-C	-9.03	104.34	113.10
1	A	186	ASN	N-CA-C	-8.52	96.35	109.64
1	A	332	ILE	N-CA-C	-8.22	104.69	112.83
1	B	119	ILE	N-CA-C	8.02	119.42	107.80
1	D	19	LEU	N-CA-C	-7.88	104.14	113.21
1	D	272	LYS	N-CA-C	7.86	119.93	111.36
1	A	363	VAL	CA-C-N	7.76	129.54	119.84
1	A	363	VAL	C-N-CA	7.76	129.54	119.84
1	B	186	ASN	N-CA-C	-7.43	96.75	109.15
1	C	181	ILE	CA-C-N	6.68	125.92	118.97
1	C	181	ILE	C-N-CA	6.68	125.92	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	332	ILE	N-CA-C	-6.40	106.09	112.17
1	B	38	SER	N-CA-C	6.17	119.30	109.24
1	B	181	ILE	CA-C-N	6.16	126.34	119.32
1	B	181	ILE	C-N-CA	6.16	126.34	119.32
1	A	119	ILE	N-CA-C	6.09	116.70	108.17
1	D	142	LEU	N-CA-C	-6.05	105.54	113.17
1	A	120	ASP	N-CA-C	-6.04	101.98	110.31
1	A	274	PRO	CA-C-N	-6.04	116.80	122.66
1	A	274	PRO	C-N-CA	-6.04	116.80	122.66
1	D	72	THR	N-CA-C	-6.00	103.11	110.31
1	D	188	MET	N-CA-C	6.00	117.81	111.28
1	B	332	ILE	N-CA-C	-5.97	106.68	112.29
1	A	142	LEU	N-CA-C	-5.96	105.59	112.92
1	B	94	LEU	N-CA-C	5.91	118.88	109.24
1	C	186	ASN	N-CA-C	-5.90	99.29	109.15
1	B	274	PRO	CA-C-N	-5.90	116.94	122.66
1	B	274	PRO	C-N-CA	-5.90	116.94	122.66
1	D	119	ILE	N-CA-C	5.82	116.32	108.17
1	C	39	LEU	N-CA-C	-5.81	104.86	112.41
1	D	128	GLU	N-CA-C	-5.69	103.02	110.53
1	D	177	LEU	N-CA-C	5.69	118.67	109.40
1	B	8	ALA	N-CA-C	-5.56	102.25	110.48
1	C	119	ILE	N-CA-C	5.56	115.90	108.11
1	C	120	ASP	N-CA-C	-5.51	102.00	110.32
1	A	298	LYS	N-CA-C	5.47	118.00	111.71
1	B	395	LYS	N-CA-C	-5.46	105.23	111.07
1	D	186	ASN	N-CA-C	-5.45	101.14	109.64
1	C	94	LEU	N-CA-C	5.41	117.34	108.52
1	C	91	TYR	N-CA-C	5.38	120.00	113.38
1	B	120	ASP	N-CA-C	-5.36	102.92	110.31
1	A	146	ILE	N-CA-C	5.29	116.19	108.58
1	B	24	LYS	N-CA-C	-5.26	106.91	113.38
1	B	223	GLU	N-CA-C	5.25	120.57	113.21
1	C	185	GLN	N-CA-C	5.23	117.46	110.35
1	A	38	SER	N-CA-C	5.17	117.66	109.24
1	C	133	ILE	N-CA-C	5.16	116.50	110.62
1	D	31	LYS	N-CA-C	-5.14	105.37	110.97
1	A	133	ILE	N-CA-C	5.13	116.47	110.62
1	A	8	ALA	N-CA-C	-5.12	102.90	110.48
1	C	128	GLU	N-CA-C	-5.06	103.72	110.55
1	A	44	PRO	N-CA-C	-5.05	103.61	111.13
1	B	341	LEU	N-CA-C	-5.05	104.33	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	ALA	N-CA-C	-5.03	105.71	111.14

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	3111	0	3162	158	0
1	B	3111	0	3162	131	0
1	C	3111	0	3162	159	0
1	D	3111	0	3162	145	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
3	A	16	0	11	2	0
3	B	16	0	11	3	0
3	C	16	0	11	1	0
3	D	16	0	11	1	0
4	A	5	0	4	0	0
4	B	5	0	4	0	0
4	C	5	0	4	0	0
4	D	5	0	4	0	0
5	A	93	0	0	12	0
5	B	120	0	0	9	0
5	C	85	0	0	10	0
5	D	84	0	0	9	0
All	All	12914	0	12708	540	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (540) 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:C:354:LEU:HD11	1:C:397:LEU:HD23	1.35	1.08
1:C:221:ARG:HD3	1:C:227:ILE:HD11	1.38	1.04
1:B:184:GLY:H	1:B:191:THR:HG22	1.25	1.01
1:B:57:ILE:HD11	1:B:286:ILE:HA	1.40	0.99
1:A:57:ILE:HD11	1:A:286:ILE:HA	1.41	0.99
1:B:221:ARG:HD2	1:B:227:ILE:HD11	1.40	0.99
1:A:12:ASN:HD21	1:C:174:LYS:H	1.11	0.99
1:A:184:GLY:H	1:A:191:THR:HG22	1.21	0.98
1:B:174:LYS:H	1:D:12:ASN:HD21	1.07	0.96
1:D:57:ILE:HD11	1:D:286:ILE:HA	1.48	0.96
1:C:241:VAL:HG13	1:C:259:ILE:HB	1.45	0.95
1:A:134:ASN:HD21	1:B:273:GLN:HG2	1.35	0.91
1:D:223:GLU:HG3	1:D:312:ARG:HH22	1.33	0.91
1:A:174:LYS:H	1:C:12:ASN:HD21	1.15	0.89
1:D:341:LEU:HD13	1:D:378:ILE:HD13	1.56	0.88
1:B:12:ASN:HD21	1:D:174:LYS:H	1.21	0.87
1:B:191:THR:HG23	5:B:421:HOH:O	1.75	0.85
1:C:72:THR:HG22	1:C:278:CYS:HB2	1.55	0.85
1:B:111:LEU:HD12	1:B:212:ILE:HD11	1.58	0.84
1:C:134:ASN:HD21	1:D:273:GLN:HG2	1.44	0.83
1:A:231:LYS:HD3	1:A:239:VAL:HG22	1.61	0.81
1:A:42:GLY:C	1:A:335:MET:HE1	2.07	0.80
1:C:97:SER:HB3	1:C:100:ASN:HD22	1.47	0.78
1:B:404:LYS:HA	1:B:404:LYS:HE2	1.65	0.77
1:A:251:THR:HG22	1:B:70:MET:HA	1.66	0.77
1:C:251:THR:HG22	1:D:70:MET:HA	1.66	0.77
1:D:404:LYS:HA	1:D:404:LYS:HE2	1.67	0.77
1:C:341:LEU:HD13	1:C:378:ILE:HD13	1.68	0.76
1:C:70:MET:HA	1:D:251:THR:HG22	1.66	0.76
1:D:384:ARG:HH11	1:D:384:ARG:HB3	1.51	0.76
1:A:75:ASN:H	1:A:75:ASN:HD22	1.30	0.76
1:D:57:ILE:HD13	1:D:289:GLU:HB2	1.68	0.75
1:A:75:ASN:HD22	1:A:75:ASN:N	1.83	0.75
1:D:2:ASP:OD2	1:D:4:THR:HB	1.87	0.75
1:B:111:LEU:CD1	1:B:212:ILE:HD11	2.17	0.75
1:D:184:GLY:H	1:D:191:THR:HG22	1.50	0.75
1:B:364:PRO:O	1:B:377:ALA:O	2.05	0.75
1:D:75:ASN:HB3	1:D:269:LEU:HD11	1.69	0.74
1:B:42:GLY:O	1:B:335:MET:HE1	1.86	0.74
1:B:125:VAL:HG13	1:B:146:ILE:HD13	1.69	0.74
1:A:246:SER:HB2	1:A:251:THR:HA	1.69	0.74
