



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:04 PM UTC

PDB ID : 2FWR / pdb_00002fwr
Title : Structure of Archaeoglobus Fulgidis XPB
Authors : Fan, L.; Arvai, A.S.; Tainer, J.A.
Deposited on : 2006-02-02
Resolution : 2.60 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

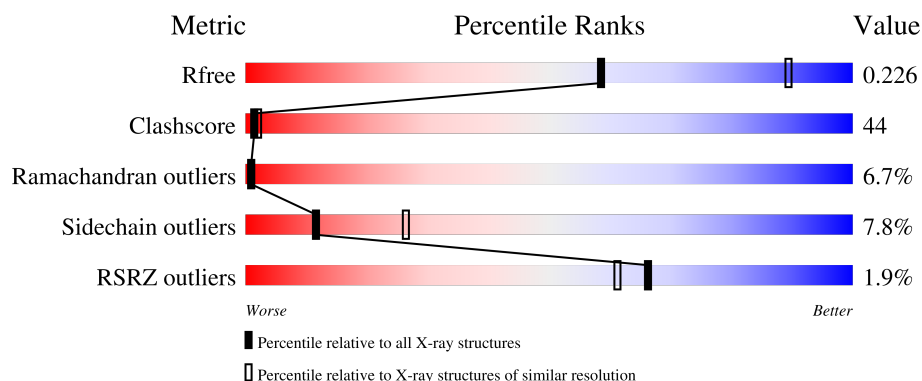
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	472	2% 35% 48% 8% 8%
1	B	472	% 39% 43% 7% 10%
1	C	472	% 29% 46% 11% 12%
1	D	472	2% 30% 48% 12% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14769 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 DNA repair protein RAD25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3513	2242	627	638	6			
1	B	423	Total	C	N	O	S	0	0	0
			3419	2181	611	619	8			
1	C	414	Total	C	N	O	S	0	0	0
			3317	2119	589	604	5			
1	D	428	Total	C	N	O	S	0	0	0
			3402	2169	604	623	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O29889
A	2	GLY	-	cloning artifact	UNP O29889
A	3	SER	-	cloning artifact	UNP O29889
A	4	SER	-	cloning artifact	UNP O29889
A	5	HIS	-	expression tag	UNP O29889
A	6	HIS	-	expression tag	UNP O29889
A	7	HIS	-	expression tag	UNP O29889
A	8	HIS	-	expression tag	UNP O29889
A	9	HIS	-	expression tag	UNP O29889
A	10	HIS	-	expression tag	UNP O29889
A	11	SER	-	cloning artifact	UNP O29889
A	12	SER	-	cloning artifact	UNP O29889
A	13	GLY	-	cloning artifact	UNP O29889
A	14	LEU	-	cloning artifact	UNP O29889
A	15	VAL	-	cloning artifact	UNP O29889
A	16	PRO	-	cloning artifact	UNP O29889
A	17	ARG	-	cloning artifact	UNP O29889
A	18	GLY	-	cloning artifact	UNP O29889
A	19	SER	-	cloning artifact	UNP O29889
A	20	HIS	-	cloning artifact	UNP O29889
B	1	MET	-	initiating methionine	UNP O29889

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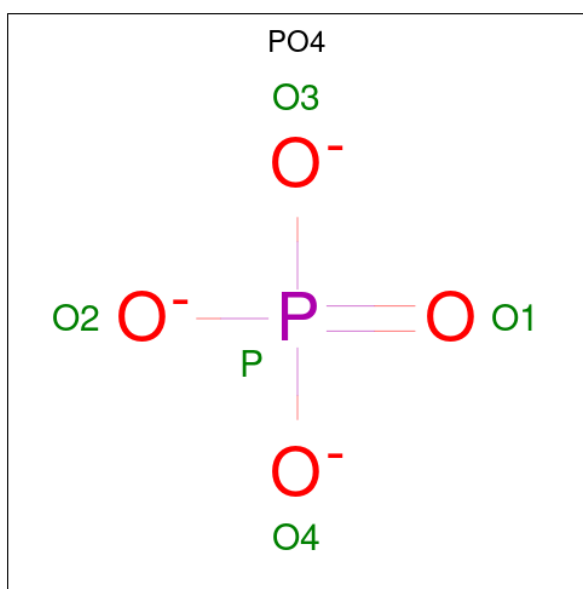
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLY	-	cloning artifact	UNP O29889
B	3	SER	-	cloning artifact	UNP O29889
B	4	SER	-	cloning artifact	UNP O29889
B	5	HIS	-	expression tag	UNP O29889
B	6	HIS	-	expression tag	UNP O29889
B	7	HIS	-	expression tag	UNP O29889
B	8	HIS	-	expression tag	UNP O29889
B	9	HIS	-	expression tag	UNP O29889
B	10	HIS	-	expression tag	UNP O29889
B	11	SER	-	cloning artifact	UNP O29889
B	12	SER	-	cloning artifact	UNP O29889
B	13	GLY	-	cloning artifact	UNP O29889
B	14	LEU	-	cloning artifact	UNP O29889
B	15	VAL	-	cloning artifact	UNP O29889
B	16	PRO	-	cloning artifact	UNP O29889
B	17	ARG	-	cloning artifact	UNP O29889
B	18	GLY	-	cloning artifact	UNP O29889
B	19	SER	-	cloning artifact	UNP O29889
B	20	HIS	-	cloning artifact	UNP O29889
C	1	MET	-	initiating methionine	UNP O29889
C	2	GLY	-	cloning artifact	UNP O29889
C	3	SER	-	cloning artifact	UNP O29889
C	4	SER	-	cloning artifact	UNP O29889
C	5	HIS	-	expression tag	UNP O29889
C	6	HIS	-	expression tag	UNP O29889
C	7	HIS	-	expression tag	UNP O29889
C	8	HIS	-	expression tag	UNP O29889
C	9	HIS	-	expression tag	UNP O29889
C	10	HIS	-	expression tag	UNP O29889
C	11	SER	-	cloning artifact	UNP O29889
C	12	SER	-	cloning artifact	UNP O29889
C	13	GLY	-	cloning artifact	UNP O29889
C	14	LEU	-	cloning artifact	UNP O29889
C	15	VAL	-	cloning artifact	UNP O29889
C	16	PRO	-	cloning artifact	UNP O29889
C	17	ARG	-	cloning artifact	UNP O29889
C	18	GLY	-	cloning artifact	UNP O29889
C	19	SER	-	cloning artifact	UNP O29889
C	20	HIS	-	cloning artifact	UNP O29889
D	1	MET	-	initiating methionine	UNP O29889
D	2	GLY	-	cloning artifact	UNP O29889
D	3	SER	-	cloning artifact	UNP O29889

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Chain	Residue	Modelled	Actual	Comment	Reference
D	4	SER	-	cloning artifact	UNP O29889
D	5	HIS	-	expression tag	UNP O29889
D	6	HIS	-	expression tag	UNP O29889
D	7	HIS	-	expression tag	UNP O29889
D	8	HIS	-	expression tag	UNP O29889
D	9	HIS	-	expression tag	UNP O29889
D	10	HIS	-	expression tag	UNP O29889
D	11	SER	-	cloning artifact	UNP O29889
D	12	SER	-	cloning artifact	UNP O29889
D	13	GLY	-	cloning artifact	UNP O29889
D	14	LEU	-	cloning artifact	UNP O29889
D	15	VAL	-	cloning artifact	UNP O29889
D	16	PRO	-	cloning artifact	UNP O29889
D	17	ARG	-	cloning artifact	UNP O29889
D	18	GLY	-	cloning artifact	UNP O29889
D	19	SER	-	cloning artifact	UNP O29889
D	20	HIS	-	cloning artifact	UNP O29889

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



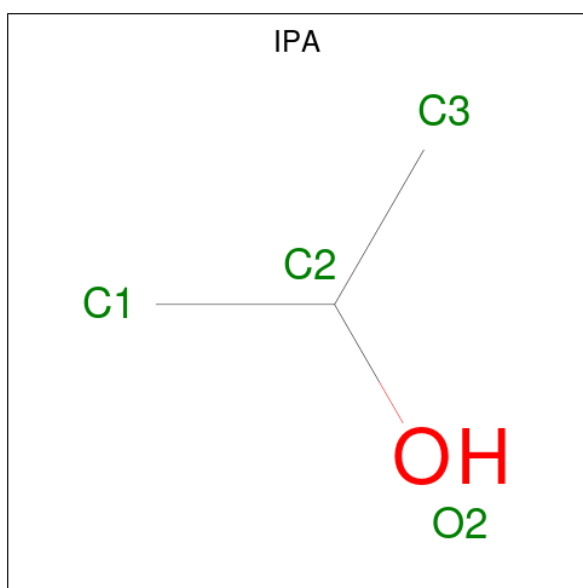
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	286	Total	O	0	0
			286	286		

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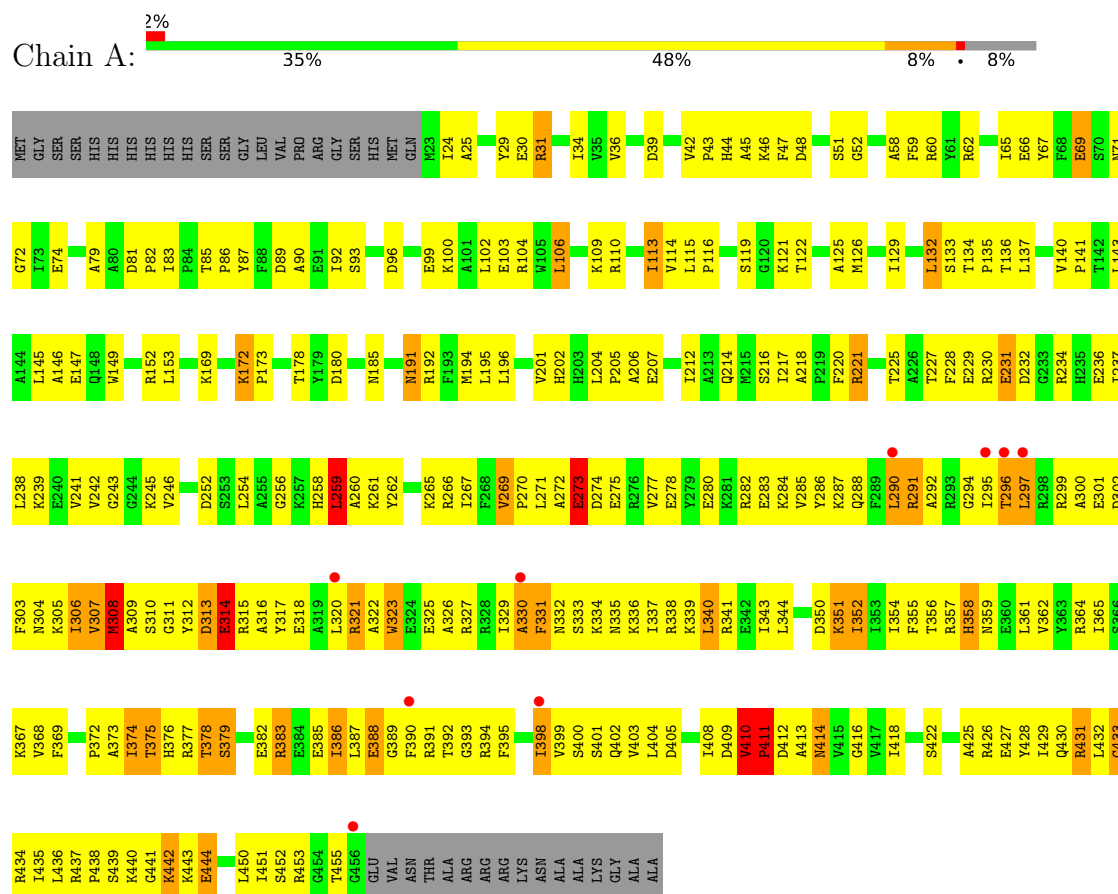
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	299	Total 299	O 299	0	0
4	C	261	Total 261	O 261	0	0
4	D	220	Total 220	O 220	0	0

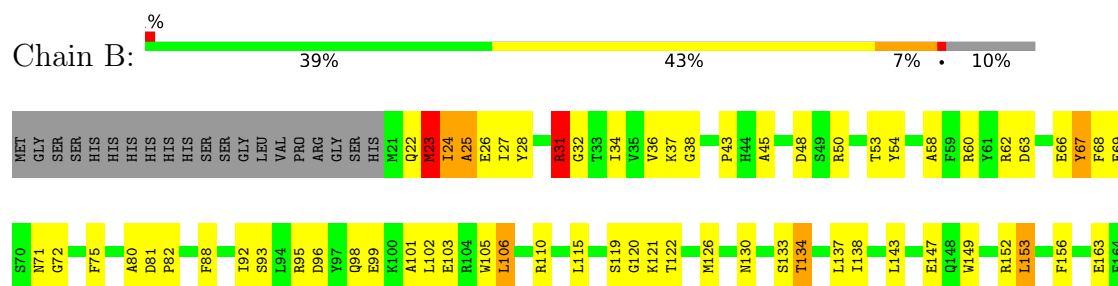
3 Residue-property plots

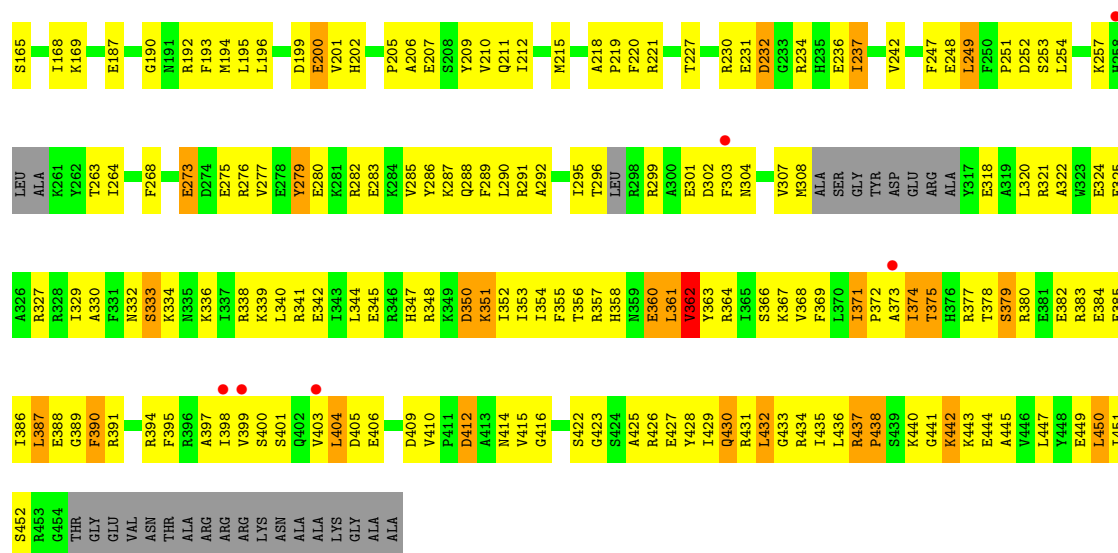
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA repair protein RAD25

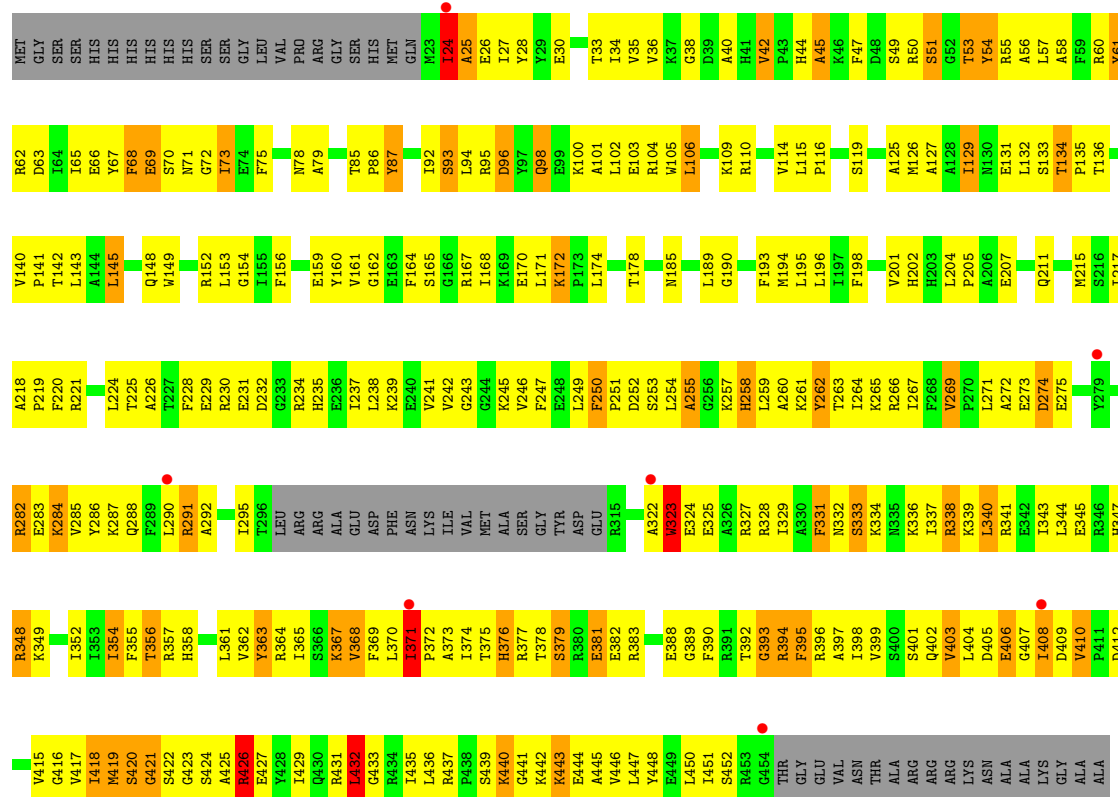


• Molecule 1: DNA repair protein RAD25





• Molecule 1: DNA repair protein RAD25



• Molecule 1: DNA repair protein RAD25



ALA	V410	D350	P411	K351	I352	I353	I354	F355	T356	R357	H358	N359	E360	L361	V362	Y363	R364	I365	S366	K367	V368	Q369	L370	I371	P372	A373	I374	T375	H376	R377	T378	S379	R380	E381	E382	R383	E384	L387	E388	G389	F390	R391	T392	G393	R394	F395	R396	A397	I398	V399	S400	S401	Q402	V403	L404	ASN	ALA	A405	E406	G407	L408	D409	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.09Å 97.96Å 113.73Å 79.03° 85.54° 89.69°	Depositor
Resolution (Å)	29.35 – 2.60 29.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.8 (29.35-2.60) 84.8 (29.35-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.300 0.215 , 0.226	Depositor DCC
R_{free} test set	2888 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 103.6	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	0.93	EDS
Total number of atoms	14769	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: IPA, PO4

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	0.60	0/3583	1.09	25/4827 (0.5%)
1	B	0.59	0/3484	1.05	21/4688 (0.4%)
1	C	0.53	0/3383	1.03	19/4562 (0.4%)
1	D	0.53	0/3466	1.02	20/4673 (0.4%)
All	All	0.56	0/13916	1.05	85/18750 (0.5%)

There are no bond length outliers.