1:D:133:ILE:HD12	1:D:134:ASN:H	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:GLU:HB3	1:C:400:LEU:HD11	1.68	0.74
1:C:61:VAL:HG21	1:C:285:TYR:HB3	1.67	0.74
1:D:390:ILE:HB	1:D:391:PRO:HD3	1.68	0.74
1:D:101:ILE:HD11	1:D:103:ILE:HD13	1.69	0.74
1:A:70:MET:HA	1:B:251:THR:HG22	1.70	0.73
1:D:399:LYS:O	1:D:403:GLU:HB2	1.89	0.73
1:B:246:SER:HB2	1:B:251:THR:HA	1.68	0.72
5:C:413:HOH:O	1:D:10:ARG:HD2	1.88	0.72
1:C:42:GLY:C	1:C:335:MET:HE1	2.13	0.72
1:D:18:ALA:C	1:D:20:ALA:H	1.97	0.72
1:A:57:ILE:HD13	1:A:289:GLU:HB2	1.70	0.72
1:A:321:ASN:HB2	5:A:486:HOH:O	1.90	0.72
1:C:136:LEU:O	1:C:140:GLU:HG3	1.89	0.71
1:C:335:MET:HE2	1:C:336:PHE:CZ	2.25	0.71
1:A:136:LEU:HD22	1:A:146:ILE:HD13	1.72	0.71
1:B:322:HIS:HB2	5:B:506:HOH:O	1.91	0.71
1:A:75:ASN:H	1:A:75:ASN:ND2	1.89	0.70
1:A:59:LYS:HE2	1:B:59:LYS:HD3	1.72	0.70
1:A:42:GLY:CA	1:A:335:MET:HE1	2.21	0.70
1:A:126:ILE:HG23	1:A:178:ILE:HG12	1.73	0.70
1:D:176:LYS:HG3	1:D:177:LEU:HG	1.73	0.70
1:A:133:ILE:HD12	1:A:134:ASN:H	1.57	0.70
1:A:75:ASN:HB3	1:A:269:LEU:HD11	1.74	0.70
1:C:297:GLU:O	1:C:302:GLU:HG2	1.91	0.70
1:B:355:MET:HE2	1:B:361:VAL:HG13	1.74	0.69
1:A:136:LEU:O	1:A:140:GLU:HG3	1.92	0.69
1:D:42:GLY:C	1:D:335:MET:HE1	2.18	0.69
1:A:377:ALA:O	1:A:378:ILE:HD12	1.92	0.69
1:C:42:GLY:O	1:C:335:MET:HE1	1.93	0.69
1:B:221:ARG:CD	1:B:227:ILE:HD11	2.21	0.68
1:A:133:ILE:HG21	5:A:495:HOH:O	1.93	0.68
1:A:191:THR:HG23	5:A:490:HOH:O	1.92	0.68
1:C:234:ASP:CG	1:C:239:VAL:HG13	2.18	0.68
1:D:391:PRO:O	1:D:395:LYS:HB2	1.94	0.67
1:C:114:LEU:HD13	1:C:258:ILE:HD13	1.77	0.67
1:A:133:ILE:HD12	1:A:134:ASN:N	2.09	0.67
1:C:273:GLN:HG2	1:D:134:ASN:HD21	1.60	0.67
1:D:343:GLU:CD	1:D:343:GLU:H	2.03	0.67
1:D:42:GLY:O	1:D:335:MET:HE1	1.94	0.67
1:B:107:GLY:O	1:B:111:LEU:HD22	1.95	0.66
1:B:231:LYS:HD3	1:B:239:VAL:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASP:CG	1:B:239:VAL:HG13	2.20	0.66
1:C:184:GLY:H	1:C:191:THR:HG22	1.59	0.66
1:C:390:ILE:HB	1:C:391:PRO:HD3	1.77	0.66
1:A:10:ARG:HD2	5:B:419:HOH:O	1.94	0.66
1:A:174:LYS:H	1:C:12:ASN:ND2	1.92	0.66
1:C:365:GLY:HA2	1:C:368:PHE:CD1	2.31	0.65
1:A:377:ALA:C	1:A:378:ILE:HD12	2.21	0.65
1:C:384:ARG:HH11	1:C:384:ARG:HB3	1.62	0.65
1:D:133:ILE:HD12	1:D:134:ASN:N	2.12	0.65
1:C:43:ASP:OD1	1:C:251:THR:HG21	1.97	0.65
1:C:314:ILE:HD11	1:C:391:PRO:HD3	1.78	0.65
1:C:264:ILE:HG13	1:D:3:TYR:HB3	1.78	0.65
1:A:217:TYR:HD2	1:A:220:MET:HE2	1.62	0.65
1:A:341:LEU:HD13	1:A:378:ILE:HD13	1.79	0.65
1:A:220:MET:HE1	1:A:335:MET:HB3	1.80	0.64
1:A:126:ILE:HD13	1:A:126:ILE:C	2.21	0.64
1:B:228:VAL:HG23	1:B:232:ALA:HB3	1.80	0.63
1:A:234:ASP:CG	1:A:239:VAL:HG13	2.24	0.63
1:A:335:MET:HE2	1:A:336:PHE:CZ	2.33	0.63
1:C:62:LEU:O	1:D:51:ARG:HB3	1.97	0.62
1:D:223:GLU:HG3	1:D:312:ARG:NH2	2.10	0.62
1:D:322:HIS:CE1	1:D:395:LYS:HZ2	2.17	0.62
1:A:79:GLU:CD	1:A:79:GLU:H	2.08	0.62
1:B:247:LYS:HZ1	3:B:409:PMP:H4A1	1.65	0.62
1:D:322:HIS:CE1	1:D:395:LYS:NZ	2.67	0.62
1:A:194:MET:HA	1:A:197:ARG:HD3	1.82	0.62
1:A:50:PRO:HB2	1:A:53:VAL:HB	1.81	0.62
1:A:221:ARG:HG2	1:A:333:ALA:HB2	1.82	0.61
1:D:231:LYS:HD3	1:D:239:VAL:HG22	1.81	0.61
1:C:191:THR:HG23	5:C:418:HOH:O	2.01	0.61
1:C:390:ILE:O	1:C:394:ILE:HG23	2.01	0.61
1:A:51:ARG:HB3	1:B:62:LEU:O	2.01	0.61
1:A:348:ILE:HG22	1:A:364:PRO:HB3	1.82	0.61
1:B:43:ASP:OD1	1:B:251:THR:HG21	1.99	0.61
1:D:366:LYS:HD3	1:D:375:LYS:HA	1.82	0.61
1:B:17:SER:HB2	1:B:137:LEU:HD21	1.82	0.61
1:C:77:ILE:HG13	1:C:80:LEU:HB2	1.83	0.61
1:C:377:ALA:O	1:C:378:ILE:HD12	2.00	0.61
1:C:253:PHE:HE2	1:D:69:VAL:HG23	1.65	0.61
1:A:266:LYS:HE3	1:A:270:MET:HE3	1.81	0.60
1:C:349:SER:HA	1:C:352:ASN:HD22	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:HIS:HE1	1:B:226:ASP:OD1	1.84	0.60
1:B:174:LYS:H	1:D:12:ASN:ND2	1.90	0.60
1:A:43:ASP:OD1	1:A:251:THR:HG21	1.99	0.60
1:B:75:ASN:HB3	1:B:269:LEU:HD11	1.84	0.60
1:B:266:LYS:HG2	1:B:270:MET:HE3	1.83	0.60
1:D:384:ARG:HB3	1:D:384:ARG:NH1	2.16	0.60
1:D:384:ARG:N	1:D:385:PRO:HD2	2.17	0.60
1:A:390:ILE:HB	1:A:391:PRO:HD3	1.83	0.60
1:C:10:ARG:HD3	5:D:436:HOH:O	2.02	0.60
1:A:227:ILE:O	1:A:227:ILE:HG13	2.01	0.60
1:C:2:ASP:OD2	1:C:4:THR:HB	2.02	0.60
1:D:18:ALA:CB	1:D:367:PRO:HG2	2.32	0.60
1:D:43:ASP:OD1	1:D:251:THR:HG21	2.02	0.60
1:A:72:THR:HG22	1:A:278:CYS:SG	2.42	0.59
1:D:392:ILE:HG22	1:D:396:LYS:HE3	1.83	0.59
1:A:5:LYS:HE2	5:C:437:HOH:O	2.02	0.59
1:B:77:ILE:H	1:B:284:GLN:HE22	1.51	0.59
1:A:72:THR:HG22	1:A:278:CYS:HB2	1.84	0.59
1:C:335:MET:HE3	1:C:381:ASN:ND2	2.18	0.58
1:A:5:LYS:HE3	1:C:208:ASP:HB3	1.85	0.58