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ILE	N-CA-C	-9.80	99.34	108.95
1	B	371	ILE	N-CA-C	9.25	117.97	107.89
1	B	390	PHE	N-CA-C	-8.94	103.20	114.56
1	A	246	VAL	N-CA-C	-8.48	104.75	112.90
1	A	90	ALA	N-CA-C	-8.16	97.70	110.36
1	D	278	GLU	N-CA-C	-7.72	104.00	113.50
1	A	96	ASP	N-CA-C	7.69	119.66	111.28
1	A	317	TYR	N-CA-C	-7.53	104.24	113.50
1	A	410	VAL	CA-C-N	7.15	128.78	119.84
1	A	410	VAL	C-N-CA	7.15	128.78	119.84
1	D	421	GLY	N-CA-C	-7.07	104.41	116.01
1	C	285	VAL	N-CA-C	-7.00	101.80	111.89
1	D	414	ASN	N-CA-C	-6.95	105.33	113.88
1	D	422	SER	N-CA-C	-6.93	105.27	113.38
1	D	382	GLU	N-CA-C	-6.83	104.95	113.28
1	A	172	LYS	CA-C-N	6.82	127.09	119.32
1	A	172	LYS	C-N-CA	6.82	127.09	119.32
1	D	362	VAL	N-CA-C	-6.62	104.06	110.42
1	A	212	ILE	N-CA-C	-6.62	104.06	110.42
1	D	190	GLY	N-CA-C	6.58	120.60	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	TYR	N-CA-C	-6.57	104.20	111.82
1	C	323	TRP	N-CA-C	-6.45	104.51	112.38
1	A	323	TRP	N-CA-C	-6.28	104.36	111.14
1	C	67	TYR	N-CA-C	-6.25	104.47	111.28
1	A	47	PHE	N-CA-C	6.17	119.29	110.10
1	B	353	ILE	N-CA-C	6.11	115.64	106.42
1	B	31	ARG	N-CA-C	6.08	118.62	111.02
1	C	373	ALA	N-CA-C	5.96	119.09	109.79
1	B	440	LYS	N-CA-C	-5.94	105.13	112.38
1	B	371	ILE	CA-C-N	5.94	127.26	119.84
1	B	371	ILE	C-N-CA	5.94	127.26	119.84
1	D	58	ALA	N-CA-C	5.92	118.50	111.33
1	C	371	ILE	N-CA-C	5.89	121.60	108.88
1	D	81	ASP	CA-C-N	5.79	125.80	119.89
1	D	81	ASP	C-N-CA	5.79	125.80	119.89
1	A	433	GLY	N-CA-C	5.79	120.18	112.77
1	C	246	VAL	N-CA-C	-5.76	106.14	113.22
1	B	96	ASP	N-CA-C	5.75	117.54	111.28
1	A	275	GLU	N-CA-C	-5.74	105.03	111.28
1	B	242	VAL	N-CA-C	-5.70	107.12	111.62
1	C	363	TYR	N-CA-C	-5.67	105.01	111.14
1	A	36	VAL	N-CA-C	5.67	116.05	108.11
1	B	387	LEU	N-CA-C	-5.66	106.33	113.18
1	D	324	GLU	N-CA-C	-5.60	105.27	111.71
1	C	388	GLU	N-CA-C	-5.60	106.43	113.20
1	B	353	ILE	CB-CA-C	-5.59	105.58	111.23
1	A	308	MET	N-CA-C	-5.55	105.32	111.71
1	D	325	GLU	N-CA-C	-5.55	104.86	111.69
1	C	129	ILE	CB-CA-C	-5.55	104.56	112.22
1	C	226	ALA	N-CA-C	-5.52	106.68	113.41
1	D	429	ILE	N-CA-C	-5.51	104.95	110.30
1	D	109	LYS	N-CA-C	-5.50	104.32	111.74
1	B	200	GLU	N-CA-C	-5.47	103.69	111.24
1	B	287	LYS	N-CA-C	-5.46	105.48	111.82
1	B	190	GLY	N-CA-C	5.45	126.10	113.18
1	B	98	GLN	N-CA-C	-5.44	105.51	111.82
1	C	421	GLY	N-CA-C	-5.43	107.29	114.95
1	B	95	ARG	N-CA-C	-5.42	103.53	110.53
1	A	132	LEU	N-CA-C	5.40	117.25	111.36
1	A	292	ALA	N-CA-C	5.37	115.63	108.38
1	B	361	LEU	N-CA-C	-5.33	105.58	111.71
1	C	432	LEU	N-CA-C	-5.33	105.64	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	376	HIS	N-CA-C	-5.31	105.94	112.90
1	D	226	ALA	N-CA-C	-5.31	106.48	113.12
1	C	193	PHE	N-CA-C	5.30	118.19	109.72
1	A	437	ARG	CA-C-N	5.28	125.44	119.90
1	A	437	ARG	C-N-CA	5.28	125.44	119.90
1	D	352	ILE	N-CA-C	5.28	117.36	108.81
1	D	136	THR	N-CA-C	5.27	118.08	109.59
1	B	23	MET	N-CA-C	5.21	121.89	110.80
1	A	375	THR	N-CA-C	5.20	118.02	110.17
1	A	284	LYS	N-CA-C	-5.17	106.67	112.87
1	C	145	LEU	N-CA-C	-5.14	105.75	111.36
1	A	453	ARG	CB-CA-C	-5.11	109.71	117.07
1	D	166	GLY	N-CA-C	-5.11	108.33	114.66
1	D	440	LYS	N-CA-C	-5.10	105.61	111.07
1	B	406	GLU	N-CA-C	5.09	117.26	109.62
1	C	250	PHE	CA-C-N	5.08	126.19	119.84
1	C	250	PHE	C-N-CA	5.08	126.19	119.84
1	B	401	SER	N-CA-C	-5.06	107.78	114.31
1	C	98	GLN	N-CA-C	-5.05	105.77	111.28
1	A	388	GLU	N-CA-C	-5.03	105.45	112.45
1	A	337	ILE	N-CA-C	-5.01	105.54	111.00
1	B	279	TYR	N-CA-C	-5.00	105.30	111.40
1	C	262	TYR	N-CA-C	5.00	117.01	109.41

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	3513	0	3546	317	0
1	B	3419	0	3446	258	0
1	C	3317	0	3324	320	0
1	D	3402	0	3401	323	0
2	A	5	0	0	0	0
2	B	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	15	0	0	0	0
3	A	12	0	24	6	0
4	A	286	0	0	14	1
4	B	299	0	0	10	3
4	C	261	0	0	12	0
4	D	220	0	0	12	1
All	All	14769	0	13741	1213	4

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 44.