1:A:315:MET:HE2	1:A:394:ILE:HD11	1.85	0.58
1:B:247:LYS:NZ	3:B:409:PMP:H4A1	2.17	0.58
1:D:234:ASP:CG	1:D:239:VAL:HG13	2.28	0.58
1:A:42:GLY:O	1:A:335:MET:HE1	2.03	0.58
1:C:322:HIS:C	1:C:324:PRO:HD3	2.28	0.58
1:A:133:ILE:HG23	1:A:368:PHE:HA	1.85	0.58
1:C:254:ARG:HA	1:C:254:ARG:NE	2.18	0.58
1:A:72:THR:OG1	1:A:77:ILE:HG23	2.04	0.58
1:D:89:LYS:C	1:D:89:LYS:HD3	2.29	0.57
1:C:323:LEU:N	1:C:324:PRO:HD3	2.18	0.57
1:D:221:ARG:HG2	1:D:333:ALA:HB2	1.86	0.57
1:A:163:GLU:HG2	5:A:474:HOH:O	2.03	0.57
1:D:81:ARG:HG2	1:D:101:ILE:HG13	1.87	0.57
1:B:42:GLY:C	1:B:335:MET:HE1	2.29	0.57
1:D:53:VAL:HG23	5:D:428:HOH:O	2.05	0.57
1:D:101:ILE:HD11	1:D:103:ILE:CD1	2.34	0.57
1:D:297:GLU:O	1:D:302:GLU:HG2	2.05	0.56
1:A:12:ASN:HD21	1:C:174:LYS:N	1.93	0.56
1:A:53:VAL:O	1:A:57:ILE:HG23	2.05	0.56
1:C:18:ALA:HB3	1:C:367:PRO:HG3	1.87	0.56
1:C:72:THR:OG1	1:C:77:ILE:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:CYS:O	1:D:254:ARG:HD2	2.05	0.56
1:D:353:GLU:HG2	1:D:357:ARG:HD3	1.87	0.56
1:D:384:ARG:H	1:D:385:PRO:HD2	1.71	0.56
1:C:372:GLU:HG2	5:C:488:HOH:O	2.04	0.56
1:D:185:GLN:HG2	1:D:186:ASN:N	2.20	0.56
1:D:167:GLU:HG2	5:D:425:HOH:O	2.05	0.56
1:B:366:LYS:HB3	1:B:367:PRO:HD3	1.88	0.56
1:D:364:PRO:O	1:D:377:ALA:O	2.23	0.56
1:C:65:GLU:OE1	1:C:66:PRO:HD2	2.06	0.56
1:C:246:SER:HB2	1:C:251:THR:HA	1.86	0.56
1:D:76:GLY:HA2	1:D:284:GLN:HE22	1.70	0.56
1:C:3:TYR:HB3	1:D:264:ILE:HG13	1.88	0.55
1:D:366:LYS:HB3	1:D:367:PRO:HD3	1.88	0.55
1:D:322:HIS:NE2	1:D:395:LYS:HD2	2.21	0.55
1:C:77:ILE:HB	1:C:79:GLU:OE1	2.07	0.55
1:C:388:GLU:O	1:C:391:PRO:HD2	2.06	0.55
1:D:244:THR:HA	1:D:256:GLY:HA2	1.88	0.55
1:C:391:PRO:O	1:C:395:LYS:HB2	2.06	0.55
1:A:354:LEU:HD22	1:A:360:VAL:HB	1.89	0.55
1:D:75:ASN:N	1:D:75:ASN:HD22	2.04	0.55
1:D:66:PRO:O	1:D:69:VAL:HG12	2.07	0.55
1:D:322:HIS:HE1	5:D:494:HOH:O	1.89	0.55
1:C:66:PRO:O	1:C:69:VAL:HG12	2.06	0.55
1:B:316:LEU:O	1:B:320:GLU:HG3	2.06	0.55
1:A:42:GLY:CA	1:A:335:MET:CE	2.84	0.54
1:A:254:ARG:HD2	1:B:278:CYS:O	2.07	0.54
1:A:72:THR:HG22	1:A:278:CYS:CB	2.38	0.54
1:C:59:LYS:HB2	1:D:59:LYS:HB2	1.89	0.54
1:C:254:ARG:HH12	3:C:409:PMP:P	2.30	0.54
1:C:399:LYS:O	1:C:403:GLU:HB2	2.08	0.54
1:A:184:GLY:N	1:A:191:THR:HG22	2.06	0.54
1:D:45:ASP:HB3	1:D:48:LEU:HG	1.90	0.54
1:A:322:HIS:CE1	1:A:395:LYS:HG2	2.42	0.54
1:A:388:GLU:O	1:A:391:PRO:HD2	2.08	0.54
1:B:220:MET:HE1	1:B:335:MET:HB3	1.90	0.54
1:B:280:PRO:O	1:B:284:GLN:HG3	2.08	0.54
1:C:253:PHE:CE2	1:D:69:VAL:HG23	2.43	0.54
1:A:194:MET:HE1	1:A:228:VAL:HG22	1.89	0.54
1:C:288:LEU:O	1:C:292:LYS:HG3	2.08	0.54
1:C:346:ASP:OD2	1:C:348:ILE:HG13	2.08	0.54
1:D:158:VAL:O	1:D:161:LEU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:475:HOH:O	1:B:10:ARG:HD2	2.08	0.53
1:D:25:LYS:CB	1:D:355:MET:HE1	2.37	0.53
1:A:4:THR:HG23	5:C:484:HOH:O	2.08	0.53
1:C:297:GLU:HA	1:C:301:LEU:HB2	1.91	0.53
1:D:328:PHE:CE1	1:D:330:LYS:HE3	2.43	0.53
1:C:194:MET:HE1	1:C:228:VAL:HG22	1.91	0.53
1:C:245:LEU:HG	1:C:257:TRP:HZ3	1.74	0.53
1:B:354:LEU:HD22	1:B:360:VAL:HB	1.90	0.53
1:C:70:MET:HA	1:D:251:THR:CG2	2.37	0.53
1:C:137:LEU:O	1:C:141:GLN:HG2	2.09	0.53
1:C:366:LYS:N	1:C:367:PRO:HD2	2.23	0.53
1:B:174:LYS:N	1:D:12:ASN:HD21	1.91	0.53
1:A:42:GLY:HA2	1:A:335:MET:CE	2.38	0.53
1:A:282:ILE:HG13	1:A:283:SER:N	2.24	0.53
1:A:384:ARG:HH11	1:A:384:ARG:HB3	1.73	0.53
1:A:72:THR:HG21	1:A:284:GLN:OE1	2.09	0.53
1:A:72:THR:CG2	1:A:278:CYS:HB2	2.39	0.52
1:B:2:ASP:OD2	1:B:4:THR:HB	2.09	0.52
1:C:78:PRO:O	1:C:82:GLU:HG3	2.09	0.52
1:C:315:MET:HE1	1:C:381:ASN:O	2.10	0.52
1:D:75:ASN:HD22	1:D:75:ASN:H	1.57	0.52
1:D:227:ILE:HG13	1:D:227:ILE:O	2.08	0.52
1:C:246:SER:HA	1:C:250:GLY:O	2.09	0.52
1:D:77:ILE:HG13	1:D:80:LEU:HB2	1.91	0.52
1:D:328:PHE:HE1	1:D:330:LYS:HE3	1.75	0.52
1:A:273:GLN:HB3	1:A:274:PRO:HD3	1.91	0.52
1:C:61:VAL:HG21	1:C:285:TYR:CB	2.37	0.52
1:D:219:PHE:O	1:D:300:HIS:HE1	1.93	0.52
1:D:297:GLU:HA	1:D:301:LEU:HB2	1.92	0.52
1:A:12:ASN:ND2	1:C:174:LYS:H	1.94	0.52
1:B:179:TYR:HA	1:B:212:ILE:HG23	1.92	0.52
1:B:377:ALA:C	1:B:378:ILE:HD12	2.35	0.52
1:C:71:TYR:N	1:D:251:THR:HG23	2.25	0.52
1:C:217:TYR:CE2	1:C:247:LYS:HE3	2.44	0.52
1:D:288:LEU:HD11	1:D:292:LYS:HE3	1.90	0.52
1:B:61:VAL:HG11	1:B:285:TYR:HB3	1.91	0.51
1:C:38:SER:HB2	1:C:361:VAL:HB	1.92	0.51
1:C:306:LEU:H	1:C:306:LEU:HD22	1.74	0.51
1:C:79:GLU:H	1:C:79:GLU:CD	2.18	0.51
1:C:88:LEU:HB3	1:C:94:LEU:HB3	1.91	0.51
5:A:482:HOH:O	1:B:59:LYS:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:HH12	3:A:409:PMP:P	2.33	0.51
1:C:185:GLN:HG2	1:C:186:ASN:N	2.25	0.51
1:C:310:GLU:OE1	1:C:387:LYS:HE2	2.10	0.51
1:A:181:ILE:HB	1:A:185:GLN:HG3	1.92	0.51
1:C:62:LEU:HD12	1:D:55:GLY:HA2	1.93	0.51
1:C:75:ASN:N	1:C:75:ASN:HD22	2.07	0.51
1:C:377:ALA:C	1:C:378:ILE:HD12	2.36	0.51
1:D:341:LEU:CD1	1:D:378:ILE:HD13	2.37	0.51
1:A:282:ILE:HG23	5:A:417:HOH:O	2.11	0.51
1:B:37:ILE:CB	5:B:515:HOH:O	2.57	0.51
1:D:181:ILE:HB	1:D:185:GLN:HG3	1.93	0.51
1:D:273:GLN:HB3	1:D:274:PRO:HD3	1.92	0.51
1:A:366:LYS:HD3	1:A:375:LYS:HA	1.93	0.51
1:B:217:TYR:HD2	1:B:220:MET:HE2	1.76	0.51
1:C:267:LYS:HE3	5:D:412:HOH:O	2.10	0.51
1:D:194:MET:HE1	1:D:228:VAL:HG22	1.93	0.51
1:B:57:ILE:HD13	1:B:289:GLU:HB2	1.92	0.51
1:D:322:HIS:CE1	5:D:494:HOH:O	2.63	0.51
1:A:310:GLU:OE1	1:A:387:LYS:HD2	2.10	0.50
1:B:136:LEU:O	1:B:140:GLU:HG3	2.11	0.50
1:B:391:PRO:O	1:B:395:LYS:HB2	2.10	0.50
1:C:75:ASN:HB3	1:C:269:LEU:HD11	1.93	0.50
1:B:60:GLU:CD	1:B:293:ARG:HH22	2.19	0.50
1:A:3:TYR:HB3	1:B:264:ILE:HG13	1.92	0.50
1:A:388:GLU:HB2	5:A:422:HOH:O	2.11	0.50
1:A:174:LYS:N	1:C:12:ASN:HD21	1.98	0.50
1:A:217:TYR:CD2	1:A:220:MET:HE2	2.45	0.50
1:B:358:GLU:HB3	1:B:396:LYS:HD3	1.92	0.50
1:A:14:ILE:HD13	1:B:271:GLN:HB3	1.93	0.50
1:A:10:ARG:HD3	5:B:447:HOH:O	2.11	0.50
1:C:75:ASN:H	1:C:75:ASN:ND2	2.10	0.50
1:D:183:THR:HA	1:D:191:THR:HB	1.94	0.50
1:A:69:VAL:HG22	1:B:250:GLY:HA3	1.94	0.50
1:A:297:GLU:HG2	1:A:301:LEU:HD12	1.92	0.49
1:C:231:LYS:HD3	1:C:239:VAL:HG22	1.93	0.49
1:C:94:LEU:HD11	1:C:231:LYS:HG3	1.94	0.49
1:D:57:ILE:HD12	1:D:61:VAL:HG23	1.95	0.49
1:D:158:VAL:HG13	1:D:203:ILE:HD12	1.94	0.49
1:A:61:VAL:HG11	1:A:285:TYR:HB3	1.94	0.49
1:A:126:ILE:HD12	1:A:178:ILE:HG12	1.95	0.49
1:B:194:MET:HA	1:B:197:ARG:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:LYS:HE3	1:C:270:MET:CE	2.41	0.49
1:C:282:ILE:O	1:C:286:ILE:HG13	2.13	0.49
1:D:364:PRO:O	1:D:378:ILE:HA	2.12	0.49
1:B:60:GLU:HG3	1:B:64:LYS:HE2	1.94	0.49
1:D:89:LYS:HA	1:D:94:LEU:O	2.12	0.49
1:B:208:ASP:HB3	1:D:5:LYS:NZ	2.27	0.49
1:B:271:GLN:O	1:B:274:PRO:HD2	2.12	0.49
1:C:194:MET:HG2	1:C:227:ILE:HG22	1.93	0.49
1:A:176:LYS:HG3	1:A:177:LEU:HG	1.94	0.49
1:A:59:LYS:CE	1:B:59:LYS:HD3	2.42	0.49
1:D:191:THR:HG23	5:D:473:HOH:O	2.13	0.49
1:B:75:ASN:HD22	1:B:75:ASN:C	2.20	0.49
1:C:91:TYR:CE2	1:C:301:LEU:HD11	2.48	0.49
1:C:300:HIS:O	1:C:305:LEU:HB2	2.13	0.49
1:D:56:GLU:O	1:D:60:GLU:HG3	2.13	0.49
1:A:128:GLU:HG3	1:A:156:MET:HE2	1.95	0.49
1:B:366:LYS:N	1:B:367:PRO:CD	2.75	0.49
1:A:53:VAL:O	1:A:57:ILE:CG2	2.61	0.48
1:B:301:LEU:HA	1:B:305:LEU:HD12	1.95	0.48
1:C:130:PRO:HD3	1:C:369:TYR:CE1	2.47	0.48
1:D:75:ASN:H	1:D:75:ASN:ND2	2.11	0.48
1:A:273:GLN:HG2	1:B:134:ASN:HD21	1.77	0.48
1:A:297:GLU:O	1:A:302:GLU:HG2	2.12	0.48
1:D:335:MET:HE2	1:D:336:PHE:CZ	2.48	0.48
1:C:69:VAL:HG23	1:D:253:PHE:CE2	2.48	0.48
1:C:364:PRO:O	1:C:377:ALA:O	2.31	0.48
1:A:322:HIS:HE1	1:A:395:LYS:HE2	1.79	0.48
1:B:289:GLU:HG2	5:B:433:HOH:O	2.12	0.48
1:D:395:LYS:NZ	5:D:494:HOH:O	2.18	0.48
1:A:57:ILE:HG13	1:A:58:ALA:N	2.25	0.48
1:A:63:GLU:HG3	1:A:64:LYS:HG3	1.95	0.48
1:C:45:ASP:OD2	1:C:47:GLU:HB2	2.14	0.48
1:C:93:HIS:NE2	5:C:494:HOH:O	2.33	0.48
1:D:327:GLU:OE1	1:D:327:GLU:HA	2.13	0.48
1:A:89:LYS:HD3	1:A:90:LYS:N	2.29	0.48
1:A:151:VAL:HG12	1:A:156:MET:HA	1.96	0.48
1:A:84:LEU:O	1:A:88:LEU:HD13	2.14	0.48
1:D:245:LEU:HG	1:D:257:TRP:HZ3	1.78	0.48
1:A:55:GLY:HA2	1:B:62:LEU:HD12	1.96	0.48
1:A:264:ILE:HG13	1:B:3:TYR:HB3	1.95	0.48
1:B:208:ASP:HB3	1:D:5:LYS:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:THR:HA	1:B:256:GLY:HA2	1.95	0.48
1:C:69:VAL:HG23	1:D:253:PHE:HE2	1.78	0.48
1:C:219:PHE:O	1:C:300:HIS:HE1	1.97	0.47
1:A:77:ILE:H	1:A:284:GLN:HE22	1.61	0.47
1:B:181:ILE:HB	1:B:185:GLN:HG3	1.97	0.47
1:C:72:THR:HG23	1:C:73:PRO:O	2.14	0.47
1:C:310:GLU:O	1:C:314:ILE:CG2	2.63	0.47
1:C:311:LYS:HA	1:C:314:ILE:HG23	1.97	0.47
1:D:335:MET:HE3	1:D:381:ASN:ND2	2.30	0.47
1:A:323:LEU:HD21	1:A:398:ALA:HB2	1.96	0.47
1:B:388:GLU:HB2	5:B:445:HOH:O	2.15	0.47
1:A:77:ILE:HB	1:A:79:GLU:OE1	2.14	0.47
1:B:384:ARG:N	1:B:385:PRO:HD2	2.30	0.47
1:C:175:VAL:HG12	5:C:484:HOH:O	2.15	0.47
1:C:180:THR:C	1:C:182:PRO:HD3	2.40	0.47
1:C:254:ARG:HD2	1:D:278:CYS:O	2.14	0.47
1:D:77:ILE:H	1:D:284:GLN:NE2	2.13	0.47
1:A:126:ILE:CG2	1:A:178:ILE:HG12	2.42	0.47
1:B:341:LEU:HD13	1:B:378:ILE:HD13	1.95	0.47
1:C:59:LYS:C	1:C:59:LYS:HD2	2.40	0.47
1:C:175:VAL:CG2	5:C:485:HOH:O	2.63	0.47
1:C:269:LEU:HD13	1:C:269:LEU:HA	1.74	0.47
1:D:323:LEU:HD21	1:D:398:ALA:HB2	1.96	0.47
1:B:343:GLU:CD	1:B:343:GLU:H	2.22	0.46