All (1213) 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:D:438:PRO:HB3	1:D:444:GLU:HA	1.31	1.08
1:A:333:SER:HB3	1:A:336:LYS:HG3	1.36	1.07
1:C:24:ILE:HD12	1:C:24:ILE:H	1.20	1.03
1:C:126:MET:HE1	1:C:152:ARG:HB3	1.40	1.03
1:D:356:THR:HG23	1:D:362:VAL:HG22	1.38	1.01
1:A:377:ARG:HG3	1:A:378:THR:H	1.23	1.01
1:D:95:ARG:HB3	1:D:259:LEU:HD11	1.39	1.01
1:A:438:PRO:HB2	1:A:443:LYS:HA	1.42	1.00
1:A:398:ILE:HD13	1:A:399:VAL:N	1.76	0.98
1:A:285:VAL:HG23	1:A:286:TYR:H	1.29	0.98
1:A:386:ILE:H	1:A:386:ILE:HD12	1.29	0.97
1:A:391:ARG:HB2	1:A:411:PRO:HG3	1.44	0.97
1:C:375:THR:HG22	1:C:378:THR:HG23	1.46	0.97
1:D:306:ILE:HG23	1:D:307:VAL:H	1.31	0.96
1:A:100:LYS:HZ2	1:A:104:ARG:HH21	1.11	0.96
1:D:132:LEU:HD23	1:D:458:VAL:HG21	1.47	0.95
1:C:408:ILE:HG23	1:C:409:ASP:H	1.32	0.94
1:C:148:GLN:HE21	1:C:152:ARG:HH12	1.15	0.94
1:D:132:LEU:HA	1:D:458:VAL:HG21	1.49	0.93
1:D:407:GLY:O	1:D:410:VAL:HG13	1.68	0.93
1:D:408:ILE:HG22	1:D:409:ASP:H	1.31	0.92
1:A:100:LYS:NZ	1:A:104:ARG:HH21	1.68	0.92
1:C:334:LYS:O	1:C:338:ARG:HD3	1.69	0.91
1:B:290:LEU:HB3	1:B:296:THR:HA	1.52	0.90
1:A:134:THR:HG22	4:A:2827:HOH:O	1.71	0.89
1:A:285:VAL:HG21	1:A:322:ALA:CB	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:GLU:HG3	1:C:329:ILE:HD13	1.53	0.89
1:C:389:GLY:HA2	1:C:392:THR:HG22	1.52	0.89
1:D:162:GLY:HA3	1:D:172:LYS:HD3	1.55	0.89
1:C:42:VAL:HG12	1:C:44:HIS:H	1.38	0.88
1:C:282:ARG:O	1:C:286:TYR:HB2	1.73	0.88
1:A:398:ILE:HD13	1:A:399:VAL:H	1.36	0.88
1:D:418:ILE:HD11	1:D:447:LEU:HD11	1.57	0.87
1:B:288:GLN:O	1:B:292:ALA:HB2	1.75	0.86
1:D:370:LEU:HD13	1:D:370:LEU:H	1.40	0.86
1:C:30:GLU:O	1:C:33:THR:HG22	1.76	0.86
1:A:405:ASP:HB2	1:A:435:ILE:HD11	1.56	0.86
1:B:352:ILE:HG22	1:B:415:VAL:HB	1.56	0.86
1:A:103:GLU:HG3	1:A:426:ARG:NH1	1.90	0.85
1:D:329:ILE:HD12	1:D:330:ALA:N	1.92	0.85
1:A:377:ARG:HG3	1:A:378:THR:N	1.90	0.84
1:D:380:ARG:O	1:D:384:GLU:HG2	1.75	0.84
1:D:405:ASP:HB3	1:D:435:ILE:HD11	1.59	0.84
1:A:66:GLU:HA	1:A:297:LEU:HD12	1.61	0.82
1:C:361:LEU:HD11	1:C:419:MET:HG3	1.61	0.82
1:D:329:ILE:HD12	1:D:330:ALA:H	1.41	0.82
1:C:27:ILE:O	1:C:27:ILE:HG13	1.79	0.82
1:C:26:GLU:HG3	1:C:78:ASN:HD22	1.44	0.81
1:C:403:VAL:HG21	1:C:431:ARG:NH2	1.94	0.81
1:D:102:LEU:O	1:D:106:LEU:HD13	1.81	0.81
1:C:383:ARG:HH22	1:C:402:GLN:NE2	1.79	0.81
1:A:89:ASP:HB3	4:A:2548:HOH:O	1.78	0.81
1:C:205:PRO:HB2	1:C:230:ARG:HH11	1.46	0.81
1:C:354:ILE:HG12	1:C:399:VAL:HG23	1.62	0.81
1:A:103:GLU:HG3	1:A:426:ARG:HH11	1.44	0.80
1:C:115:LEU:HD23	1:C:249:LEU:HB3	1.60	0.80
1:D:305:LYS:HZ2	1:D:305:LYS:HB3	1.45	0.80
1:C:259:LEU:HD11	1:C:262:TYR:CE2	2.16	0.80
1:C:62:ARG:O	1:C:66:GLU:HG3	1.82	0.79
1:B:115:LEU:O	1:B:121:LYS:HE3	1.83	0.79
1:A:259:LEU:HD13	1:A:260:ALA:N	1.98	0.79
1:B:377:ARG:HD2	1:B:377:ARG:O	1.83	0.79
1:D:132:LEU:HA	1:D:458:VAL:CG2	2.11	0.79
1:A:207:GLU:HG2	3:A:6002:IPA:H12	1.62	0.79
1:A:358:HIS:O	1:A:362:VAL:HG23	1.83	0.79
1:D:352:ILE:HD12	1:D:353:ILE:N	1.98	0.79
1:A:295:ILE:HB	1:A:299:ARG:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:SER:HB3	1:B:336:LYS:HG2	1.64	0.78
1:B:389:GLY:O	1:B:394:ARG:HB3	1.83	0.78
1:D:356:THR:CG2	1:D:362:VAL:HG22	2.12	0.78
1:D:100:LYS:HD3	1:D:426:ARG:HH22	1.49	0.78
1:C:272:ALA:HB3	1:C:275:GLU:HG3	1.67	0.77
1:B:126:MET:HE3	1:B:152:ARG:HG2	1.65	0.77
1:B:121:LYS:HG3	2:B:4002:PO4:O4	1.85	0.77
1:D:232:ASP:OD1	1:D:234:ARG:HG3	1.84	0.77
1:C:420:SER:HB3	1:C:450:LEU:O	1.84	0.77
1:D:379:SER:HB3	1:D:382:GLU:HB2	1.67	0.76
1:A:42:VAL:HG13	1:A:43:PRO:HD2	1.67	0.76
1:D:321:ARG:O	1:D:325:GLU:HB2	1.84	0.76
1:C:257:LYS:NZ	1:C:260:ALA:HB3	2.00	0.76
1:C:257:LYS:HZ2	1:C:260:ALA:HB3	1.49	0.76
1:D:205:PRO:HA	1:D:237:ILE:HD11	1.68	0.76
1:A:285:VAL:HG21	1:A:322:ALA:HB3	1.64	0.76
1:A:122:THR:HG21	1:A:152:ARG:CD	2.15	0.76
1:B:99:GLU:O	1:B:103:GLU:HG2	1.86	0.75
1:C:205:PRO:HA	1:C:237:ILE:HD11	1.67	0.75
1:C:95:ARG:HB2	1:C:98:GLN:HG3	1.69	0.75
1:C:115:LEU:HD21	1:C:247:PHE:HE1	1.50	0.75
1:D:325:GLU:O	1:D:329:ILE:HG13	1.85	0.75
1:D:388:GLU:HA	1:D:391:ARG:CG	2.17	0.75
1:B:27:ILE:HG22	1:B:36:VAL:HG22	1.68	0.75
1:D:269:VAL:HG21	1:D:336:LYS:HG2	1.68	0.75
1:C:28:TYR:HA	1:C:79:ALA:HB2	1.68	0.75
1:C:412:ASP:HB2	1:C:437:ARG:HD2	1.68	0.74
1:B:332:ASN:CG	1:B:333:SER:H	1.93	0.74
1:B:351:LYS:H	1:B:351:LYS:HD2	1.52	0.74
1:B:325:GLU:O	1:B:329:ILE:HG13	1.87	0.74
1:C:57:LEU:H	1:C:57:LEU:HD22	1.52	0.74
1:D:45:ALA:HB1	1:D:54:TYR:HB3	1.70	0.74
1:D:201:VAL:HG12	1:D:225:THR:HB	1.70	0.74
1:D:361:LEU:O	1:D:365:ILE:HG13	1.87	0.74
1:D:440:LYS:HE3	1:D:440:LYS:HA	1.67	0.74
1:A:45:ALA:C	1:A:46:LYS:HD2	2.13	0.74
1:D:70:SER:HA	1:D:292:ALA:HB2	1.68	0.73
1:D:290:LEU:H	1:D:290:LEU:HD22	1.53	0.73
1:C:267:ILE:HG21	1:C:339:LYS:HE2	1.70	0.73
1:B:303:PHE:O	1:B:307:VAL:HG23	1.89	0.73
1:C:392:THR:HG23	1:C:393:GLY:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:ILE:HA	1:C:378:THR:HG21	1.71	0.72
1:D:305:LYS:HB3	1:D:305:LYS:NZ	2.04	0.72
1:A:386:ILE:H	1:A:386:ILE:CD1	2.02	0.72
1:D:424:SER:OG	1:D:429:ILE:HD11	1.88	0.72
1:C:148:GLN:HG2	1:C:152:ARG:NH1	2.04	0.72
1:D:165:SER:HB2	4:D:2598:HOH:O	1.89	0.72
1:B:23:MET:HB2	1:B:38:GLY:HA2	1.71	0.72
1:B:24:ILE:O	1:B:24:ILE:HG22	1.89	0.72
1:C:71:ASN:O	1:C:73:ILE:HG13	1.89	0.72
1:A:66:GLU:HG3	1:A:297:LEU:HD13	1.71	0.72
1:A:305:LYS:HZ3	1:A:323:TRP:CG	2.08	0.72
1:A:285:VAL:HG23	1:A:286:TYR:N	2.04	0.71
1:C:383:ARG:HH22	1:C:402:GLN:HE21	1.38	0.71
1:D:34:ILE:HG12	1:D:58:ALA:HA	1.72	0.71
1:B:332:ASN:CG	1:B:333:SER:N	2.46	0.71
1:B:366:SER:HB2	1:B:373:ALA:HB2	1.72	0.71
1:C:185:ASN:O	1:C:189:LEU:HG	1.90	0.71
1:A:241:VAL:HG23	1:A:242:VAL:HG23	1.73	0.71
1:A:295:ILE:HD13	1:A:300:ALA:HB3	1.73	0.71
1:A:333:SER:HB3	1:A:336:LYS:CG	2.19	0.71
1:C:263:THR:CG2	1:C:446:VAL:HG22	2.19	0.71
1:A:295:ILE:O	1:A:295:ILE:HG13	1.90	0.71
1:C:389:GLY:CA	1:C:392:THR:HG22	2.20	0.71
1:D:388:GLU:HA	1:D:391:ARG:HG2	1.73	0.71
1:D:32:GLY:HA3	1:D:215:MET:HE2	1.72	0.71
1:B:405:ASP:HB3	1:B:435:ILE:HD11	1.71	0.70
1:D:60:ARG:HA	4:D:2516:HOH:O	1.91	0.70
1:D:323:TRP:HA	1:D:326:ALA:HB3	1.72	0.70
1:B:375:THR:HG23	1:B:377:ARG:H	1.57	0.70
1:B:404:LEU:N	1:B:404:LEU:HD22	2.07	0.70
1:A:304:ASN:HA	1:A:307:VAL:HG22	1.73	0.70
1:C:230:ARG:HG3	1:C:235:HIS:HB3	1.74	0.70
1:D:234:ARG:HG2	1:D:234:ARG:HH11	1.56	0.70
1:B:143:LEU:O	1:B:147:GLU:HG3	1.92	0.70
1:B:37:LYS:HG2	1:B:53:THR:HG22	1.74	0.70
1:B:320:LEU:O	1:B:324:GLU:HG3	1.92	0.70
1:D:172:LYS:HB3	1:D:173:PRO:HD2	1.73	0.70
1:A:314:GLU:HG2	1:A:316:ALA:H	1.55	0.70
1:B:273:GLU:O	1:B:277:VAL:HG23	1.92	0.69
1:D:149:TRP:HE3	1:D:153:LEU:HD11	1.56	0.69
1:C:126:MET:CE	1:C:152:ARG:HB3	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ALA:C	1:D:82:PRO:HD3	2.17	0.69
1:A:282:ARG:HH21	1:A:322:ALA:HA	1.57	0.69
1:B:286:TYR:HA	1:B:289:PHE:HB2	1.74	0.69
1:A:69:GLU:HG2	1:A:297:LEU:HG	1.75	0.69
1:D:425:ALA:O	1:D:429:ILE:HG13	1.92	0.69
1:D:333:SER:O	1:D:337:ILE:HG12	1.92	0.69
1:C:109:LYS:HD3	1:C:132:LEU:HD21	1.76	0.68
1:D:418:ILE:HD12	1:D:447:LEU:HD21	1.73	0.68
1:D:43:PRO:O	1:D:44:HIS:HB2	1.92	0.68
1:D:95:ARG:HB3	1:D:259:LEU:CD1	2.21	0.68
1:A:259:LEU:O	1:A:261:LYS:HG3	1.93	0.68
1:B:340:LEU:HD21	1:B:354:ILE:HD13	1.73	0.68
1:C:336:LYS:HE3	1:C:452:SER:HB3	1.74	0.68
1:D:283:GLU:HB3	1:D:286:TYR:CZ	2.28	0.68
1:B:358:HIS:CE1	1:B:360:GLU:HB3	2.29	0.68
1:C:332:ASN:HD22	1:C:364:ARG:HD2	1.59	0.68
1:C:439:SER:HB2	1:C:442:LYS:HD2	1.76	0.68
1:D:432:LEU:O	1:D:432:LEU:HD23	1.94	0.68
1:A:274:ASP:O	1:A:277:VAL:HG12	1.93	0.68
1:B:34:ILE:HG12	1:B:58:ALA:HA	1.76	0.68
1:B:102:LEU:HG	1:B:106:LEU:HD22	1.75	0.68
1:C:443:LYS:HG3	1:C:444:GLU:H	1.58	0.68
1:D:91:GLU:HB3	1:D:265:LYS:HD3	1.76	0.68
1:A:296:THR:O	1:A:297:LEU:HB2	1.92	0.68
1:B:321:ARG:HA	1:B:324:GLU:OE1	1.94	0.68
1:D:404:LEU:N	1:D:404:LEU:HD22	2.08	0.68
1:C:394:ARG:HE	1:C:394:ARG:HA	1.60	0.67
1:B:384:GLU:O	1:B:388:GLU:HG2	1.94	0.67
1:C:341:ARG:O	1:C:345:GLU:HG3	1.94	0.67
1:C:26:GLU:HG3	1:C:78:ASN:ND2	2.09	0.67
1:D:273:GLU:O	1:D:274:ASP:HB3	1.95	0.67
1:D:369:PHE:CE1	1:D:370:LEU:HD22	2.30	0.67
1:A:234:ARG:HH22	3:A:6002:IPA:H2	1.59	0.67
1:B:62:ARG:HB2	4:B:2009:HOH:O	1.95	0.67
1:D:362:VAL:HG13	1:D:399:VAL:HG22	1.77	0.67
1:A:110:ARG:HD2	1:A:221:ARG:HG3	1.78	0.66
1:A:402:GLN:O	1:A:404:LEU:HD22	1.96	0.66
1:C:418:ILE:HG12	1:C:425:ALA:HB2	1.75	0.66
1:C:339:LYS:O	1:C:343:ILE:HG13	1.95	0.66
1:D:260:ALA:HB2	4:D:2799:HOH:O	1.94	0.66
1:C:333:SER:HB3	1:C:336:LYS:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:PHE:C	1:D:291:ARG:H	2.04	0.66
1:B:37:LYS:HG2	1:B:53:THR:CG2	2.26	0.66
1:C:68:PHE:O	1:C:70:SER:N	2.28	0.66
1:A:100:LYS:NZ	1:A:104:ARG:NH2	2.43	0.66
1:A:359:ASN:HA	1:A:362:VAL:HB	1.78	0.66
1:B:50:ARG:HH21	1:B:50:ARG:HG2	1.60	0.66
1:B:364:ARG:O	1:B:368:VAL:HG23	1.96	0.66
1:D:365:ILE:HD12	1:D:399:VAL:HG21	1.77	0.66
1:D:372:PRO:HB2	1:D:398:ILE:HG22	1.77	0.66
1:C:263:THR:HG22	1:C:445:ALA:O	1.95	0.66
1:D:368:VAL:HG12	1:D:368:VAL:O	1.95	0.66
1:B:122:THR:HG21	1:B:152:ARG:HD3	1.77	0.65
1:A:393:GLY:C	1:A:395:PHE:H	2.03	0.65
1:A:444:GLU:HB3	4:A:2628:HOH:O	1.96	0.65
1:C:375:THR:HG23	1:C:377:ARG:H	1.61	0.65
1:C:24:ILE:H	1:C:24:ILE:CD1	1.98	0.65
1:A:305:LYS:HG2	1:A:323:TRP:CD2	2.32	0.65
1:B:273:GLU:O	1:B:276:ARG:HG2	1.97	0.65
1:B:279:TYR:CE1	1:B:330:ALA:HB2	2.32	0.65
1:D:134:THR:HB	1:D:194:MET:HB2	1.79	0.65
1:D:158:GLU:HB3	4:D:2667:HOH:O	1.97	0.65
1:C:356:THR:HB	1:C:419:MET:HG2	1.79	0.65
1:A:413:ALA:CB	1:A:436:LEU:HD23	2.27	0.65
1:A:442:LYS:NZ	1:A:442:LYS:HA	2.12	0.65
1:B:283:GLU:C	1:B:285:VAL:H	2.05	0.65
1:B:372:PRO:HG2	1:B:395:PHE:CG	2.31	0.65
1:C:134:THR:HG21	4:C:2617:HOH:O	1.96	0.64
1:D:340:LEU:HA	1:D:343:ILE:CD1	2.27	0.64
1:D:213:ALA:O	1:D:221:ARG:NH2	2.29	0.64
1:A:46:LYS:HA	1:A:46:LYS:HE3	1.79	0.64
1:A:66:GLU:HA	1:A:297:LEU:CD1	2.27	0.64
1:D:418:ILE:CD1	1:D:429:ILE:HA	2.27	0.64
1:B:23:MET:C	1:B:25:ALA:H	2.06	0.64
1:B:387:LEU:HD23	1:B:387:LEU:O	1.97	0.64
1:D:350:ASP:HB3	1:D:414:ASN:HB3	1.78	0.64
1:B:434:ARG:NH2	1:B:434:ARG:HB2	2.12	0.64
1:D:325:GLU:C	1:D:327:ARG:H	2.05	0.64
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.60	0.64
1:B:165:SER:O	1:B:169:LYS:HD2	1.98	0.64
1:D:33:THR:HG23	1:D:56:ALA:O	1.98	0.64
1:D:149:TRP:O	1:D:153:LEU:HD13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:SER:HA	1:A:265:LYS:HG2	1.80	0.64
1:A:334:LYS:O	1:A:338:ARG:HG2	1.98	0.64
1:A:438:PRO:HB2	1:A:443:LYS:CA	2.25	0.63
1:D:340:LEU:O	1:D:343:ILE:HG12	1.97	0.63
1:A:357:ARG:HD3	1:A:428:TYR:OH	1.97	0.63
1:B:307:VAL:O	1:B:308:MET:HE2	1.98	0.63
1:C:148:GLN:HG2	1:C:152:ARG:CZ	2.27	0.63
1:C:69:GLU:HG3	1:C:75:PHE:CZ	2.33	0.63
1:A:425:ALA:O	1:A:429:ILE:HG12	1.97	0.63
1:B:351:LYS:HB2	1:B:390:PHE:CZ	2.34	0.63
1:D:37:LYS:HA	1:D:53:THR:HG22	1.81	0.63
1:D:45:ALA:CB	1:D:54:TYR:HB3	2.27	0.63
1:D:340:LEU:HG	1:D:343:ILE:HD11	1.79	0.63
1:D:336:LYS:O	1:D:340:LEU:HB2	1.98	0.63
1:D:36:VAL:HG11	1:D:42:VAL:HG21	1.81	0.63
1:A:69:GLU:OE1	1:A:297:LEU:HD11	1.99	0.63
1:A:386:ILE:HD12	1:A:386:ILE:N	2.08	0.63
1:C:334:LYS:HG2	1:C:338:ARG:HE	1.62	0.63
1:D:369:PHE:CD1	1:D:371:ILE:HB	2.34	0.63
1:A:65:ILE:HG22	1:A:297:LEU:HD11	1.81	0.62
1:C:389:GLY:HA2	1:C:392:THR:CG2	2.28	0.62
1:B:234:ARG:O	1:B:237:ILE:HG23	1.99	0.62
1:A:285:VAL:HG21	1:A:322:ALA:HB1	1.81	0.62
1:C:148:GLN:NE2	1:C:152:ARG:HH12	1.94	0.62
1:B:289:PHE:O	1:B:292:ALA:HB3	1.99	0.62
1:C:143:LEU:HD13	1:C:167:ARG:HD2	1.82	0.62
1:D:408:ILE:HG22	1:D:409:ASP:N	2.08	0.62
1:C:161:VAL:O	1:C:172:LYS:HG2	2.00	0.62
1:D:394:ARG:HD3	1:D:394:ARG:N	2.15	0.62
1:B:122:THR:HG21	1:B:152:ARG:CD	2.30	0.62
1:B:149:TRP:O	1:B:153:LEU:HD22	1.99	0.61
1:B:374:ILE:HG22	1:B:374:ILE:O	1.99	0.61
1:B:433:GLY:HA2	1:B:436:LEU:HD12	1.81	0.61
1:A:357:ARG:HD3	1:A:428:TYR:CZ	2.35	0.61
1:B:352:ILE:CG2	1:B:415:VAL:HB	2.29	0.61
1:C:408:ILE:HG23	1:C:409:ASP:N	2.10	0.61
1:B:23:MET:HE3	1:B:38:GLY:C	2.25	0.61
1:C:148:GLN:O	1:C:152:ARG:HG3	2.00	0.61
1:C:378:THR:O	1:C:379:SER:O	2.19	0.61
1:A:413:ALA:HB3	1:A:436:LEU:HD23	1.82	0.61
1:B:322:ALA:C	1:B:324:GLU:H	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:LEU:O	1:C:255:ALA:HB2	2.00	0.61
1:A:382:GLU:O	1:A:383:ARG:HG2	2.01	0.61
1:C:100:LYS:HE2	1:C:104:ARG:HE	1.65	0.61
1:B:301:GLU:O	1:B:303:PHE:N	2.29	0.61
1:D:96:ASP:OD2	1:D:259:LEU:HD13	2.01	0.61
1:A:351:LYS:HD3	1:A:412:ASP:O	1.99	0.60
1:A:109:LYS:HD3	1:A:132:LEU:HD21	1.82	0.60
1:A:340:LEU:HA	1:A:343:ILE:HD12	1.83	0.60
1:C:229:GLU:OE2	1:C:229:GLU:HA	2.02	0.60
1:D:256:GLY:C	1:D:258:HIS:H	2.09	0.60
1:A:307:VAL:HG23	1:A:308:MET:H	1.66	0.60
1:C:205:PRO:HB2	1:C:230:ARG:NH1	2.15	0.60
1:D:191:ASN:OD1	1:D:192:ARG:HD2	2.02	0.60
1:A:320:LEU:HD23	1:A:320:LEU:C	2.26	0.60
1:A:330:ALA:O	1:A:331:PHE:C	2.44	0.60
1:D:269:VAL:HG21	1:D:336:LYS:CG	2.30	0.60
1:A:125:ALA:O	1:A:129:ILE:HG13	2.01	0.60
1:A:377:ARG:NH1	1:A:378:THR:HA	2.16	0.60
1:A:408:ILE:O	1:A:408:ILE:HG22	2.01	0.60
1:B:333:SER:HB3	1:B:336:LYS:CG	2.29	0.60
1:C:418:ILE:HG12	1:C:425:ALA:CB	2.32	0.60
1:A:387:LEU:O	1:A:411:PRO:HG2	2.02	0.60
1:C:332:ASN:O	1:C:333:SER:C	2.44	0.60
1:D:37:LYS:HA	1:D:53:THR:CG2	2.32	0.60
1:D:210:VAL:HG21	1:D:237:ILE:HD12	1.82	0.60
1:A:191:ASN:HD22	1:A:191:ASN:H	1.50	0.60