1:B:208:ASP:HB3	1:D:5:LYS:CE	2.45	0.46
1:B:276:ASP:OD1	1:B:276:ASP:C	2.59	0.46
1:D:94:LEU:HD11	1:D:231:LYS:HG3	1.96	0.46
1:A:89:LYS:HD3	1:A:89:LYS:C	2.41	0.46
1:C:140:GLU:HG2	1:C:146:ILE:HD13	1.97	0.46
1:C:297:GLU:HA	1:C:301:LEU:HD12	1.97	0.46
1:B:75:ASN:HB3	1:B:269:LEU:CD1	2.45	0.46
1:A:132:TYR:CZ	1:A:134:ASN:HB2	2.50	0.46
1:A:176:LYS:CG	1:A:177:LEU:HG	2.46	0.46
1:B:231:LYS:CD	1:B:239:VAL:HG22	2.45	0.46
1:A:110:ALA:O	1:A:114:LEU:HD22	2.16	0.46
1:B:175:VAL:HG22	1:B:176:LYS:N	2.30	0.46
1:C:354:LEU:HD21	1:C:397:LEU:HA	1.96	0.46
1:A:156:MET:SD	1:A:161:LEU:HG	2.56	0.46
1:B:228:VAL:CG2	1:B:233:LEU:HD13	2.46	0.46
1:C:273:GLN:HB3	1:C:274:PRO:HD3	1.97	0.46
5:A:418:HOH:O	1:B:267:LYS:HE3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ASN:HD22	1:C:75:ASN:H	1.62	0.46
1:B:228:VAL:HG21	1:B:233:LEU:HD13	1.97	0.46
1:C:57:ILE:O	1:C:61:VAL:HG12	2.16	0.46
1:D:231:LYS:CD	1:D:239:VAL:HG22	2.46	0.46
1:C:354:LEU:HD12	1:C:362:VAL:HG21	1.98	0.45
1:D:161:LEU:HD13	1:D:203:ILE:HG21	1.97	0.45
1:D:322:HIS:HE1	1:D:395:LYS:NZ	2.12	0.45
1:B:93:HIS:NE2	1:B:226:ASP:OD2	2.49	0.45
1:B:185:GLN:HG2	1:B:186:ASN:N	2.32	0.45
1:C:310:GLU:O	1:C:314:ILE:HG22	2.17	0.45
1:B:254:ARG:HH12	3:B:409:PMP:P	2.39	0.45
1:A:384:ARG:N	1:A:385:PRO:HD2	2.32	0.45
1:C:245:LEU:HG	1:C:257:TRP:CZ3	2.52	0.45
1:A:182:PRO:O	1:A:191:THR:HA	2.16	0.45
1:A:278:CYS:O	1:B:254:ARG:HD2	2.16	0.45
1:C:231:LYS:CD	1:C:239:VAL:HG22	2.46	0.45
1:D:221:ARG:HD3	1:D:227:ILE:CD1	2.46	0.45
1:D:305:LEU:HD23	1:D:305:LEU:O	2.17	0.45
1:D:341:LEU:HB3	1:D:345:ALA:HB3	1.98	0.45
1:D:366:LYS:N	1:D:367:PRO:CD	2.79	0.45
1:A:2:ASP:OD2	1:A:4:THR:HG22	2.17	0.45
1:B:57:ILE:HD12	1:B:61:VAL:HG23	1.99	0.45
1:C:221:ARG:NH2	1:C:225:GLY:O	2.48	0.45
1:A:322:HIS:CE1	1:A:395:LYS:HE2	2.52	0.45
1:C:386:SER:OG	1:C:389:GLU:HG3	2.17	0.45
1:A:57:ILE:HD12	1:A:61:VAL:HG23	1.98	0.45
1:C:167:GLU:O	1:C:171:LYS:HG3	2.17	0.45
1:C:282:ILE:HG13	5:C:438:HOH:O	2.17	0.45
1:B:60:GLU:OE1	1:B:293:ARG:NH2	2.46	0.44
1:D:281:ALA:HB3	5:D:447:HOH:O	2.16	0.44
1:A:219:PHE:O	1:A:300:HIS:HE1	2.00	0.44
1:B:219:PHE:O	1:B:300:HIS:HE1	2.00	0.44
1:B:273:GLN:HB3	1:B:274:PRO:HD3	1.98	0.44
1:C:394:ILE:HD12	1:C:394:ILE:O	2.17	0.44
1:A:72:THR:HG23	1:A:73:PRO:O	2.17	0.44
1:B:180:THR:C	1:B:182:PRO:HD3	2.43	0.44
1:C:135:THR:HG21	1:C:179:TYR:CE1	2.52	0.44
1:C:135:THR:HG21	1:C:179:TYR:CZ	2.52	0.44
1:A:65:GLU:OE1	1:A:66:PRO:HD2	2.18	0.44
1:D:18:ALA:C	1:D:20:ALA:N	2.66	0.44
1:D:137:LEU:O	1:D:141:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:THR:C	1:D:182:PRO:HD3	2.43	0.44
1:A:29:LEU:HA	5:A:481:HOH:O	2.18	0.44
1:A:112:ASP:O	1:A:116:ARG:HG3	2.18	0.44
1:A:231:LYS:CD	1:A:239:VAL:HG22	2.42	0.44
1:A:312:ARG:HD2	1:A:312:ARG:C	2.43	0.44
1:A:362:VAL:HG22	5:A:429:HOH:O	2.17	0.44
1:B:57:ILE:HG13	1:B:58:ALA:N	2.33	0.44
1:C:220:MET:HE1	1:C:335:MET:HB3	1.99	0.44
1:B:323:LEU:N	1:B:324:PRO:CD	2.81	0.44
1:A:133:ILE:HG13	1:A:368:PHE:CE2	2.52	0.44
1:B:77:ILE:CG1	1:B:80:LEU:HB2	2.48	0.44
1:D:296:PHE:O	1:D:300:HIS:HB3	2.18	0.44
1:A:102:VAL:O	1:A:257:TRP:HA	2.18	0.44
1:A:136:LEU:CD2	1:A:146:ILE:HD13	2.45	0.44
5:A:496:HOH:O	1:C:4:THR:CG2	2.66	0.44
1:B:112:ASP:O	1:B:116:ARG:HG3	2.18	0.44
1:C:154:ASP:O	1:C:192:MET:HA	2.18	0.44
1:D:310:GLU:O	1:D:314:ILE:HG13	2.18	0.44
1:D:354:LEU:HA	1:D:400:LEU:HD12	2.00	0.44
1:A:384:ARG:HB3	1:A:384:ARG:NH1	2.32	0.43
1:B:93:HIS:CE1	1:B:226:ASP:OD1	2.69	0.43
1:A:397:LEU:HD13	1:A:397:LEU:C	2.43	0.43
1:B:328:PHE:CE1	1:B:330:LYS:HE3	2.53	0.43
1:C:14:ILE:HD13	1:D:271:GLN:HB3	1.99	0.43
1:A:80:LEU:HD12	1:A:284:GLN:HB3	2.00	0.43
1:B:192:MET:HG2	1:B:197:ARG:HG3	1.99	0.43
1:B:228:VAL:HA	1:B:229:PRO:HD3	1.91	0.43
1:C:402:LYS:C	1:C:404:LYS:H	2.26	0.43
1:D:238:ARG:HG2	1:D:238:ARG:NH2	2.34	0.43
1:A:300:HIS:O	1:A:305:LEU:HB2	2.18	0.43
1:C:84:LEU:HD23	1:C:84:LEU:HA	1.92	0.43
1:D:31:LYS:C	1:D:33:GLY:H	2.26	0.43
1:D:77:ILE:H	1:D:284:GLN:HE22	1.67	0.43
1:A:271:GLN:O	1:A:274:PRO:HD2	2.19	0.43
1:C:220:MET:CE	1:C:335:MET:HB3	2.49	0.43
1:C:335:MET:HA	1:C:382:PHE:CZ	2.53	0.43
1:A:266:LYS:HE3	1:A:270:MET:CE	2.48	0.42
1:C:158:VAL:CG1	1:C:203:ILE:HD12	2.48	0.42
1:C:162:GLU:HG2	1:C:166:LYS:HD2	2.01	0.42
1:A:97:SER:HB3	1:A:100:ASN:HD22	1.83	0.42
1:A:128:GLU:HG3	1:A:156:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HG13	1:B:203:ILE:HD12	2.01	0.42
1:B:254:ARG:HA	1:B:254:ARG:NE	2.34	0.42
1:C:161:LEU:HD22	1:C:165:ILE:HD11	2.01	0.42
1:A:45:ASP:OD2	1:A:311:LYS:NZ	2.41	0.42
1:A:282:ILE:O	1:A:286:ILE:HG13	2.19	0.42