1:B:110:ARG:HH12	1:B:219:PRO:HA	1.67	0.60
1:D:160:TYR:O	1:D:172:LYS:HB3	2.01	0.59
1:D:368:VAL:O	1:D:369:PHE:HB2	2.01	0.59
1:A:391:ARG:HB2	1:A:411:PRO:CG	2.26	0.59
1:A:393:GLY:C	1:A:395:PHE:N	2.59	0.59
1:B:415:VAL:HG12	1:B:416:GLY:N	2.17	0.59
1:C:116:PRO:HG2	1:C:251:PRO:HA	1.84	0.59
1:C:379:SER:OG	1:C:382:GLU:HG3	2.02	0.59
1:A:295:ILE:HB	1:A:299:ARG:N	2.16	0.59
1:C:322:ALA:HA	1:C:324:GLU:HG2	1.82	0.59
1:B:450:LEU:N	1:B:450:LEU:HD22	2.17	0.59
1:D:109:LYS:HD3	1:D:132:LEU:HD21	1.85	0.59
1:D:366:SER:O	1:D:369:PHE:O	2.20	0.59
1:C:69:GLU:HG3	1:C:75:PHE:HZ	1.67	0.59
1:D:418:ILE:HD11	1:D:429:ILE:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:VAL:HG21	1:A:336:LYS:HG2	1.84	0.59
1:C:393:GLY:O	1:C:394:ARG:O	2.21	0.59
1:A:372:PRO:HG3	1:A:395:PHE:HE2	1.68	0.59
1:B:442:LYS:HE3	4:B:3002:HOH:O	2.01	0.59
1:C:87:TYR:HE2	4:C:2561:HOH:O	1.85	0.59
1:B:115:LEU:HB3	1:B:119:SER:OG	2.02	0.58
1:C:110:ARG:HG3	1:C:242:VAL:O	2.03	0.58
1:C:231:GLU:HB2	4:C:2883:HOH:O	2.02	0.58
1:A:122:THR:HG22	1:A:126:MET:CE	2.33	0.58
1:C:267:ILE:CG2	1:C:339:LYS:HE2	2.33	0.58
1:C:340:LEU:HD11	1:C:354:ILE:HD13	1.85	0.58
1:A:432:LEU:HD13	1:A:432:LEU:O	2.03	0.58
1:A:361:LEU:O	1:A:361:LEU:HD23	2.04	0.58
1:B:290:LEU:HB3	1:B:296:THR:CA	2.27	0.58
1:C:194:MET:HA	1:C:219:PRO:HD2	1.85	0.58
1:C:194:MET:HE3	1:C:219:PRO:HG3	1.86	0.58
1:D:84:PRO:HG2	4:D:2119:HOH:O	2.03	0.58
1:A:283:GLU:C	1:A:285:VAL:N	2.61	0.58
1:C:134:THR:HB	1:C:194:MET:HB2	1.85	0.58
1:C:323:TRP:CE2	1:C:327:ARG:HB2	2.38	0.58
1:D:149:TRP:CE3	1:D:153:LEU:HD11	2.38	0.58
1:D:346:ARG:HG3	1:D:347:HIS:CD2	2.38	0.58
1:C:160:TYR:O	1:C:172:LYS:HB3	2.03	0.58
1:A:143:LEU:O	1:A:147:GLU:HG3	2.03	0.58
1:B:273:GLU:HA	1:B:276:ARG:HG2	1.85	0.58
1:B:441:GLY:O	1:B:442:LYS:C	2.45	0.58
1:D:305:LYS:HD2	1:D:305:LYS:N	2.18	0.58
1:A:295:ILE:CB	1:A:299:ARG:HB3	2.34	0.58
1:A:404:LEU:HB3	1:A:410:VAL:HG11	1.86	0.58
1:B:103:GLU:HG3	1:B:426:ARG:NH1	2.19	0.58
1:C:375:THR:HG23	1:C:377:ARG:N	2.17	0.58
1:D:77:ASP:OD2	1:D:80:ALA:HB3	2.03	0.58
1:A:278:GLU:O	1:A:282:ARG:HG2	2.03	0.58
1:B:122:THR:CG2	1:B:152:ARG:HD3	2.34	0.58
1:A:230:ARG:NH2	3:A:6001:IPA:H2	2.18	0.58
1:C:211:GLN:HG2	1:C:215:MET:SD	2.44	0.58
1:C:432:LEU:O	1:C:436:LEU:HG	2.04	0.58
1:A:375:THR:OG1	1:A:376:HIS:N	2.35	0.57
1:D:239:LYS:O	1:D:243:GLY:HA2	2.04	0.57
1:D:404:LEU:HD22	1:D:404:LEU:H	1.69	0.57
1:B:372:PRO:HB2	1:B:398:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:PHE:HB3	1:C:75:PHE:CD2	2.39	0.57
1:A:31:ARG:HH11	1:A:31:ARG:HB2	1.68	0.57
1:A:115:LEU:HD12	1:A:121:LYS:HG2	1.87	0.57
1:A:205:PRO:O	1:A:206:ALA:C	2.46	0.57
1:B:62:ARG:O	1:B:66:GLU:HG3	2.04	0.57
1:D:132:LEU:CD2	1:D:458:VAL:HG11	2.35	0.57
1:A:259:LEU:HD21	1:A:262:TYR:HD2	1.69	0.57
1:D:238:LEU:O	1:D:243:GLY:N	2.37	0.57
1:A:318:GLU:OE1	1:A:318:GLU:HA	2.04	0.57
1:A:374:ILE:HD11	1:A:386:ILE:HG21	1.85	0.57
1:D:45:ALA:HB3	1:D:54:TYR:HD2	1.70	0.57
1:D:306:ILE:HG23	1:D:307:VAL:N	2.12	0.57
1:D:376:HIS:CD2	1:D:377:ARG:HG2	2.40	0.57
1:B:202:HIS:O	1:B:230:ARG:HD2	2.05	0.57
1:A:114:VAL:HA	1:A:225:THR:O	2.05	0.57
1:A:301:GLU:O	1:A:302:ASP:HB2	2.05	0.57
1:B:340:LEU:HD21	1:B:354:ILE:CD1	2.35	0.57
1:B:187:GLU:CD	1:B:187:GLU:H	2.13	0.57
1:B:414:ASN:O	1:B:445:ALA:HB1	2.05	0.57
1:C:259:LEU:C	1:C:261:LYS:H	2.13	0.57
1:C:352:ILE:O	1:C:397:ALA:HA	2.04	0.57
1:A:295:ILE:HG22	1:A:299:ARG:HB3	1.87	0.56
1:B:362:VAL:HG23	1:B:363:TYR:H	1.69	0.56
1:C:263:THR:HG21	1:C:446:VAL:HG22	1.86	0.56
1:D:278:GLU:O	1:D:282:ARG:HG2	2.05	0.56
1:B:103:GLU:HG3	1:B:426:ARG:CZ	2.34	0.56
1:C:49:SER:HB3	1:C:53:THR:OG1	2.05	0.56
1:A:280:GLU:C	1:A:282:ARG:H	2.13	0.56
1:B:187:GLU:HG3	1:B:215:MET:HE1	1.88	0.56
1:B:432:LEU:HD12	1:B:436:LEU:HG	1.87	0.56
1:C:333:SER:HB3	1:C:336:LYS:CG	2.34	0.56
1:C:418:ILE:HD12	1:C:419:MET:N	2.21	0.56
1:B:354:ILE:HG22	1:B:355:PHE:N	2.19	0.56
1:C:24:ILE:HD12	1:C:24:ILE:N	2.05	0.56
1:C:93:SER:HA	1:C:265:LYS:HG2	1.86	0.56
1:D:369:PHE:HD1	1:D:371:ILE:HB	1.71	0.56
1:B:450:LEU:HD22	1:B:450:LEU:H	1.71	0.56
1:D:172:LYS:HE2	4:D:2211:HOH:O	2.04	0.56
1:A:285:VAL:O	1:A:290:LEU:HD23	2.04	0.56
1:A:393:GLY:O	1:A:395:PHE:N	2.39	0.56
1:B:23:MET:HB2	1:B:38:GLY:CA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLU:O	1:A:287:LYS:HG2	2.05	0.56
1:B:268:PHE:HA	1:B:451:ILE:O	2.05	0.56
1:B:400:SER:HB3	1:B:404:LEU:HD21	1.87	0.56
1:C:361:LEU:HD22	1:C:361:LEU:O	2.05	0.56
1:C:425:ALA:O	1:C:427:GLU:N	2.37	0.56
1:D:24:ILE:O	1:D:24:ILE:HG22	2.06	0.56
1:D:234:ARG:HG2	1:D:234:ARG:NH1	2.21	0.56
1:A:113:ILE:HG22	1:A:113:ILE:O	2.06	0.56
1:D:305:LYS:N	1:D:305:LYS:HZ3	2.03	0.56
1:A:205:PRO:HB2	1:A:230:ARG:NH1	2.21	0.56
1:C:103:GLU:HB3	1:C:426:ARG:NH2	2.21	0.56
1:C:250:PHE:HD1	1:C:251:PRO:HD2	1.71	0.56
1:C:358:HIS:HD2	1:C:361:LEU:H	1.52	0.56
1:D:95:ARG:HB2	1:D:98:GLN:HG3	1.88	0.56
1:C:42:VAL:HB	1:C:45:ALA:HB2	1.88	0.55
1:C:286:TYR:C	1:C:288:GLN:H	2.14	0.55
1:D:93:SER:HA	1:D:264:ILE:O	2.06	0.55
1:D:379:SER:HB3	1:D:382:GLU:CB	2.35	0.55
1:C:148:GLN:NE2	1:C:152:ARG:HH22	2.04	0.55
1:A:282:ARG:HG3	1:A:329:ILE:HD11	1.86	0.55
1:D:180:ASP:O	1:D:184:VAL:HG23	2.06	0.55
1:D:259:LEU:C	1:D:261:LYS:H	2.13	0.55
1:D:306:ILE:HG13	1:D:307:VAL:N	2.20	0.55
1:A:391:ARG:HG3	1:A:391:ARG:NH1	2.21	0.55
1:B:290:LEU:CB	1:B:296:THR:HA	2.33	0.55
1:B:374:ILE:HG12	1:B:386:ILE:HD12	1.88	0.55
1:C:261:LYS:O	1:C:444:GLU:HB3	2.06	0.55
1:C:263:THR:HG22	1:C:446:VAL:HA	1.87	0.55
1:A:442:LYS:HA	1:A:442:LYS:HZ3	1.70	0.55
1:B:32:GLY:HA3	1:B:215:MET:HE2	1.87	0.55
1:B:126:MET:CE	1:B:152:ARG:HG2	2.36	0.55
1:C:136:THR:HB	1:C:174:LEU:HD23	1.88	0.55
1:C:406:GLU:HG2	1:C:406:GLU:O	2.06	0.55
1:D:372:PRO:HD3	1:D:395:PHE:CE1	2.41	0.55
1:A:334:LYS:O	1:A:338:ARG:CG	2.54	0.55
1:C:361:LEU:O	1:C:365:ILE:HG13	2.07	0.55
1:A:283:GLU:C	1:A:285:VAL:H	2.13	0.55
1:B:291:ARG:N	1:B:296:THR:HG22	2.22	0.55
1:A:350:ASP:HB3	1:A:414:ASN:HB3	1.89	0.55
1:C:36:VAL:O	1:C:54:TYR:HB2	2.07	0.55
1:C:85:THR:HG23	1:C:86:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:PHE:CD1	1:C:395:PHE:O	2.60	0.55
1:B:69:GLU:HG2	1:B:291:ARG:HH11	1.71	0.55
1:B:120:GLY:HA2	4:B:2256:HOH:O	2.07	0.55
1:D:360:GLU:O	1:D:363:TYR:HB3	2.06	0.55
1:A:122:THR:HG22	1:A:126:MET:HE1	1.88	0.54
1:A:234:ARG:C	1:A:236:GLU:H	2.15	0.54
1:B:301:GLU:C	1:B:303:PHE:H	2.14	0.54
1:B:382:GLU:O	1:B:386:ILE:HG13	2.07	0.54
1:C:152:ARG:C	1:C:154:GLY:H	2.15	0.54
1:B:88:PHE:HB3	1:B:156:PHE:CD1	2.43	0.54
1:B:264:ILE:HD12	1:B:264:ILE:N	2.22	0.54
1:C:50:ARG:O	1:C:51:SER:HB2	2.06	0.54
1:D:62:ARG:NH1	1:D:219:PRO:O	2.37	0.54
1:D:373:ALA:O	1:D:374:ILE:HG13	2.07	0.54
1:C:228:PHE:CD1	1:C:245:LYS:HE2	2.43	0.54
1:D:378:THR:HG22	1:D:379:SER:N	2.22	0.54
1:A:230:ARG:HH22	3:A:6001:IPA:H2	1.72	0.54
1:A:321:ARG:O	1:A:321:ARG:HD3	2.06	0.54
1:B:290:LEU:C	1:B:296:THR:HG22	2.33	0.54
1:D:336:LYS:HZ1	1:D:420:SER:CB	2.21	0.54
1:A:122:THR:HG21	1:A:152:ARG:HD3	1.89	0.54
1:A:314:GLU:HG2	1:A:315:ARG:N	2.23	0.54
1:A:338:ARG:O	1:A:341:ARG:HB3	2.07	0.54
1:A:356:THR:HG23	1:A:362:VAL:HG22	1.89	0.54
1:B:351:LYS:HB2	1:B:390:PHE:CE1	2.43	0.54
1:C:50:ARG:HG2	1:C:50:ARG:HH11	1.73	0.54
1:C:63:ASP:HA	1:C:66:GLU:OE2	2.08	0.54
1:D:227:THR:HG23	4:D:2756:HOH:O	2.08	0.54
1:A:295:ILE:HB	1:A:299:ARG:HB3	1.90	0.54
1:B:110:ARG:NH1	1:B:219:PRO:HA	2.22	0.54
1:C:451:ILE:HG22	1:C:452:SER:N	2.22	0.54
1:B:253:SER:C	1:B:254:LEU:HD22	2.33	0.54
1:C:272:ALA:HB3	1:C:275:GLU:CG	2.35	0.54
1:D:328:ARG:HG3	1:D:328:ARG:HH11	1.73	0.54
1:A:74:GLU:OE2	1:A:74:GLU:HA	2.08	0.54
1:B:31:ARG:CG	1:B:187:GLU:HB3	2.38	0.54
1:B:62:ARG:N	4:B:2009:HOH:O	2.21	0.54
1:B:122:THR:HG21	1:B:152:ARG:CZ	2.38	0.54
1:B:247:PHE:C	1:B:247:PHE:CD1	2.86	0.54
1:B:334:LYS:O	1:B:338:ARG:HG3	2.08	0.54
1:B:344:LEU:CD2	1:B:352:ILE:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:LYS:HE3	1:D:438:PRO:HG3	1.89	0.54
1:D:418:ILE:HG12	1:D:432:LEU:HD13	1.89	0.54
1:A:99:GLU:HG3	1:A:426:ARG:NH2	2.23	0.54
1:D:409:ASP:O	1:D:410:VAL:O	2.25	0.54
1:A:44:HIS:CG	1:A:60:ARG:HD2	2.43	0.53
1:A:24:ILE:HG22	1:A:25:ALA:N	2.22	0.53
1:B:23:MET:HE3	1:B:38:GLY:O	2.09	0.53
1:A:180:ASP:OD2	4:A:2475:HOH:O	2.19	0.53
1:C:381:GLU:HG3	1:C:382:GLU:H	1.73	0.53
1:D:105:TRP:CD1	1:D:222:LEU:HD13	2.44	0.53
1:D:388:GLU:OE2	1:D:391:ARG:NE	2.42	0.53
1:B:50:ARG:HG2	1:B:50:ARG:NH2	2.23	0.53
1:C:149:TRP:O	1:C:153:LEU:HD22	2.08	0.53
1:C:325:GLU:OE2	1:C:328:ARG:HD3	2.09	0.53
1:D:351:LYS:HB2	1:D:413:ALA:HA	1.91	0.53
1:C:140:VAL:O	1:C:178:THR:HA	2.08	0.53
1:D:162:GLY:O	1:D:175:THR:HA	2.09	0.53
1:A:62:ARG:HH11	1:A:110:ARG:HD3	1.73	0.53
1:A:323:TRP:O	1:A:327:ARG:HG2	2.09	0.53
1:A:427:GLU:HB2	1:A:431:ARG:HH21	1.74	0.53
1:D:389:GLY:O	1:D:395:PHE:HB2	2.08	0.53
1:A:309:ALA:O	1:A:310:SER:CB	2.55	0.53
1:A:409:ASP:O	1:A:410:VAL:HB	2.09	0.53
1:A:426:ARG:HH11	1:A:426:ARG:HG3	1.74	0.53
1:D:340:LEU:CG	1:D:343:ILE:HD11	2.39	0.53
1:A:304:ASN:C	1:A:306:ILE:H	2.18	0.52
1:C:217:ILE:O	1:C:218:ALA:C	2.51	0.52
1:D:356:THR:O	1:D:401:SER:HA	2.09	0.52
1:D:387:LEU:O	1:D:391:ARG:HG2	2.10	0.52
1:B:254:LEU:HD22	1:B:254:LEU:N	2.24	0.52
1:C:259:LEU:O	1:C:261:LYS:N	2.36	0.52
1:D:33:THR:HG21	1:D:55:ARG:HG2	1.92	0.52
1:A:259:LEU:C	1:A:259:LEU:HD22	2.34	0.52
1:B:24:ILE:O	1:B:24:ILE:CG2	2.58	0.52
1:C:201:VAL:O	1:C:205:PRO:HD3	2.09	0.52
1:C:263:THR:HG22	1:C:446:VAL:HG22	1.90	0.52
1:D:336:LYS:NZ	1:D:420:SER:HB2	2.24	0.52
1:C:126:MET:HE1	1:C:152:ARG:CB	2.28	0.52
1:D:27:ILE:C	1:D:27:ILE:HD12	2.34	0.52
1:D:163:GLU:O	1:D:170:GLU:HB2	2.10	0.52
1:C:389:GLY:O	1:C:392:THR:HG22	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:OE2	1:A:31:ARG:NH1	2.42	0.52
1:A:46:LYS:HD2	1:A:46:LYS:N	2.24	0.52
1:A:172:LYS:HD3	1:B:50:ARG:NE	2.25	0.52
1:A:344:LEU:HD12	1:A:369:PHE:CD2	2.45	0.52
1:B:449:GLU:O	1:B:451:ILE:HG13	2.10	0.52
1:D:95:ARG:CB	1:D:259:LEU:HD11	2.27	0.52
1:B:248:GLU:HG3	1:B:249:LEU:N	2.24	0.52
1:C:35:VAL:HA	1:C:54:TYR:O	2.09	0.52
1:C:68:PHE:O	1:C:69:GLU:C	2.53	0.52
1:C:96:ASP:N	1:C:96:ASP:OD2	2.40	0.52
1:D:150:LYS:HD3	1:D:163:GLU:HB2	1.91	0.52
1:D:441:GLY:O	1:D:442:LYS:HB2	2.09	0.52
1:A:102:LEU:O	1:A:106:LEU:HD22	2.09	0.52
1:B:67:TYR:CD1	1:B:67:TYR:C	2.87	0.52
1:C:356:THR:HG23	1:C:362:VAL:HG22	1.91	0.52
1:D:81:ASP:N	1:D:82:PRO:HD3	2.25	0.52
1:D:378:THR:HG22	1:D:382:GLU:HB3	1.92	0.52
1:A:359:ASN:HA	1:A:362:VAL:CG2	2.40	0.52
1:A:416:GLY:HA3	1:A:436:LEU:HD11	1.91	0.52
1:B:122:THR:HG21	1:B:152:ARG:NH2	2.24	0.52
1:C:426:ARG:HG3	1:C:426:ARG:HH11	1.75	0.52
1:B:299:ARG:C	1:B:301:GLU:H	2.17	0.52
1:C:329:ILE:HD11	4:C:2804:HOH:O	2.10	0.52
1:C:334:LYS:CG	1:C:338:ARG:HE	2.23	0.52
1:A:252:ASP:HB3	4:A:2835:HOH:O	2.11	0.51
1:A:269:VAL:HG22	1:A:336:LYS:HE3	1.91	0.51
1:C:356:THR:CG2	1:C:362:VAL:HG22	2.40	0.51
1:D:194:MET:HA	1:D:219:PRO:HD2	1.91	0.51
1:A:45:ALA:HB3	4:A:2010:HOH:O	2.10	0.51
1:B:248:GLU:HG3	1:B:249:LEU:H	1.74	0.51
1:C:232:ASP:HB2	4:C:2589:HOH:O	2.11	0.51
1:C:347:HIS:O	1:C:349:LYS:N	2.44	0.51
1:A:290:LEU:O	1:A:291:ARG:CB	2.58	0.51
1:B:378:THR:HB	1:B:382:GLU:HB2	1.92	0.51
1:A:121:LYS:HE2	1:A:225:THR:C	2.36	0.51
1:C:69:GLU:H	1:C:75:PHE:HE2	1.58	0.51
1:C:394:ARG:HA	1:C:394:ARG:NE	2.24	0.51
1:B:350:ASP:O	1:B:352:ILE:HG23	2.10	0.51
1:B:366:SER:CB	1:B:373:ALA:HB2	2.40	0.51
1:D:230:ARG:HH21	1:D:234:ARG:HD3	1.75	0.51
1:A:42:VAL:HG22	1:A:67:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLU:O	1:A:392:THR:HG23	2.10	0.51
1:C:33:THR:HG21	1:C:55:ARG:HE	1.76	0.51
1:C:152:ARG:C	1:C:154:GLY:N	2.69	0.51
1:A:295:ILE:CG2	1:A:299:ARG:HB3	2.41	0.51
1:B:391:ARG:HG3	4:B:2869:HOH:O	2.10	0.51
1:C:57:LEU:HD22	1:C:57:LEU:N	2.23	0.51
1:D:67:TYR:HA	1:D:70:SER:OG	2.09	0.51
1:D:249:LEU:HB3	1:D:254:LEU:HD21	1.93	0.51
1:D:450:LEU:N	1:D:450:LEU:HD23	2.24	0.51
1:A:34:ILE:HG12	1:A:58:ALA:HA	1.92	0.51
1:A:62:ARG:HB3	4:A:2002:HOH:O	2.10	0.51
1:A:172:LYS:HD3	1:B:50:ARG:HE	1.76	0.51
1:C:349:LYS:O	1:C:349:LYS:HG2	2.11	0.51
1:D:361:LEU:CD1	1:D:365:ILE:HD11	2.40	0.51
1:A:110:ARG:HG3	1:A:242:VAL:O	2.11	0.51
1:A:327:ARG:HH21	1:A:422:SER:HB3	1.76	0.51
1:B:130:ASN:ND2	1:B:268:PHE:HE1	2.09	0.51
1:B:434:ARG:NH2	1:B:434:ARG:CB	2.73	0.51
1:B:438:PRO:HA	1:B:445:ALA:HB2	1.93	0.51
1:C:164:PHE:HE1	1:C:185:ASN:CG	2.18	0.51
1:D:259:LEU:C	1:D:261:LYS:N	2.67	0.51
1:B:367:LYS:C	1:B:369:PHE:N	2.67	0.50
1:C:371:ILE:CG2	1:C:399:VAL:HG12	2.41	0.50
1:D:59:PHE:HA	1:D:216:SER:O	2.11	0.50
1:A:267:ILE:HB	1:A:450:LEU:HD22	1.92	0.50
1:B:369:PHE:HB2	1:B:371:ILE:CD1	2.41	0.50
1:C:57:LEU:O	1:C:60:ARG:HG2	2.12	0.50
1:D:136:THR:N	1:D:173:PRO:O	2.42	0.50
1:A:377:ARG:O	1:A:378:THR:C	2.53	0.50
1:B:63:ASP:OD1	4:B:2110:HOH:O	2.18	0.50
1:C:259:LEU:O	1:C:259:LEU:HD23	2.11	0.50
1:D:44:HIS:ND1	1:D:60:ARG:HD2	2.26	0.50
1:D:152:ARG:HH11	1:D:152:ARG:CG	2.25	0.50
1:D:318:GLU:O	1:D:319:ALA:HB2	2.11	0.50
1:A:42:VAL:CG1	1:A:43:PRO:HD2	2.37	0.50
1:C:284:LYS:C	1:C:286:TYR:N	2.66	0.50
1:C:343:ILE:HD11	1:C:450:LEU:HD21	1.93	0.50
1:A:327:ARG:O	1:A:330:ALA:HB3	2.12	0.50
1:C:57:LEU:H	1:C:57:LEU:CD2	2.22	0.50
1:C:331:PHE:CE2	1:C:421:GLY:HA2	2.47	0.50
1:C:426:ARG:HA	1:C:429:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:LYS:HG2	4:D:2604:HOH:O	2.11	0.50
1:C:347:HIS:O	1:C:348:ARG:C	2.55	0.50
1:D:258:HIS:C	1:D:260:ALA:H	2.20	0.50