1:B:75:ASN:C	1:B:75:ASN:ND2	2.76	0.42
1:C:175:VAL:HG23	5:C:485:HOH:O	2.19	0.42
1:B:1:MET:N	5:B:524:HOH:O	2.53	0.42
1:C:53:VAL:O	1:C:57:ILE:HG13	2.19	0.42
1:D:53:VAL:O	1:D:57:ILE:HG23	2.20	0.42
1:B:100:ASN:N	1:B:100:ASN:HD22	2.17	0.42
1:B:111:LEU:HD12	1:B:212:ILE:CD1	2.38	0.42
1:B:194:MET:HG2	1:B:227:ILE:HG22	2.01	0.42
1:D:238:ARG:HG2	1:D:238:ARG:HH21	1.84	0.42
1:B:164:LYS:O	1:B:168:LEU:HD22	2.19	0.42
1:B:399:LYS:O	1:B:403:GLU:HG2	2.19	0.42
1:C:276:ASP:OD1	1:C:276:ASP:C	2.63	0.42
1:A:77:ILE:HG13	1:A:80:LEU:HB2	2.02	0.42
1:B:65:GLU:HA	1:B:66:PRO:HD2	1.90	0.42
1:C:392:ILE:HG22	1:C:396:LYS:HE3	2.02	0.42
1:D:57:ILE:HD13	1:D:289:GLU:CB	2.44	0.42
1:A:57:ILE:HD13	1:A:289:GLU:CB	2.45	0.42
1:A:314:ILE:HD11	1:A:387:LYS:HZ2	1.85	0.42
1:C:72:THR:HG21	1:C:284:GLN:OE1	2.19	0.42
1:D:62:LEU:HD23	1:D:68:SER:OG	2.19	0.42
1:A:17:SER:HB2	1:A:137:LEU:HD21	2.01	0.42
1:A:282:ILE:HG21	1:B:253:PHE:CE1	2.55	0.42
1:D:184:GLY:H	1:D:191:THR:CG2	2.25	0.42
1:D:254:ARG:HH12	3:D:409:PMP:P	2.43	0.42
1:A:18:ALA:HB3	1:A:367:PRO:HG2	2.01	0.41
1:B:42:GLY:CA	1:B:335:MET:CE	2.98	0.41
1:C:9:GLY:H	1:D:120:ASP:CG	2.28	0.41
1:C:192:MET:HG2	1:C:197:ARG:HG3	2.02	0.41
1:C:342:PRO:HG2	1:C:405:PHE:CD2	2.55	0.41
1:D:112:ASP:O	1:D:116:ARG:HG3	2.20	0.41
1:B:61:VAL:HG11	1:B:285:TYR:CB	2.51	0.41
1:B:113:LEU:HD12	1:B:113:LEU:HA	1.74	0.41
1:A:134:ASN:ND2	1:B:273:GLN:HG2	2.17	0.41
1:B:18:ALA:C	1:B:20:ALA:H	2.28	0.41
1:C:97:SER:HB3	1:C:100:ASN:ND2	2.24	0.41
1:A:94:LEU:HD11	1:A:231:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:HB3	1:A:230:LEU:HD23	2.02	0.41
1:A:221:ARG:HA	1:A:333:ALA:CB	2.50	0.41
1:B:357:ARG:NH1	1:B:403:GLU:OE2	2.53	0.41
1:D:77:ILE:HA	1:D:78:PRO:HD3	1.94	0.41
1:D:194:MET:HA	1:D:197:ARG:HD3	2.01	0.41
1:D:354:LEU:HD22	1:D:354:LEU:O	2.21	0.41
1:C:45:ASP:OD2	1:C:48:LEU:HG	2.21	0.41
1:C:126:ILE:O	1:C:126:ILE:HG13	2.21	0.41
1:C:194:MET:HA	1:C:197:ARG:HD3	2.02	0.41
1:D:47:GLU:CD	1:D:51:ARG:HH22	2.29	0.41
1:A:366:LYS:N	1:A:367:PRO:CD	2.83	0.41
1:B:53:VAL:O	1:B:57:ILE:HG23	2.21	0.41
1:B:110:ALA:HB1	1:B:258:ILE:HG13	2.03	0.41
1:B:394:ILE:HA	1:B:397:LEU:HB3	2.02	0.41
1:C:76:GLY:HA2	1:C:284:GLN:HE22	1.86	0.41
1:D:392:ILE:O	1:D:396:LYS:HG3	2.21	0.41
1:C:3:TYR:HA	1:C:6:TYR:HD1	1.86	0.41
1:C:26:ALA:HB2	1:C:355:MET:SD	2.61	0.41
1:C:185:GLN:OE1	1:C:188:MET:HB2	2.20	0.41
1:D:402:LYS:HD3	1:D:402:LYS:HA	1.90	0.41
1:B:161:LEU:O	1:B:165:ILE:HG13	2.21	0.41
1:B:198:LYS:HE3	5:B:518:HOH:O	2.20	0.41
1:B:221:ARG:HD2	1:B:227:ILE:CD1	2.30	0.41
1:C:38:SER:CB	1:C:361:VAL:HB	2.51	0.41
1:D:78:PRO:O	1:D:82:GLU:HG3	2.21	0.41
1:D:360:VAL:CG2	1:D:396:LYS:HD2	2.51	0.41
1:A:69:VAL:HG23	1:B:253:PHE:CE2	2.56	0.41
1:A:276:ASP:OD1	1:A:276:ASP:C	2.64	0.41
1:B:135:THR:HG21	1:B:179:TYR:CE1	2.56	0.41
1:C:227:ILE:H	1:C:227:ILE:HG12	1.69	0.41
1:D:132:TYR:CZ	1:D:134:ASN:HB2	2.56	0.41
1:D:305:LEU:HD23	1:D:305:LEU:C	2.45	0.41
1:A:335:MET:HE3	1:A:381:ASN:ND2	2.35	0.40
1:B:132:TYR:CZ	1:B:134:ASN:HB2	2.56	0.40
1:C:267:LYS:HD3	1:C:267:LYS:HA	1.88	0.40
1:A:40:ALA:HB2	1:A:361:VAL:HG12	2.03	0.40
1:D:83:GLU:HG3	1:D:288:LEU:HD12	2.04	0.40
1:A:282:ILE:HD13	1:B:253:PHE:CD1	2.56	0.40
1:A:2:ASP:CG	1:A:4:THR:HG22	2.47	0.40
1:A:31:LYS:C	1:A:33:GLY:H	2.29	0.40
1:A:254:ARG:NH1	3:A:409:PMP:O2P	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PRO:HG3	1:B:280:PRO:HG2	2.03	0.40
1:B:77:ILE:HG13	1:B:80:LEU:H	1.85	0.40
1:C:69:VAL:HG21	1:D:49:ILE:HG21	2.03	0.40
1:D:331:PRO:HG2	1:D:336:PHE:O	2.22	0.40
1:A:126:ILE:HD13	1:A:126:ILE:O	2.22	0.40
1:C:369:TYR:CD2	1:C:374:GLY:HA3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	403/407 (99%)	387 (96%)	14 (4%)	2 (0%)	24	31
1	B	403/407 (99%)	377 (94%)	24 (6%)	2 (0%)	24	31
1	C	403/407 (99%)	380 (94%)	19 (5%)	4 (1%)	12	15
1	D	403/407 (99%)	374 (93%)	25 (6%)	4 (1%)	12	15
All	All	1612/1628 (99%)	1518 (94%)	82 (5%)	12 (1%)	18	23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	VAL
1	D	33	GLY
1	D	41	ALA
1	B	32	LYS
1	B	41	ALA
1	C	31	LYS
1	C	224	GLY
1	A	364	PRO
1	A	225	GLY

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Mol	Chain	Res	Type
1	D	234	ASP
1	D	303	GLY
1	C	303	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	321/338 (95%)	285 (89%)	36 (11%)	6	7
1	B	321/338 (95%)	283 (88%)	38 (12%)	5	6
1	C	321/338 (95%)	283 (88%)	38 (12%)	5	6
1	D	321/338 (95%)	285 (89%)	36 (11%)	6	7
All	All	1284/1352 (95%)	1136 (88%)	148 (12%)	5	6

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	56	GLU