1:D:305:LYS:NZ	1:D:305:LYS:CB	2.73	0.50
1:A:351:LYS:NZ	1:A:351:LYS:HB3	2.27	0.50
1:A:377:ARG:HG3	1:A:377:ARG:HH11	1.76	0.50
1:C:60:ARG:O	1:C:61:TYR:C	2.54	0.50
1:C:239:LYS:HA	1:C:243:GLY:C	2.36	0.50
1:C:418:ILE:CG1	1:C:425:ALA:HB2	2.40	0.50
1:A:364:ARG:O	1:A:368:VAL:HG23	2.12	0.50
1:B:199:ASP:O	1:B:200:GLU:C	2.53	0.50
1:C:221:ARG:NH2	1:C:241:VAL:O	2.45	0.50
1:D:336:LYS:NZ	1:D:452:SER:HB2	2.27	0.50
1:D:340:LEU:O	1:D:344:LEU:HG	2.11	0.50
1:A:430:GLN:O	1:A:433:GLY:N	2.43	0.50
1:A:140:VAL:O	1:A:178:THR:HA	2.12	0.49
1:A:400:SER:OG	1:A:401:SER:N	2.45	0.49
1:C:126:MET:SD	1:C:153:LEU:HD13	2.52	0.49
1:C:390:PHE:CE2	1:C:398:ILE:HG12	2.48	0.49
1:D:112:CYS:O	1:D:246:VAL:HG22	2.12	0.49
1:A:357:ARG:HD3	1:A:428:TYR:CE2	2.47	0.49
1:A:414:ASN:OD1	1:A:439:SER:HB2	2.12	0.49
1:A:115:LEU:O	1:A:121:LYS:HE3	2.12	0.49
1:A:259:LEU:HD21	1:A:262:TYR:CD2	2.47	0.49
1:B:88:PHE:CD2	1:B:133:SER:HA	2.47	0.49
1:B:110:ARG:HD2	1:B:221:ARG:HG3	1.94	0.49
1:B:134:THR:HB	1:B:194:MET:HB2	1.95	0.49
1:C:229:GLU:OE2	1:C:235:HIS:NE2	2.45	0.49
1:A:141:PRO:HD2	1:A:145:LEU:HD12	1.92	0.49
1:B:251:PRO:O	1:B:254:LEU:HD23	2.11	0.49
1:C:389:GLY:C	1:C:392:THR:HG22	2.36	0.49
1:A:39:ASP:HB3	1:A:42:VAL:HG23	1.94	0.49
1:B:336:LYS:HE3	1:B:452:SER:OG	2.13	0.49
1:B:450:LEU:H	1:B:450:LEU:CD2	2.25	0.49
1:A:180:ASP:OD1	1:D:143:LEU:HB2	2.13	0.49
1:A:330:ALA:O	1:A:332:ASN:N	2.45	0.49
1:B:322:ALA:C	1:B:324:GLU:N	2.71	0.49
1:C:262:TYR:CE2	1:C:433:GLY:HA3	2.48	0.49
1:C:364:ARG:O	1:C:368:VAL:HG23	2.13	0.49
1:D:441:GLY:O	1:D:442:LYS:CB	2.61	0.49
1:A:256:GLY:O	1:A:258:HIS:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ARG:HG3	1:C:349:LYS:H	1.77	0.49
1:A:191:ASN:H	1:A:191:ASN:ND2	2.11	0.49
1:A:379:SER:HB2	1:A:382:GLU:HB2	1.94	0.49
1:A:432:LEU:HD13	1:A:432:LEU:C	2.38	0.49
1:B:433:GLY:O	1:B:436:LEU:HB2	2.12	0.49
1:C:61:TYR:O	1:C:65:ILE:HG12	2.13	0.49
1:C:96:ASP:CG	1:C:259:LEU:HD22	2.38	0.49
1:C:196:LEU:HG	1:C:218:ALA:HB3	1.94	0.49
1:C:259:LEU:C	1:C:261:LYS:N	2.69	0.49
1:D:27:ILE:O	1:D:27:ILE:HG13	2.13	0.49
1:A:288:GLN:C	1:A:290:LEU:H	2.21	0.49
1:B:99:GLU:OE1	1:B:99:GLU:HA	2.12	0.49
1:C:291:ARG:O	1:C:292:ALA:HB3	2.13	0.49
1:D:325:GLU:C	1:D:327:ARG:N	2.71	0.49
1:A:194:MET:HE2	1:A:194:MET:HA	1.94	0.49
1:A:304:ASN:HD22	1:A:307:VAL:CG2	2.26	0.49
1:B:382:GLU:HA	1:B:385:GLU:HB3	1.94	0.49
1:C:28:TYR:CA	1:C:79:ALA:HB2	2.40	0.49
1:C:375:THR:OG1	1:C:376:HIS:N	2.43	0.49
1:A:389:GLY:O	1:A:395:PHE:HB2	2.12	0.48
1:B:210:VAL:HG21	1:B:237:ILE:HD12	1.94	0.48
1:B:350:ASP:HB3	1:B:414:ASN:OD1	2.13	0.48
1:B:434:ARG:CB	1:B:434:ARG:HH21	2.25	0.48
1:C:42:VAL:HG12	1:C:45:ALA:H	1.77	0.48
1:C:431:ARG:O	1:C:435:ILE:HG13	2.13	0.48
1:D:383:ARG:O	1:D:387:LEU:HG	2.13	0.48
1:C:333:SER:O	1:C:337:ILE:HG12	2.13	0.48
1:D:340:LEU:CD2	1:D:343:ILE:HD11	2.43	0.48
1:D:352:ILE:HD12	1:D:353:ILE:H	1.78	0.48
1:C:34:ILE:HG12	1:C:58:ALA:HA	1.95	0.48
1:D:96:ASP:H	1:D:259:LEU:CD1	2.26	0.48
1:D:267:ILE:O	1:D:451:ILE:N	2.36	0.48
1:C:196:LEU:HG	1:C:218:ALA:CB	2.44	0.48
1:A:136:THR:N	1:A:173:PRO:O	2.32	0.48
1:A:259:LEU:HD22	1:A:261:LYS:HG3	1.95	0.48
1:B:105:TRP:HE3	1:B:106:LEU:HD13	1.78	0.48
1:C:159:GLU:OE2	1:C:159:GLU:N	2.39	0.48
1:C:204:LEU:N	1:C:205:PRO:CD	2.77	0.48
1:D:449:GLU:HG2	1:D:451:ILE:CG1	2.43	0.48
1:C:418:ILE:CD1	1:C:425:ALA:HB2	2.44	0.48
1:A:305:LYS:C	1:A:306:ILE:HG13	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LEU:HB3	1:C:119:SER:HB2	1.94	0.48
1:D:369:PHE:O	1:D:371:ILE:N	2.41	0.48
1:D:391:ARG:HG3	1:D:392:THR:H	1.79	0.48
1:D:421:GLY:C	1:D:423:GLY:N	2.72	0.48
1:B:299:ARG:C	1:B:301:GLU:N	2.72	0.48
1:B:304:ASN:HA	1:B:307:VAL:HB	1.96	0.48
1:C:361:LEU:HD22	1:C:365:ILE:HG13	1.96	0.48
1:C:440:LYS:HG2	1:C:441:GLY:N	2.27	0.48
1:D:65:ILE:O	1:D:68:PHE:HB2	2.13	0.48
1:D:352:ILE:HA	1:D:415:VAL:O	2.14	0.48
1:A:102:LEU:HG	1:A:106:LEU:CD2	2.44	0.48
1:A:439:SER:O	1:A:441:GLY:N	2.46	0.48
1:C:132:LEU:O	1:C:133:SER:HB2	2.14	0.48
1:C:338:ARG:O	1:C:341:ARG:HB3	2.14	0.48
1:C:356:THR:HB	1:C:419:MET:CG	2.44	0.48
1:D:339:LYS:O	1:D:343:ILE:HG23	2.14	0.48
1:A:295:ILE:HB	1:A:299:ARG:CB	2.44	0.47
1:B:283:GLU:C	1:B:285:VAL:N	2.68	0.47
1:C:272:ALA:O	1:C:274:ASP:N	2.45	0.47
1:D:116:PRO:CG	1:D:251:PRO:HG3	2.44	0.47
1:A:234:ARG:NH2	3:A:6002:IPA:H2	2.29	0.47
1:B:110:ARG:NH1	1:B:219:PRO:O	2.44	0.47
1:B:282:ARG:O	1:B:322:ALA:HB1	2.14	0.47
1:C:171:LEU:C	1:C:172:LYS:HE2	2.39	0.47
1:C:237:ILE:HG13	1:C:238:LEU:N	2.27	0.47
1:A:259:LEU:HD22	1:A:261:LYS:H	1.79	0.47
1:B:105:TRP:CE3	1:B:106:LEU:HD13	2.49	0.47
1:C:71:ASN:O	1:C:73:ILE:N	2.42	0.47
1:C:72:GLY:O	1:C:73:ILE:C	2.56	0.47
1:C:254:LEU:O	1:C:255:ALA:CB	2.62	0.47
1:C:361:LEU:CD1	1:C:419:MET:HG3	2.40	0.47
1:D:68:PHE:C	1:D:70:SER:H	2.22	0.47
1:D:266:ARG:HB3	1:D:451:ILE:HD12	1.95	0.47
1:A:261:LYS:NZ	1:A:261:LYS:HB3	2.29	0.47
1:A:426:ARG:NH2	4:A:2471:HOH:O	2.46	0.47
1:B:102:LEU:CD1	1:B:106:LEU:HD22	2.44	0.47
1:D:84:PRO:HB3	4:D:2177:HOH:O	2.14	0.47
1:D:140:VAL:O	1:D:178:THR:HA	2.14	0.47
1:D:149:TRP:HE3	1:D:153:LEU:CD1	2.24	0.47
1:D:361:LEU:HD13	1:D:365:ILE:HG13	1.95	0.47
1:A:355:PHE:CD2	1:A:356:THR:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ALA:C	1:B:82:PRO:HD3	2.39	0.47
1:B:333:SER:CB	1:B:336:LYS:HG2	2.40	0.47
1:B:412:ASP:OD2	1:B:437:ARG:HG2	2.15	0.47
1:D:74:GLU:OE1	1:D:74:GLU:HA	2.14	0.47
1:D:460:THR:O	1:D:461:ALA:HB2	2.15	0.47
1:B:350:ASP:HB2	1:B:414:ASN:HB3	1.95	0.47
1:C:105:TRP:O	1:C:109:LYS:N	2.46	0.47
1:C:125:ALA:O	1:C:129:ILE:HG13	2.13	0.47
1:C:426:ARG:HA	1:C:429:ILE:CD1	2.44	0.47
1:D:344:LEU:O	1:D:346:ARG:N	2.48	0.47
1:A:258:HIS:O	1:A:259:LEU:C	2.58	0.47
1:A:325:GLU:O	1:A:326:ALA:C	2.56	0.47
1:A:352:ILE:HD11	1:A:354:ILE:HD11	1.97	0.47
1:A:389:GLY:HA2	1:A:392:THR:OG1	2.14	0.47
1:A:390:PHE:HA	1:A:395:PHE:CB	2.44	0.47
1:B:28:TYR:HE1	1:B:37:LYS:HD2	1.79	0.47
1:B:405:ASP:CB	1:B:435:ILE:HD11	2.41	0.47
1:C:348:ARG:HG3	1:C:349:LYS:N	2.29	0.47
1:C:363:TYR:O	1:C:367:LYS:HG2	2.15	0.47
1:D:250:PHE:O	1:D:253:SER:HB2	2.15	0.47
1:D:289:PHE:C	1:D:291:ARG:N	2.71	0.47
1:A:295:ILE:HD13	1:A:300:ALA:CB	2.43	0.47
1:A:404:LEU:O	1:A:410:VAL:HG11	2.15	0.47
1:B:31:ARG:HG2	1:B:187:GLU:HB3	1.95	0.47
1:C:26:GLU:HG2	1:C:27:ILE:N	2.29	0.47
1:C:254:LEU:C	1:C:254:LEU:HD23	2.40	0.47
1:D:132:LEU:HD23	1:D:458:VAL:CG2	2.32	0.47
1:A:239:LYS:HA	1:A:243:GLY:C	2.39	0.47
1:A:307:VAL:HG23	1:A:308:MET:N	2.29	0.47
1:B:279:TYR:OH	1:B:422:SER:HB3	2.15	0.47
1:D:327:ARG:NH2	1:D:358:HIS:NE2	2.63	0.47
1:D:418:ILE:CG1	1:D:432:LEU:HD13	2.45	0.47
1:B:60:ARG:NH1	4:B:2110:HOH:O	2.43	0.47
1:B:81:ASP:O	1:B:192:ARG:HA	2.14	0.47
1:B:290:LEU:HD22	1:B:296:THR:C	2.40	0.47
1:B:405:ASP:HB3	1:B:435:ILE:CD1	2.43	0.47
1:C:290:LEU:HD23	1:C:290:LEU:H	1.80	0.47
1:A:359:ASN:HA	1:A:362:VAL:CB	2.44	0.46
1:A:403:VAL:HG23	1:A:403:VAL:O	2.15	0.46
1:B:375:THR:HG23	1:B:377:ARG:N	2.28	0.46
1:A:122:THR:HG21	1:A:152:ARG:NE	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:PRO:HA	1:B:237:ILE:HD11	1.97	0.46
1:B:403:VAL:HG21	1:B:431:ARG:HE	1.80	0.46
1:C:168:ILE:HG12	1:C:170:GLU:HG3	1.97	0.46
1:A:374:ILE:HD11	1:A:386:ILE:CG2	2.45	0.46
1:B:369:PHE:HB2	1:B:371:ILE:HG13	1.98	0.46
1:C:267:ILE:HD11	1:C:448:TYR:HD2	1.79	0.46
1:A:191:ASN:ND2	4:A:2501:HOH:O	2.47	0.46
1:A:220:PHE:C	1:A:221:ARG:HG2	2.39	0.46
1:A:365:ILE:O	1:A:369:PHE:HD1	1.99	0.46
1:D:43:PRO:HG3	1:D:67:TYR:CD2	2.50	0.46
1:D:100:LYS:HD3	1:D:426:ARG:NH2	2.25	0.46
1:D:403:VAL:HG11	1:D:431:ARG:HD3	1.96	0.46
1:A:205:PRO:HA	1:A:237:ILE:HD11	1.96	0.46
1:A:259:LEU:CD1	1:A:260:ALA:N	2.77	0.46
1:B:102:LEU:CG	1:B:106:LEU:HD22	2.43	0.46
1:B:205:PRO:O	1:B:206:ALA:C	2.57	0.46
1:C:27:ILE:HG22	1:C:36:VAL:HG13	1.96	0.46
1:C:220:PHE:C	1:C:221:ARG:HG3	2.40	0.46
1:D:66:GLU:O	1:D:68:PHE:N	2.48	0.46
1:D:261:LYS:C	1:D:444:GLU:HB3	2.41	0.46
1:D:376:HIS:HB3	1:D:402:GLN:HE22	1.80	0.46
1:A:277:VAL:HG13	1:A:278:GLU:N	2.29	0.46
1:D:198:PHE:CE1	1:D:204:LEU:HD13	2.50	0.46
1:D:333:SER:HB3	1:D:336:LYS:HG3	1.97	0.46
1:D:404:LEU:O	1:D:411:PRO:HD2	2.15	0.46
1:B:45:ALA:HB1	1:B:54:TYR:HB3	1.97	0.46
1:D:443:LYS:O	1:D:444:GLU:HG3	2.15	0.46
1:A:191:ASN:HD22	1:A:191:ASN:N	2.10	0.46
1:B:371:ILE:HA	1:B:372:PRO:HD3	1.68	0.46
1:C:258:HIS:C	1:C:260:ALA:H	2.24	0.46
1:B:434:ARG:HB2	1:B:434:ARG:CZ	2.44	0.46
1:C:419:MET:HE1	1:C:450:LEU:HD12	1.97	0.46
1:D:167:ARG:C	1:D:168:ILE:CG1	2.88	0.46
1:D:274:ASP:HA	1:D:277:VAL:CG2	2.46	0.46
1:D:424:SER:HA	1:D:449:GLU:OE2	2.16	0.46
1:D:432:LEU:HD23	1:D:432:LEU:C	2.41	0.46
1:A:254:LEU:N	1:A:254:LEU:HD12	2.31	0.46
1:A:304:ASN:HA	1:A:307:VAL:CG2	2.44	0.46
1:A:451:ILE:HG22	1:A:452:SER:N	2.31	0.46
1:C:162:GLY:HA3	1:C:172:LYS:HB2	1.98	0.46
1:D:268:PHE:HA	1:D:451:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:HG3	1:A:329:ILE:CD1	2.46	0.45
1:A:340:LEU:O	1:A:344:LEU:HG	2.16	0.45
1:C:149:TRP:O	1:C:152:ARG:N	2.50	0.45
1:D:217:ILE:O	1:D:218:ALA:C	2.59	0.45
1:A:358:HIS:C	1:A:362:VAL:HG23	2.39	0.45
1:A:390:PHE:HA	1:A:395:PHE:HB3	1.98	0.45
1:B:344:LEU:O	1:B:348:ARG:HG3	2.15	0.45
1:D:110:ARG:HE	1:D:221:ARG:HG3	1.81	0.45
1:A:149:TRP:HA	1:A:152:ARG:HH11	1.81	0.45
1:A:388:GLU:O	1:A:392:THR:N	2.48	0.45
1:B:378:THR:O	1:B:379:SER:HB2	2.17	0.45
1:C:116:PRO:HD2	1:C:119:SER:OG	2.16	0.45
1:C:263:THR:HG23	1:C:446:VAL:HG13	1.99	0.45
1:C:407:GLY:O	1:C:408:ILE:HB	2.17	0.45
1:D:172:LYS:HB3	1:D:173:PRO:CD	2.44	0.45
1:D:256:GLY:O	1:D:258:HIS:N	2.40	0.45
1:D:336:LYS:HZ1	1:D:420:SER:HB2	1.82	0.45
1:A:271:LEU:HD21	1:A:452:SER:HB3	1.99	0.45
1:B:71:ASN:O	1:B:72:GLY:C	2.59	0.45
1:C:94:LEU:N	1:C:264:ILE:O	2.39	0.45
1:C:423:GLY:O	1:C:424:SER:HB2	2.16	0.45
1:D:357:ARG:HE	1:D:428:TYR:HE2	1.65	0.45
1:B:390:PHE:CE2	1:B:398:ILE:HG12	2.51	0.45
1:B:415:VAL:CG1	1:B:416:GLY:N	2.79	0.45
1:C:412:ASP:HB2	1:C:437:ARG:NH1	2.32	0.45
1:D:457:GLU:O	1:D:458:VAL:HB	2.16	0.45
1:A:62:ARG:NH1	1:A:110:ARG:HD3	2.31	0.45
1:A:372:PRO:HG3	1:A:395:PHE:CE2	2.49	0.45
1:A:443:LYS:O	1:A:444:GLU:HG3	2.17	0.45
1:B:26:GLU:HG2	1:B:27:ILE:N	2.31	0.45
1:B:427:GLU:HG2	1:B:428:TYR:CD2	2.52	0.45
1:D:43:PRO:O	1:D:44:HIS:CB	2.63	0.45
1:A:196:LEU:HG	1:A:218:ALA:CB	2.47	0.45
1:A:312:TYR:O	1:A:313:ASP:C	2.60	0.45
1:B:31:ARG:HG2	1:B:187:GLU:CG	2.46	0.45
1:B:43:PRO:C	1:B:45:ALA:H	2.24	0.45
1:B:375:THR:O	1:B:383:ARG:NH2	2.49	0.45
1:C:101:ALA:HB2	1:C:247:PHE:CE1	2.52	0.45
1:C:358:HIS:HB3	1:C:361:LEU:HB3	1.99	0.45
1:D:195:LEU:HD23	1:D:220:PHE:HB2	1.99	0.45
1:A:430:GLN:O	1:A:431:ARG:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ARG:HD3	1:A:431:ARG:N	2.32	0.45
1:B:347:HIS:ND1	1:B:415:VAL:HG21	2.32	0.45
1:C:271:LEU:HD12	1:C:271:LEU:HA	1.81	0.45
1:D:261:LYS:HA	1:D:444:GLU:HG2	1.99	0.45
1:D:430:GLN:O	1:D:431:ARG:C	2.60	0.45
1:A:241:VAL:HG23	1:A:242:VAL:N	2.32	0.45
1:A:398:ILE:CD1	1:A:399:VAL:N	2.66	0.45
1:B:339:LYS:O	1:B:342:GLU:HB2	2.17	0.45
1:C:95:ARG:O	1:C:96:ASP:C	2.60	0.45
1:C:232:ASP:OD1	1:C:234:ARG:HB2	2.16	0.45
1:C:234:ARG:HG3	1:C:234:ARG:HH11	1.81	0.45
1:D:116:PRO:HG3	1:D:251:PRO:HG3	1.99	0.45
1:A:266:ARG:HH21	1:A:266:ARG:HG2	1.82	0.45
1:A:339:LYS:O	1:A:343:ILE:HG13	2.17	0.45
1:B:329:ILE:O	1:B:332:ASN:OD1	2.35	0.45
1:B:430:GLN:HE21	1:B:430:GLN:HB2	1.53	0.45
1:C:286:TYR:C	1:C:288:GLN:N	2.75	0.45
1:D:42:VAL:HB	1:D:54:TYR:CD2	2.51	0.45
1:D:394:ARG:O	1:D:394:ARG:HG2	2.17	0.45
1:A:217:ILE:O	1:A:218:ALA:C	2.60	0.44
1:C:325:GLU:HG3	1:C:329:ILE:CD1	2.36	0.44
1:D:29:TYR:H	1:D:79:ALA:HA	1.82	0.44
1:D:328:ARG:HG3	1:D:328:ARG:NH1	2.32	0.44
1:D:352:ILE:HD11	1:D:354:ILE:HG12	1.99	0.44
1:A:311:GLY:C	1:A:312:TYR:HD2	2.25	0.44
1:D:172:LYS:CB	1:D:173:PRO:HD2	2.43	0.44
1:A:81:ASP:O	1:A:192:ARG:HA	2.17	0.44
1:A:85:THR:HG23	1:A:86:PRO:HD2	1.99	0.44
4:A:2006:HOH:O	1:D:142:THR:HG22	2.16	0.44
1:B:429:ILE:HD11	1:B:449:GLU:OE2	2.18	0.44
1:C:148:GLN:CD	1:C:152:ARG:HH22	2.25	0.44
1:C:190:GLY:O	1:C:217:ILE:HG23	2.17	0.44
1:D:109:LYS:O	1:D:220:PHE:HA	2.17	0.44
1:B:404:LEU:N	1:B:404:LEU:CD2	2.77	0.44
1:C:327:ARG:O	1:C:331:PHE:HB2	2.16	0.44
1:D:372:PRO:CB	1:D:398:ILE:HG22	2.45	0.44
1:A:204:LEU:HB3	1:A:205:PRO:HD3	1.98	0.44
1:A:259:LEU:HD13	1:A:261:LYS:H	1.83	0.44
1:A:288:GLN:HB2	1:A:290:LEU:HD22	1.99	0.44
1:A:320:LEU:HD23	1:A:320:LEU:O	2.17	0.44
1:A:377:ARG:HG3	1:A:377:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:HG2	1:B:187:GLU:HG2	1.99	0.44
1:C:202:HIS:O	1:C:205:PRO:HD2	2.17	0.44
1:C:250:PHE:CD1	1:C:251:PRO:HD2	2.50	0.44
1:C:266:ARG:HB2	4:C:2247:HOH:O	2.17	0.44
1:B:399:VAL:O	1:B:399:VAL:HG13	2.18	0.44
1:C:247:PHE:CE1	1:C:249:LEU:HB2	2.53	0.44
1:D:66:GLU:C	1:D:68:PHE:N	2.75	0.44
1:D:421:GLY:C	1:D:423:GLY:H	2.26	0.44
1:A:232:ASP:C	1:A:234:ARG:H	2.26	0.44
1:A:234:ARG:C	1:A:236:GLU:N	2.75	0.44
1:A:269:VAL:HG23	4:A:2285:HOH:O	2.17	0.44
1:A:326:ALA:O	1:A:329:ILE:HB	2.17	0.44
1:A:359:ASN:O	1:A:362:VAL:N	2.51	0.44
1:B:207:GLU:HG2	1:B:234:ARG:NH1	2.32	0.44
1:B:248:GLU:CG	1:B:249:LEU:N	2.80	0.44
1:B:290:LEU:C	1:B:292:ALA:H	2.25	0.44
1:C:100:LYS:HD3	1:C:100:LYS:C	2.43	0.44
1:C:322:ALA:C	1:C:324:GLU:N	2.70	0.44
1:C:356:THR:O	1:C:401:SER:HA	2.18	0.44
1:D:305:LYS:N	1:D:305:LYS:CD	2.81	0.44
1:D:361:LEU:HD22	1:D:364:ARG:HD2	1.99	0.44
1:A:116:PRO:O	1:A:119:SER:OG	2.33	0.44
1:A:431:ARG:HD3	1:A:431:ARG:H	1.81	0.44
1:C:252:ASP:O	1:C:253:SER:C	2.60	0.44
1:D:26:GLU:HG2	1:D:27:ILE:N	2.32	0.44
1:D:420:SER:OG	1:D:421:GLY:N	2.47	0.44
1:A:66:GLU:CG	1:A:297:LEU:HD13	2.44	0.44
1:A:134:THR:HB	1:A:135:PRO:HD2	2.00	0.44
1:A:300:ALA:HB1	1:A:304:ASN:HB2	1.99	0.44
1:B:354:ILE:HG22	1:B:355:PHE:H	1.81	0.44
1:B:366:SER:HA	1:B:371:ILE:HB	2.00	0.44
1:D:83:ILE:HD13	1:D:171:LEU:O	2.18	0.44
1:D:290:LEU:N	1:D:290:LEU:HD13	2.33	0.44
1:D:449:GLU:O	1:D:451:ILE:HG13	2.17	0.44
1:A:205:PRO:HB2	1:A:230:ARG:HH11	1.81	0.43
1:B:22:GLN:O	1:B:24:ILE:HG13	2.17	0.43
1:B:425:ALA:O	1:B:429:ILE:HG13	2.18	0.43
1:C:92:ILE:HG21	1:C:127:ALA:HB2	1.99	0.43
1:C:95:ARG:O	1:C:98:GLN:N	2.51	0.43
1:C:154:GLY:C	1:C:156:PHE:N	2.75	0.43
1:C:405:ASP:HA	1:C:410:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:ARG:HG3	1:C:426:ARG:NH1	2.33	0.43
1:D:239:LYS:HA	1:D:243:GLY:C	2.43	0.43
1:A:29:TYR:H	1:A:79:ALA:HA	1.82	0.43
1:B:62:ARG:HH11	1:B:110:ARG:HD3	1.83	0.43
1:B:276:ARG:HG3	1:B:277:VAL:N	2.32	0.43
1:C:38:GLY:C	1:C:40:ALA:N	2.76	0.43
1:C:103:GLU:OE2	1:C:103:GLU:HA	2.16	0.43
1:C:340:LEU:HD11	1:C:354:ILE:CD1	2.48	0.43
1:D:47:PHE:O	1:D:48:ASP:C	2.61	0.43
1:D:280:GLU:O	1:D:282:ARG:N	2.37	0.43
1:D:405:ASP:HB3	1:D:435:ILE:CD1	2.39	0.43
1:D:456:GLY:O	1:D:457:GLU:HB2	2.18	0.43
1:A:85:THR:HG22	1:A:86:PRO:O	2.18	0.43
1:A:103:GLU:HG3	1:A:426:ARG:HD3	2.00	0.43
1:A:286:TYR:CE2	1:A:323:TRP:HA	2.53	0.43
1:A:418:ILE:HD12	1:A:429:ILE:HD13	1.99	0.43
1:A:430:GLN:HG3	4:A:2471:HOH:O	2.18	0.43
1:B:391:ARG:HD2	1:B:391:ARG:O	2.18	0.43
1:C:361:LEU:O	1:C:365:ILE:CG1	2.67	0.43
1:C:392:THR:HG23	1:C:393:GLY:H	1.82	0.43
1:D:404:LEU:N	1:D:404:LEU:CD2	2.78	0.43
1:D:417:VAL:HG12	1:D:419:MET:HE2	2.00	0.43
1:A:270:PRO:O	1:A:335:ASN:ND2	2.52	0.43
1:A:385:GLU:O	1:A:388:GLU:N	2.47	0.43
1:A:425:ALA:HB1	1:A:428:TYR:HD2	1.83	0.43
1:B:280:GLU:C	1:B:282:ARG:H	2.26	0.43
1:C:323:TRP:CZ2	1:C:327:ARG:HB2	2.53	0.43
1:C:331:PHE:CE1	1:C:358:HIS:HB2	2.54	0.43
1:C:403:VAL:HG21	1:C:431:ARG:CZ	2.48	0.43
1:D:417:VAL:HG12	1:D:419:MET:CE	2.49	0.43
1:D:458:VAL:HG12	1:D:459:ASN:N	2.33	0.43
1:A:351:LYS:NZ	1:A:390:PHE:CE1	2.87	0.43
1:A:425:ALA:HB1	1:A:428:TYR:CD2	2.53	0.43
1:C:284:LYS:C	1:C:286:TYR:H	2.27	0.43
1:D:73:ILE:HG22	1:D:74:GLU:N	2.33	0.43
1:D:261:LYS:CA	1:D:444:GLU:HG2	2.49	0.43
1:D:269:VAL:O	1:D:269:VAL:HG23	2.17	0.43
1:D:376:HIS:HB3	1:D:402:GLN:NE2	2.34	0.43
1:A:285:VAL:CG2	1:A:286:TYR:H	2.12	0.43
1:B:357:ARG:O	1:B:357:ARG:HG3	2.18	0.43
1:C:283:GLU:O	1:C:284:LYS:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:GLY:O	1:C:422:SER:CB	2.66	0.43
1:D:110:ARG:NE	1:D:221:ARG:HG3	2.33	0.43
1:D:132:LEU:HD23	1:D:458:VAL:HG11	2.00	0.43
1:D:355:PHE:C	1:D:356:THR:HG22	2.43	0.43
1:D:356:THR:HB	1:D:419:MET:CG	2.49	0.43
1:A:169:LYS:NZ	1:A:185:ASN:HD21	2.16	0.43
1:A:228:PHE:CD1	1:A:245:LYS:HD3	2.54	0.43
1:A:428:TYR:O	1:A:432:LEU:HB3	2.19	0.43
1:B:103:GLU:OE1	1:B:426:ARG:HD2	2.19	0.43
1:C:229:GLU:HG3	4:C:2633:HOH:O	2.18	0.43
1:C:393:GLY:O	1:C:394:ARG:C	2.61	0.43
1:C:447:LEU:C	1:C:447:LEU:HD23	2.44	0.43
1:A:201:VAL:HG22	1:A:201:VAL:O	2.17	0.43
1:B:357:ARG:HD3	1:B:428:TYR:OH	2.18	0.43
1:B:437:ARG:O	1:B:438:PRO:O	2.36	0.43
1:C:361:LEU:O	1:C:361:LEU:HD13	2.18	0.43
1:D:371:ILE:HD12	1:D:371:ILE:HA	1.92	0.43
1:D:388:GLU:OE2	1:D:391:ARG:CZ	2.67	0.43
1:A:103:GLU:HA	1:A:106:LEU:HD23	2.01	0.43
1:A:141:PRO:HD2	1:A:145:LEU:CD1	2.49	0.43
1:A:238:LEU:O	1:A:239:LYS:C	2.61	0.43
1:A:256:GLY:C	1:A:258:HIS:H	2.27	0.43
1:A:336:LYS:O	1:A:340:LEU:HB2	2.19	0.43
1:B:273:GLU:HG3	1:B:276:ARG:HD3	2.00	0.43
1:B:400:SER:CB	1:B:404:LEU:HD11	2.49	0.43
1:C:96:ASP:OD1	1:C:259:LEU:HB2	2.19	0.43
1:A:202:HIS:O	1:A:205:PRO:HD2	2.19	0.43
1:B:231:GLU:OE2	1:B:232:ASP:N	2.52	0.43
1:B:332:ASN:O	1:B:333:SER:O	2.36	0.43
1:C:354:ILE:HD11	1:C:419:MET:SD	2.58	0.43
1:D:329:ILE:CD1	1:D:330:ALA:N	2.72	0.43
1:D:340:LEU:HD23	1:D:343:ILE:HD11	1.99	0.43
1:C:202:HIS:C	1:C:205:PRO:HD2	2.44	0.42
1:C:269:VAL:HG21	1:C:336:LYS:HD3	2.01	0.42
1:D:34:ILE:HD13	1:D:34:ILE:HA	1.85	0.42
1:D:52:GLY:O	1:D:53:THR:HG23	2.18	0.42
1:D:62:ARG:HD3	1:D:110:ARG:NH1	2.33	0.42
1:D:378:THR:HG23	1:D:382:GLU:CD	2.43	0.42
1:A:46:LYS:HE2	4:A:2260:HOH:O	2.18	0.42
1:A:231:GLU:HG3	1:D:118:GLY:HA2	2.00	0.42
1:B:48:ASP:OD1	1:B:50:ARG:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:TYR:OH	1:C:142:THR:HB	2.18	0.42
1:B:329:ILE:O	1:B:329:ILE:HG22	2.18	0.42
1:C:375:THR:CG2	1:C:378:THR:HG23	2.31	0.42
1:D:115:LEU:HD12	1:D:121:LYS:HG2	2.00	0.42
1:B:295:ILE:O	1:B:295:ILE:HG23	2.19	0.42
1:B:435:ILE:O	1:B:437:ARG:HD2	2.18	0.42
1:C:357:ARG:NH1	4:C:2340:HOH:O	2.52	0.42
1:C:404:LEU:C	1:C:406:GLU:H	2.27	0.42
1:D:413:ALA:HB3	1:D:436:LEU:HD23	2.01	0.42
1:B:102:LEU:HG	1:B:106:LEU:CD2	2.46	0.42
1:B:122:THR:O	1:B:122:THR:HG22	2.18	0.42
1:B:187:GLU:HG3	1:B:215:MET:CE	2.49	0.42
1:C:148:GLN:HE21	1:C:152:ARG:NH1	1.97	0.42
1:C:196:LEU:HD13	1:C:198:PHE:CZ	2.54	0.42
1:C:269:VAL:HG22	1:C:452:SER:HB3	2.01	0.42
1:C:358:HIS:O	1:C:362:VAL:HG23	2.19	0.42
1:D:191:ASN:OD1	1:D:192:ARG:CD	2.65	0.42
1:D:453:ARG:HB2	1:D:454:GLY:H	1.69	0.42
1:A:65:ILE:HG22	1:A:297:LEU:CD1	2.47	0.42
1:A:335:ASN:O	1:A:339:LYS:HB2	2.19	0.42
1:B:68:PHE:HB3	1:B:75:PHE:CE2	2.54	0.42
1:B:93:SER:HA	1:B:264:ILE:O	2.20	0.42
1:B:211:GLN:O	1:B:212:ILE:C	2.60	0.42
1:B:275:GLU:O	1:B:276:ARG:C	2.62	0.42
1:B:372:PRO:HG2	1:B:395:PHE:CD1	2.54	0.42
1:C:100:LYS:HD2	1:C:247:PHE:HE2	1.84	0.42
1:D:309:ALA:O	1:D:311:GLY:N	2.52	0.42
1:D:336:LYS:NZ	1:D:420:SER:CB	2.82	0.42
1:A:59:PHE:HA	1:A:216:SER:O	2.20	0.42
1:A:92:ILE:N	1:A:92:ILE:HD12	2.34	0.42
1:A:269:VAL:CG2	1:A:336:LYS:HE3	2.50	0.42
1:D:33:THR:HG21	1:D:55:ARG:CG	2.50	0.42
1:D:44:HIS:HE1	1:D:63:ASP:OD1	2.01	0.42
1:D:68:PHE:CD1	1:D:75:PHE:CD2	3.06	0.42
1:A:272:ALA:O	1:A:273:GLU:C	2.62	0.42
1:B:163:GLU:OE1	1:B:168:ILE:HG22	2.19	0.42
1:B:196:LEU:HG	1:B:218:ALA:HB3	2.01	0.42
1:B:356:THR:OG1	1:B:361:LEU:HD13	2.20	0.42
1:C:24:ILE:HG13	4:C:2709:HOH:O	2.18	0.42
1:C:267:ILE:CD1	1:C:448:TYR:HD2	2.32	0.42
1:C:372:PRO:HD2	1:C:398:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:LYS:HE2	1:D:458:VAL:CG1	2.50	0.42
1:D:138:ILE:N	1:D:138:ILE:HD12	2.35	0.42
1:D:152:ARG:HH11	1:D:152:ARG:HB2	1.85	0.42
1:A:301:GLU:O	1:A:302:ASP:CB	2.68	0.42
1:B:168:ILE:HG13	4:B:2122:HOH:O	2.18	0.42
1:B:201:VAL:O	1:B:201:VAL:HG22	2.18	0.42
1:B:220:PHE:C	1:B:221:ARG:HG2	2.45	0.42
1:B:367:LYS:C	1:B:369:PHE:H	2.27	0.42
1:B:382:GLU:O	1:B:385:GLU:HB3	2.20	0.42
1:C:65:ILE:O	1:C:69:GLU:HB2	2.20	0.42
1:C:418:ILE:HD12	1:C:419:MET:H	1.85	0.42
1:D:337:ILE:HD11	1:D:361:LEU:HD21	2.01	0.42
1:A:48:ASP:OD1	1:A:51:SER:OG	2.31	0.42
1:A:81:ASP:N	1:A:82:PRO:HD3	2.35	0.42
1:B:263:THR:HG23	1:B:444:GLU:HB3	2.02	0.42
1:B:367:LYS:O	1:B:369:PHE:N	2.53	0.42
1:C:50:ARG:HG2	1:C:50:ARG:NH1	2.34	0.42
1:C:62:ARG:NH1	1:C:219:PRO:O	2.51	0.42
1:C:325:GLU:HA	1:C:328:ARG:HB3	2.02	0.42
1:C:340:LEU:HD22	1:C:344:LEU:HG	2.02	0.42
1:C:396:ARG:HG2	1:C:396:ARG:HH11	1.83	0.42
1:D:276:ARG:O	1:D:279:TYR:HB3	2.20	0.42
1:D:403:VAL:HG21	1:D:431:ARG:NH1	2.34	0.42
1:A:43:PRO:C	1:A:45:ALA:H	2.28	0.42
1:B:99:GLU:OE1	1:B:99:GLU:CA	2.68	0.42
1:B:115:LEU:HD21	1:B:247:PHE:HE1	1.85	0.42
1:B:338:ARG:O	1:B:342:GLU:HG3	2.20	0.42
1:C:355:PHE:CD2	1:C:418:ILE:HD13	2.54	0.42
1:C:415:VAL:CG1	1:C:416:GLY:N	2.83	0.42
1:D:26:GLU:CG	1:D:27:ILE:N	2.82	0.42
1:D:57:LEU:HD22	4:D:2560:HOH:O	2.19	0.42
1:D:152:ARG:HH11	1:D:152:ARG:CB	2.33	0.42
1:D:164:PHE:O	1:D:164:PHE:HD1	2.03	0.42
1:D:395:PHE:O	1:D:397:ALA:N	2.53	0.42
1:A:340:LEU:HD22	1:A:344:LEU:HD11	2.02	0.41
1:B:360:GLU:N	1:B:362:VAL:HG22	2.35	0.41
1:B:436:LEU:HD11	1:B:447:LEU:HB2	2.02	0.41
1:C:399:VAL:O	1:C:399:VAL:HG13	2.20	0.41
1:D:26:GLU:C	1:D:27:ILE:CG2	2.92	0.41
1:D:312:TYR:O	1:D:317:TYR:HB2	2.19	0.41
1:D:368:VAL:O	1:D:368:VAL:CG1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLY:HA3	4:A:2818:HOH:O	2.19	0.41
1:A:234:ARG:HG2	1:A:234:ARG:HH11	1.85	0.41
1:A:303:PHE:O	1:A:303:PHE:CD1	2.73	0.41
1:B:405:ASP:HA	1:B:410:VAL:HG12	2.01	0.41
1:B:450:LEU:N	1:B:450:LEU:CD2	2.81	0.41
1:C:415:VAL:HG12	1:C:416:GLY:N	2.34	0.41
1:D:105:TRP:HE3	1:D:106:LEU:HD12	1.85	0.41
1:D:306:ILE:C	1:D:308:MET:H	2.28	0.41
1:D:364:ARG:HG3	1:D:368:VAL:HG21	2.01	0.41
1:D:390:PHE:CE2	1:D:398:ILE:HG12	2.55	0.41
1:D:449:GLU:HG2	1:D:451:ILE:HD11	2.02	0.41
1:A:230:ARG:HH22	3:A:6001:IPA:C3	2.33	0.41
1:A:266:ARG:HD3	1:A:451:ILE:HD12	2.02	0.41
1:A:267:ILE:HG21	1:A:339:LYS:HE2	2.03	0.41
1:A:373:ALA:O	1:A:374:ILE:HG13	2.20	0.41
1:B:31:ARG:HG3	1:B:187:GLU:HB3	2.03	0.41
1:B:137:LEU:HB2	1:B:193:PHE:CD2	2.56	0.41
1:B:389:GLY:C	1:B:394:ARG:HB3	2.43	0.41
1:C:154:GLY:C	1:C:156:PHE:H	2.29	0.41
1:B:101:ALA:HA	1:B:247:PHE:CD2	2.55	0.41
1:B:207:GLU:HG3	4:B:2032:HOH:O	2.20	0.41
1:B:327:ARG:NH1	1:B:423:GLY:H	2.17	0.41
1:C:153:LEU:O	1:C:156:PHE:HB2	2.19	0.41
1:D:283:GLU:HB3	1:D:286:TYR:CE1	2.56	0.41
1:D:418:ILE:CD1	1:D:447:LEU:HD21	2.47	0.41
1:A:60:ARG:HH21	1:A:60:ARG:HG3	1.85	0.41
1:B:67:TYR:CD1	1:B:68:PHE:N	2.89	0.41
1:B:88:PHE:HB3	1:B:156:PHE:CE1	2.55	0.41
1:B:232:ASP:OD1	1:B:234:ARG:HB2	2.20	0.41
1:B:257:LYS:HD3	1:B:257:LYS:HA	1.82	0.41
1:C:141:PRO:HD2	1:C:145:LEU:HD13	2.02	0.41
1:D:28:TYR:N	1:D:28:TYR:CD1	2.88	0.41
1:D:115:LEU:O	1:D:121:LYS:NZ	2.41	0.41
1:D:305:LYS:HE3	1:D:320:LEU:HD11	2.02	0.41
1:D:355:PHE:CG	1:D:356:THR:N	2.89	0.41
1:A:434:ARG:H	1:A:434:ARG:HG2	1.75	0.41
1:C:38:GLY:C	1:C:40:ALA:H	2.27	0.41
1:C:102:LEU:O	1:C:106:LEU:HB2	2.20	0.41
1:C:134:THR:O	1:C:135:PRO:C	2.62	0.41
1:C:257:LYS:HZ3	1:C:260:ALA:HB3	1.84	0.41
1:D:167:ARG:C	1:D:168:ILE:HG13	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HG22	1:A:25:ALA:H	1.86	0.41
1:A:122:THR:HG22	1:A:126:MET:HE2	2.03	0.41
1:B:152:ARG:NH1	4:B:2621:HOH:O	2.53	0.41
1:C:24:ILE:HB	1:C:25:ALA:H	1.66	0.41
1:D:27:ILE:HD12	1:D:79:ALA:HB2	2.03	0.41
1:D:66:GLU:C	1:D:68:PHE:H	2.29	0.41
1:A:30:GLU:CD	1:A:31:ARG:NH1	2.78	0.41
1:A:305:LYS:HG2	1:A:323:TRP:CE3	2.56	0.41
1:A:305:LYS:HE2	1:A:320:LEU:HG	2.02	0.41
1:C:56:ALA:O	1:C:57:LEU:C	2.62	0.41
1:C:337:ILE:HG21	1:C:364:ARG:HH12	1.85	0.41
1:C:405:ASP:OD1	1:C:405:ASP:N	2.54	0.41
1:C:421:GLY:O	1:C:422:SER:HB2	2.21	0.41
1:D:438:PRO:HB3	1:D:444:GLU:CA	2.22	0.41
1:A:59:PHE:CD2	1:A:214:GLN:HA	2.56	0.41
1:A:100:LYS:HZ1	1:A:104:ARG:NH2	2.16	0.41
1:A:230:ARG:C	1:A:232:ASP:H	2.29	0.41
1:A:259:LEU:HD11	1:A:262:TYR:CD2	2.56	0.41
1:A:426:ARG:HA	1:A:429:ILE:CG1	2.51	0.41
1:B:23:MET:C	1:B:25:ALA:N	2.75	0.41
1:B:102:LEU:O	1:B:106:LEU:HD22	2.20	0.41
1:B:344:LEU:HD23	1:B:352:ILE:HD11	2.03	0.41
1:B:414:ASN:HA	1:B:437:ARG:O	2.20	0.41
1:C:114:VAL:HA	1:C:225:THR:O	2.21	0.41
1:C:143:LEU:CD1	1:C:167:ARG:HD2	2.48	0.41
1:C:224:LEU:O	1:C:225:THR:HB	2.21	0.41
1:C:284:LYS:HG2	4:C:2887:HOH:O	2.20	0.41
1:C:337:ILE:HG21	1:C:364:ARG:NH1	2.36	0.41
1:C:358:HIS:CD2	1:C:361:LEU:H	2.36	0.41
1:C:361:LEU:HD13	1:C:365:ILE:HD12	2.02	0.41
1:D:46:LYS:HE3	1:D:55:ARG:O	2.20	0.41
1:D:68:PHE:HD2	1:D:68:PHE:HA	1.72	0.41
1:D:282:ARG:NH1	1:D:322:ALA:HA	2.35	0.41
1:A:71:ASN:O	1:A:72:GLY:C	2.63	0.41
1:A:74:GLU:OE2	1:A:74:GLU:CA	2.66	0.41
1:A:149:TRP:CD1	1:A:152:ARG:HH12	2.38	0.41
1:A:204:LEU:HD23	1:A:242:VAL:HG21	2.03	0.41
1:B:427:GLU:HG2	1:B:428:TYR:N	2.36	0.41
1:C:61:TYR:C	1:C:61:TYR:CD1	2.99	0.41
1:C:165:SER:HB2	4:C:2529:HOH:O	2.21	0.41
1:C:331:PHE:CD1	1:C:358:HIS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:LEU:HD22	1:C:344:LEU:HD11	2.03	0.41
1:C:361:LEU:HD13	1:C:361:LEU:C	2.45	0.41
1:D:29:TYR:HB2	1:D:79:ALA:HB1	2.01	0.41
1:D:67:TYR:CD1	1:D:67:TYR:O	2.74	0.41
1:D:167:ARG:O	1:D:168:ILE:HG12	2.21	0.41
1:D:264:ILE:HG22	1:D:265:LYS:N	2.35	0.41
1:A:29:TYR:N	1:A:79:ALA:HA	2.36	0.40
1:A:344:LEU:HD12	1:A:369:PHE:CE2	2.56	0.40
1:B:285:VAL:HG11	1:B:322:ALA:HB2	2.03	0.40
1:C:354:ILE:HG23	1:C:399:VAL:HA	2.03	0.40
1:C:412:ASP:HB2	1:C:437:ARG:CD	2.47	0.40
1:D:226:ALA:HB2	4:D:2283:HOH:O	2.20	0.40
1:A:140:VAL:HG21	1:A:146:ALA:HB2	2.03	0.40
1:A:385:GLU:O	1:A:386:ILE:C	2.64	0.40
1:C:340:LEU:HD22	1:C:344:LEU:CD1	2.51	0.40
1:C:389:GLY:HA3	1:C:395:PHE:CZ	2.57	0.40
1:D:227:THR:CG2	4:D:2756:HOH:O	2.69	0.40
1:D:405:ASP:C	1:D:410:VAL:HG11	2.46	0.40
1:B:92:ILE:N	1:B:92:ILE:HD12	2.35	0.40
1:C:68:PHE:HB3	1:C:75:PHE:CE2	2.56	0.40
1:D:264:ILE:HG23	1:D:447:LEU:HD22	2.03	0.40
1:D:340:LEU:HA	1:D:343:ILE:HD11	2.01	0.40
1:D:361:LEU:HD13	1:D:365:ILE:CG1	2.51	0.40
1:A:303:PHE:O	1:A:303:PHE:HD1	2.04	0.40
1:B:122:THR:HG21	1:B:152:ARG:NE	2.36	0.40
1:B:340:LEU:O	1:B:341:ARG:C	2.65	0.40
1:C:409:ASP:O	1:C:410:VAL:HB	2.21	0.40
1:C:441:GLY:HA3	4:C:3007:HOH:O	2.22	0.40
1:D:40:ALA:O	1:D:41:HIS:C	2.62	0.40
1:D:250:PHE:HA	1:D:251:PRO:HD3	1.91	0.40
1:D:330:ALA:O	1:D:331:PHE:C	2.64	0.40
1:D:372:PRO:CG	1:D:398:ILE:HG22	2.51	0.40
1:A:65:ILE:HD13	1:A:65:ILE:HA	1.93	0.40
1:B:234:ARG:C	1:B:236:GLU:H	2.29	0.40
1:C:262:TYR:HE1	1:C:264:ILE:HD11	1.86	0.40
1:D:35:VAL:HG22	1:D:55:ARG:HG3	2.03	0.40
1:D:97:TYR:HE1	1:D:259:LEU:HD21	1.86	0.40
1:D:140:VAL:HG22	1:D:177:SER:O	2.22	0.40
1:D:371:ILE:HA	1:D:372:PRO:HD3	1.94	0.40