1	A	57	ILE
1	A	75	ASN
1	A	80	LEU
1	A	111	LEU
1	A	113	LEU
1	A	114	LEU
1	A	125	VAL
1	A	126	ILE
1	A	133	ILE
1	A	137	LEU
1	A	161	LEU
1	A	168	LEU
1	A	198	LYS
1	A	210	LEU
1	A	221	ARG
1	A	233	LEU

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Mol	Chain	Res	Type
1	A	239	VAL
1	A	241	VAL
1	A	251	THR
1	A	261	GLU
1	A	269	LEU
1	A	275	ILE
1	A	297	GLU
1	A	305	LEU
1	A	320	GLU
1	A	327	GLU
1	A	343	GLU
1	A	354	LEU
1	A	372	GLU
1	A	384	ARG
1	A	394	ILE
1	A	397	LEU
1	A	400	LEU
1	A	404	LYS
1	B	4	THR
1	B	5	LYS
1	B	39	LEU
1	B	57	ILE
1	B	59	LYS
1	B	69	VAL
1	B	75	ASN
1	B	80	LEU
1	B	88	LEU
1	B	100	ASN
1	B	111	LEU
1	B	113	LEU
1	B	114	LEU
1	B	125	VAL
1	B	137	LEU
1	B	161	LEU
1	B	168	LEU
1	B	187	PRO
1	B	210	LEU
1	B	212	ILE
1	B	227	ILE
1	B	228	VAL
1	B	233	LEU
1	B	239	VAL

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Mol	Chain	Res	Type
1	B	241	VAL
1	B	251	THR
1	B	268	VAL
1	B	275	ILE
1	B	302	GLU
1	B	341	LEU
1	B	343	GLU
1	B	354	LEU
1	B	372	GLU
1	B	384	ARG
1	B	388	GLU
1	B	394	ILE
1	B	400	LEU
1	B	404	LYS
1	C	4	THR
1	C	72	THR
1	C	75	ASN
1	C	80	LEU
1	C	88	LEU
1	C	93	HIS
1	C	111	LEU
1	C	113	LEU
1	C	114	LEU
1	C	117	VAL
1	C	125	VAL
1	C	126	ILE
1	C	137	LEU
1	C	161	LEU
1	C	168	LEU
1	C	187	PRO
1	C	191	THR
1	C	198	LYS
1	C	210	LEU
1	C	221	ARG
1	C	223	GLU
1	C	233	LEU
1	C	239	VAL
1	C	241	VAL
1	C	251	THR
1	C	261	GLU
1	C	269	LEU
1	C	282	ILE

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Mol	Chain	Res	Type
1	C	305	LEU
1	C	314	ILE
1	C	323	LEU
1	C	341	LEU
1	C	378	ILE
1	C	384	ARG
1	C	388	GLU
1	C	394	ILE
1	C	397	LEU
1	C	400	LEU
1	D	4	THR
1	D	56	GLU
1	D	57	ILE
1	D	70	MET
1	D	75	ASN
1	D	80	LEU
1	D	88	LEU
1	D	93	HIS
1	D	101	ILE
1	D	111	LEU
1	D	113	LEU
1	D	114	LEU
1	D	121	PRO
1	D	125	VAL
1	D	133	ILE
1	D	137	LEU
1	D	161	LEU
1	D	167	GLU
1	D	168	LEU
1	D	187	PRO
1	D	191	THR
1	D	210	LEU
1	D	233	LEU
1	D	239	VAL
1	D	241	VAL
1	D	247	LYS
1	D	269	LEU
1	D	282	ILE
1	D	317	LYS
1	D	327	GLU
1	D	343	GLU
1	D	354	LEU

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Mol	Chain	Res	Type
1	D	378	ILE
1	D	384	ARG
1	D	397	LEU
1	D	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	75	ASN
1	A	100	ASN
1	A	134	ASN
1	A	173	GLN
1	A	284	GLN
1	A	300	HIS
1	A	321	ASN
1	A	322	HIS
1	B	12	ASN
1	B	75	ASN
1	B	93	HIS
1	B	100	ASN
1	B	173	GLN
1	B	271	GLN
1	B	284	GLN
1	B	300	HIS
1	C	12	ASN
1	C	75	ASN
1	C	100	ASN
1	C	134	ASN
1	C	173	GLN
1	C	300	HIS
1	C	321	ASN
1	C	322	HIS
1	C	352	ASN
1	C	381	ASN
1	D	12	ASN
1	D	75	ASN
1	D	100	ASN
1	D	134	ASN
1	D	173	GLN
1	D	271	GLN
1	D	284	GLN

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Mol	Chain	Res	Type
1	D	300	HIS
1	D	322	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	PMP	A	409	-	16,16,16	5.79	9 (56%)	22,23,23	1.66	4 (18%)
3	PMP	D	409	-	16,16,16	5.87	8 (50%)	22,23,23	1.84	5 (22%)
3	PMP	B	409	-	16,16,16	5.80	9 (56%)	22,23,23	1.68	4 (18%)
4	IMD	C	410	2	5,5,5	0.30	0	5,5,5	0.48	0
3	PMP	C	409	-	16,16,16	5.71	7 (43%)	22,23,23	1.66	4 (18%)
4	IMD	A	410	2	5,5,5	0.19	0	5,5,5	0.45	0
4	IMD	D	410	2	5,5,5	0.37	0	5,5,5	0.47	0
4	IMD	B	410	2	5,5,5	0.31	0	5,5,5	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PMP	A	409	-	-	4/8/8/8	0/1/1/1
3	PMP	D	409	-	-	5/8/8/8	0/1/1/1
3	PMP	B	409	-	-	4/8/8/8	0/1/1/1
4	IMD	C	410	2	-	-	0/1/1/1
3	PMP	C	409	-	-	3/8/8/8	0/1/1/1
4	IMD	A	410	2	-	-	0/1/1/1
4	IMD	D	410	2	-	-	0/1/1/1
4	IMD	B	410	2	-	-	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	409	PMP	P-O1P	12.72	1.90	1.50
3	D	409	PMP	P-O1P	12.65	1.89	1.50
3	C	409	PMP	P-O1P	12.65	1.89	1.50
3	B	409	PMP	P-O1P	12.39	1.89	1.50
3	D	409	PMP	C5-C4	10.67	1.55	1.40
3	B	409	PMP	C5-C4	10.51	1.55	1.40
3	A	409	PMP	C5-C4	10.13	1.54	1.40
3	A	409	PMP	P-O2P	9.89	1.91	1.54
3	C	409	PMP	P-O2P	9.88	1.91	1.54
3	B	409	PMP	P-O2P	9.86	1.91	1.54
3	D	409	PMP	P-O2P	9.79	1.91	1.54
3	C	409	PMP	C5-C4	9.62	1.54	1.40
3	D	409	PMP	O4P-C5A	-9.56	1.09	1.44
3	C	409	PMP	O4P-C5A	-9.36	1.10	1.44
3	B	409	PMP	O4P-C5A	-9.24	1.10	1.44
3	A	409	PMP	O4P-C5A	-9.12	1.11	1.44
3	D	409	PMP	P-O3P	7.38	1.82	1.54
3	C	409	PMP	P-O3P	7.34	1.82	1.54
3	A	409	PMP	P-O3P	7.29	1.81	1.54
3	B	409	PMP	P-O3P	7.29	1.81	1.54
3	D	409	PMP	C3-C4	3.66	1.45	1.40
3	B	409	PMP	C3-C4	3.65	1.45	1.40
3	A	409	PMP	C3-C4	3.35	1.45	1.40
3	C	409	PMP	C3-C4	3.14	1.44	1.40
3	A	409	PMP	C6-N1	2.50	1.39	1.34
3	B	409	PMP	C6-N1	2.43	1.39	1.34
3	D	409	PMP	C6-N1	2.30	1.39	1.34
3	A	409	PMP	P-O4P	2.30	1.67	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	409	PMP	P-O4P	2.28	1.67	1.60