All (4) 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)
4:A:2319:HOH:O	4:B:2932:HOH:O[1_455]	1.98	0.22
4:B:2454:HOH:O	4:B:2522:HOH:O[1_655]	2.16	0.04
4:B:2433:HOH:O	4:B:2745:HOH:O[1_455]	2.18	0.02
4:D:2465:HOH:O	4:D:2580:HOH:O[1_655]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	432/472 (92%)	343 (79%)	67 (16%)	22 (5%)	1	2
1	B	415/472 (88%)	341 (82%)	57 (14%)	17 (4%)	2	3
1	C	410/472 (87%)	304 (74%)	64 (16%)	42 (10%)	0	0
1	D	422/472 (89%)	313 (74%)	77 (18%)	32 (8%)	1	1
All	All	1679/1888 (89%)	1301 (78%)	265 (16%)	113 (7%)	1	1

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	LEU
1	A	297	LEU
1	A	307	VAL
1	A	313	ASP
1	A	331	PHE
1	A	440	LYS
1	A	455	THR
1	B	23	MET
1	B	302	ASP
1	B	333	SER
1	B	375	THR
1	B	438	PRO
1	B	443	LYS
1	C	24	ILE

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Mol	Chain	Res	Type
1	C	47	PHE
1	C	61	TYR
1	C	69	GLU
1	C	73	ILE
1	C	255	ALA
1	C	258	HIS
1	C	274	ASP
1	C	284	LYS
1	C	295	ILE
1	C	348	ARG
1	C	379	SER
1	C	394	ARG
1	C	395	PHE
1	C	406	GLU
1	C	408	ILE
1	D	39	ASP
1	D	48	ASP
1	D	346	ARG
1	D	372	PRO
1	D	396	ARG
1	D	410	VAL
1	D	442	LYS
1	A	291	ARG
1	A	294	GLY
1	A	314	GLU
1	A	374	ILE
1	A	378	THR
1	A	379	SER
1	A	394	ARG
1	A	411	PRO
1	B	25	ALA
1	B	360	GLU
1	B	409	ASP
1	B	412	ASP
1	C	25	ALA
1	C	51	SER
1	C	68	PHE
1	C	273	GLU
1	C	282	ARG
1	C	368	VAL
1	C	393	GLY
1	C	419	MET