3	D	409	PMP	P-O4P	2.23	1.67	1.60
3	C	409	PMP	C6-N1	2.22	1.38	1.34
3	A	409	PMP	C6-C5	2.17	1.42	1.37
3	B	409	PMP	C2A-C2	2.10	1.53	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	409	PMP	O4P-P-O1P	5.11	120.25	106.44
3	C	409	PMP	O4P-P-O1P	4.35	118.19	106.44
3	A	409	PMP	O4P-P-O1P	4.31	118.09	106.44
3	B	409	PMP	O4P-P-O1P	4.08	117.47	106.44
3	C	409	PMP	C5-C6-N1	-3.45	118.22	123.83
3	D	409	PMP	C6-N1-C2	3.34	125.25	119.20
3	B	409	PMP	C6-N1-C2	3.33	125.23	119.20
3	A	409	PMP	C5-C6-N1	-3.26	118.53	123.83
3	D	409	PMP	C5-C6-N1	-3.23	118.57	123.83
3	B	409	PMP	C5-C6-N1	-3.23	118.58	123.83
3	A	409	PMP	C6-N1-C2	3.23	125.05	119.20
3	C	409	PMP	C6-N1-C2	3.21	125.03	119.20
3	B	409	PMP	O3P-P-O4P	2.76	113.86	106.67
3	A	409	PMP	O3P-P-O4P	2.52	113.24	106.67
3	D	409	PMP	O4P-C5A-C5	2.28	113.63	109.36
3	C	409	PMP	O3P-P-O4P	2.09	112.11	106.67
3	D	409	PMP	C4A-C4-C5	2.07	124.42	120.27

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	409	PMP	C5A-O4P-P-O1P
3	A	409	PMP	C5A-O4P-P-O2P
3	A	409	PMP	C5A-O4P-P-O3P
3	B	409	PMP	C5A-O4P-P-O1P
3	B	409	PMP	C5A-O4P-P-O2P
3	B	409	PMP	C5A-O4P-P-O3P
3	C	409	PMP	C5A-O4P-P-O1P
3	C	409	PMP	C5A-O4P-P-O2P
3	C	409	PMP	C5A-O4P-P-O3P
3	D	409	PMP	C4-C5-C5A-O4P
3	D	409	PMP	C6-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
3	D	409	PMP	C5A-O4P-P-O1P
3	D	409	PMP	C5A-O4P-P-O2P
3	D	409	PMP	C5A-O4P-P-O3P
3	A	409	PMP	C5-C4-C4A-N4A
3	B	409	PMP	C5-C4-C4A-N4A

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	409	PMP	2	0
3	D	409	PMP	1	0
3	B	409	PMP	3	0
3	C	409	PMP	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	405/407 (99%)	0.47	27 (6%)	24	26	24, 46, 75, 102	0
1	B	405/407 (99%)	0.29	16 (3%)	42	44	23, 42, 69, 100	0
1	C	405/407 (99%)	0.60	37 (9%)	15	16	26, 48, 98, 109	0
1	D	405/407 (99%)	0.58	34 (8%)	17	18	24, 49, 83, 102	0
All	All	1620/1628 (99%)	0.48	114 (7%)	22	24	23, 46, 85, 109	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	LEU	5.8
1	D	19	LEU	5.3
1	B	20	ALA	4.9
1	C	282	ILE	4.6
1	C	19	LEU	4.4
1	D	22	VAL	4.1
1	B	22	VAL	3.8
1	C	249	LEU	3.8
1	B	224	GLY	3.6
1	A	19	LEU	3.5
1	C	397	LEU	3.5
1	A	20	ALA	3.4
1	C	296	PHE	3.4
1	C	37	ILE	3.3
1	C	405	PHE	3.3
1	D	20	ALA	3.3
1	D	393	GLY	3.2
1	A	21	ASP	3.2
1	C	323	LEU	3.2
1	C	36	LEU	3.2
1	C	34	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	37	ILE	3.1
1	A	25	LYS	3.0
1	D	66	PRO	3.0
1	C	356	GLU	3.0
1	C	29	LEU	3.0
1	D	57	ILE	3.0
1	B	21	ASP	3.0
1	C	402	LYS	2.9
1	C	30	GLN	2.9
1	A	225	GLY	2.9
1	C	22	VAL	2.9
1	C	348	ILE	2.9
1	A	224	GLY	2.8
1	B	18	ALA	2.8
1	B	405	PHE	2.8
1	B	34	VAL	2.8
1	C	394	ILE	2.7
1	C	321	ASN	2.7
1	A	326	ALA	2.7
1	C	350	PHE	2.6
1	D	392	ILE	2.6
1	D	394	ILE	2.6
1	D	323	LEU	2.6
1	A	402	LYS	2.6
1	D	62	LEU	2.6
1	C	33	GLY	2.6
1	A	37	ILE	2.6
1	D	94	LEU	2.5
1	C	20	ALA	2.5
1	A	27	SER	2.5
1	B	91	TYR	2.5
1	B	327	GLU	2.5
1	D	60	GLU	2.5
1	C	401	TYR	2.5
1	C	347	GLY	2.5
1	C	314	ILE	2.4
1	C	360	VAL	2.4
1	C	322	HIS	2.4
1	B	364	PRO	2.4
1	C	27	SER	2.4
1	D	17	SER	2.4
1	A	348	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	355	MET	2.4
1	C	354	LEU	2.4
1	C	21	ASP	2.4
1	B	402	LYS	2.4
1	A	17	SER	2.4
1	A	55	GLY	2.3
1	C	41	ALA	2.3
1	C	399	LYS	2.3
1	C	23	MET	2.3
1	A	30	GLN	2.3
1	A	405	PHE	2.3
1	A	153	ASN	2.3
1	D	222	TYR	2.3
1	D	23	MET	2.3
1	D	27	SER	2.3
1	A	22	VAL	2.3
1	D	29	LEU	2.3
1	B	322	HIS	2.3
1	D	93	HIS	2.2
1	D	402	LYS	2.2
1	A	29	LEU	2.2
1	A	60	GLU	2.2
1	D	299	TYR	2.2
1	A	36	LEU	2.2
1	D	397	LEU	2.2
1	B	66	PRO	2.2
1	A	249	LEU	2.2
1	C	59	LYS	2.2
1	D	388	GLU	2.2
1	D	400	LEU	2.1
1	D	404	LYS	2.1
1	D	18	ALA	2.1
1	A	401	TYR	2.1
1	D	71	TYR	2.1
1	A	57	ILE	2.1
1	D	227	ILE	2.1
1	D	61	VAL	2.1
1	B	23	MET	2.1
1	D	354	LEU	2.1
1	D	295	TYR	2.1
1	C	53	VAL	2.1
1	C	351	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	327	GLU	2.1
1	A	397	LEU	2.1
1	D	34	VAL	2.1
1	C	25	LYS	2.0
1	A	350	PHE	2.0
1	A	198	LYS	2.0
1	B	399	LYS	2.0
1	D	249	LEU	2.0
1	D	291	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
3	PMP	D	409	16/16	0.88	0.16	56,61,62,63	0
3	PMP	C	409	16/16	0.89	0.17	57,62,63,63	0
3	PMP	A	409	16/16	0.89	0.16	48,59,61,66	0
3	PMP	B	409	16/16	0.90	0.15	41,54,57,61	0
4	IMD	A	410	5/5	0.92	0.12	44,44,44,45	0
4	IMD	C	410	5/5	0.95	0.09	52,52,52,53	0
2	ZN	A	408	1/1	0.97	0.09	46,46,46,46	0
4	IMD	D	410	5/5	0.97	0.07	51,51,52,53	0
4	IMD	B	410	5/5	0.98	0.07	44,45,46,46	0
2	ZN	D	408	1/1	0.99	0.06	45,45,45,45	0
2	ZN	B	408	1/1	0.99	0.06	38,38,38,38	0
2	ZN	C	408	1/1	0.99	0.04	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.