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Mol	Chain	Res	Type
1	C	420	SER
1	C	426	ARG
1	D	52	GLY
1	D	67	TYR
1	D	72	GLY
1	D	281	LYS
1	D	293	ARG
1	D	310	SER
1	D	319	ALA
1	D	374	ILE
1	D	408	ILE
1	D	458	VAL
1	A	290	LEU
1	A	330	ALA
1	A	444	GLU
1	B	380	ARG
1	C	96	ASP
1	C	131	GLU
1	C	291	ARG
1	C	367	LYS
1	C	443	LYS
1	D	86	PRO
1	D	257	LYS
1	D	426	ARG
1	A	273	GLU
1	A	410	VAL
1	B	397	ALA
1	C	42	VAL
1	C	45	ALA
1	C	53	THR
1	C	333	SER
1	C	371	ILE
1	C	410	VAL
1	D	41	HIS
1	D	46	LYS
1	D	49	SER
1	B	379	SER
1	B	442	LYS
1	C	440	LYS
1	D	259	LEU
1	D	307	VAL
1	D	369	PHE

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Mol	Chain	Res	Type
1	D	407	GLY
1	D	457	GLU
1	A	383	ARG
1	B	374	ILE
1	C	287	LYS
1	C	370	LEU
1	C	403	VAL
1	B	24	ILE
1	D	242	VAL
1	D	306	ILE
1	B	362	VAL
1	A	306	ILE
1	C	417	VAL
1	D	251	PRO
1	D	368	VAL

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	366/398 (92%)	334 (91%)	32 (9%)	9	21
1	B	357/398 (90%)	334 (94%)	23 (6%)	16	35
1	C	343/398 (86%)	322 (94%)	21 (6%)	17	37
1	D	349/398 (88%)	315 (90%)	34 (10%)	8	17
All	All	1415/1592 (89%)	1305 (92%)	110 (8%)	11	26

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	69	GLU
1	A	87	TYR
1	A	106	LEU
1	A	113	ILE
1	A	133	SER

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Mol	Chain	Res	Type
1	A	137	LEU
1	A	153	LEU
1	A	191	ASN
1	A	195	LEU
1	A	221	ARG
1	A	227	THR
1	A	229	GLU
1	A	231	GLU
1	A	259	LEU
1	A	269	VAL
1	A	273	GLU
1	A	296	THR
1	A	308	MET
1	A	314	GLU
1	A	321	ARG
1	A	340	LEU
1	A	351	LYS
1	A	352	ILE
1	A	358	HIS
1	A	367	LYS
1	A	386	ILE
1	A	398	ILE
1	A	411	PRO
1	A	414	ASN
1	A	431	ARG
1	A	442	LYS
1	B	31	ARG
1	B	67	TYR
1	B	106	LEU
1	B	134	THR
1	B	138	ILE
1	B	153	LEU
1	B	195	LEU
1	B	227	THR
1	B	232	ASP
1	B	237	ILE
1	B	249	LEU
1	B	252	ASP
1	B	273	GLU
1	B	318	GLU
1	B	345	GLU
1	B	350	ASP

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Mol	Chain	Res	Type
1	B	351	LYS
1	B	362	VAL
1	B	404	LEU
1	B	430	GLN
1	B	432	LEU
1	B	437	ARG
1	B	450	LEU
1	C	24	ILE
1	C	54	TYR
1	C	87	TYR
1	C	93	SER
1	C	106	LEU
1	C	134	THR
1	C	172	LYS
1	C	195	LEU
1	C	207	GLU
1	C	269	VAL
1	C	323	TRP
1	C	331	PHE
1	C	338	ARG
1	C	340	LEU
1	C	354	ILE
1	C	356	THR
1	C	369	PHE
1	C	381	GLU
1	C	418	ILE
1	C	426	ARG
1	C	432	LEU
1	D	27	ILE
1	D	57	LEU
1	D	68	PHE
1	D	100	LYS
1	D	114	VAL
1	D	152	ARG
1	D	155	ILE
1	D	195	LEU
1	D	221	ARG
1	D	229	GLU
1	D	232	ASP
1	D	239	LYS
1	D	274	ASP
1	D	290	LEU

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Mol	Chain	Res	Type
1	D	305	LYS
1	D	306	ILE
1	D	328	ARG
1	D	329	ILE
1	D	346	ARG
1	D	352	ILE
1	D	356	THR
1	D	357	ARG
1	D	358	HIS
1	D	361	LEU
1	D	367	LYS
1	D	370	LEU
1	D	392	THR
1	D	403	VAL
1	D	404	LEU
1	D	405	ASP
1	D	409	ASP
1	D	414	ASN
1	D	440	LYS
1	D	453	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	44	HIS
1	A	78	ASN
1	A	130	ASN
1	A	185	ASN
1	A	191	ASN
1	A	211	GLN
1	A	214	GLN
1	A	304	ASN
1	B	22	GLN
1	B	44	HIS
1	B	71	ASN
1	B	130	ASN
1	B	185	ASN
1	B	214	GLN
1	B	430	GLN
1	C	71	ASN
1	C	78	ASN

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Mol	Chain	Res	Type
1	C	98	GLN
1	C	148	GLN
1	C	332	ASN
1	C	402	GLN
1	D	78	ASN
1	D	185	ASN
1	D	211	GLN
1	D	335	ASN
1	D	359	ASN
1	D	402	GLN

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 ⓘ

11 ligands 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	$\# Z > 2$
3	IPA	A	6001	-	3,3,3	0.45	0	3,3,3	0.38	0
3	IPA	A	6002	-	3,3,3	0.44	0	3,3,3	0.38	0
2	PO4	D	4006	-	4,4,4	1.66	0	6,6,6	0.51	0
3	IPA	A	6003	-	3,3,3	0.40	0	3,3,3	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	D	4005	-	4,4,4	1.69	0	6,6,6	0.46	0
2	PO4	D	4004	-	4,4,4	1.87	3 (75%)	6,6,6	0.46	0
2	PO4	B	4007	-	4,4,4	1.76	2 (50%)	6,6,6	0.45	0
2	PO4	A	4001	-	4,4,4	1.72	1 (25%)	6,6,6	0.46	0
2	PO4	B	4008	-	4,4,4	1.71	1 (25%)	6,6,6	0.43	0
2	PO4	B	4002	-	4,4,4	1.74	1 (25%)	6,6,6	0.45	0
2	PO4	C	4003	-	4,4,4	1.81	2 (50%)	6,6,6	0.45	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4004	PO4	P-O4	-2.15	1.48	1.54
2	B	4008	PO4	P-O3	-2.13	1.48	1.54
2	A	4001	PO4	P-O2	-2.13	1.48	1.54
2	D	4004	PO4	P-O2	-2.10	1.48	1.54
2	D	4004	PO4	P-O3	-2.07	1.48	1.54
2	C	4003	PO4	P-O3	-2.06	1.48	1.54
2	B	4002	PO4	P-O3	-2.05	1.48	1.54
2	C	4003	PO4	P-O2	-2.05	1.48	1.54
2	B	4007	PO4	P-O2	-2.01	1.48	1.54
2	B	4007	PO4	P-O4	-2.01	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.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	6001	IPA	3	0
3	A	6002	IPA	3	0
2	B	4002	PO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	434/472 (91%)	-0.03	9 (2%) 63 58	12, 46, 121, 131	0
1	B	423/472 (89%)	-0.08	6 (1%) 73 69	11, 47, 122, 129	0
1	C	414/472 (87%)	0.14	7 (1%) 69 64	19, 68, 120, 132	0
1	D	428/472 (90%)	0.25	11 (2%) 57 51	18, 70, 123, 131	0
All	All	1699/1888 (89%)	0.07	33 (1%) 66 61	11, 58, 122, 132	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	403	VAL	3.3
1	D	312	TYR	2.9
1	C	454	GLY	2.8
1	D	52	GLY	2.7
1	C	279	TYR	2.7
1	D	260	ALA	2.6
1	A	296	THR	2.6
1	D	295	ILE	2.6
1	C	24	ILE	2.6
1	C	408	ILE	2.6
1	C	322	ALA	2.5
1	D	316	ALA	2.5
1	B	373	ALA	2.5
1	D	256	GLY	2.4
1	A	320	LEU	2.3
1	D	320	LEU	2.3
1	B	258	HIS	2.3
1	A	290	LEU	2.3
1	D	319	ALA	2.3
1	A	456	GLY	2.3
1	A	398	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	290	LEU	2.3
1	A	390	PHE	2.2
1	D	329	ILE	2.2
1	A	330	ALA	2.2
1	A	297	LEU	2.1
1	B	398	ILE	2.1
1	D	38	GLY	2.1
1	D	403	VAL	2.1
1	C	371	ILE	2.0
1	B	399	VAL	2.0
1	B	303	PHE	2.0
1	A	295	ILE	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($\text{\AA}^2$)	Q<0.9
2	PO4	A	4001	5/5	0.77	0.13	85,86,87,87	0
3	IPA	A	6003	4/4	0.81	0.13	58,59,59,60	0
3	IPA	A	6002	4/4	0.85	0.14	40,41,41,41	0
2	PO4	B	4008	5/5	0.86	0.13	82,83,84,84	0
2	PO4	D	4005	5/5	0.88	0.15	113,114,114,114	0
2	PO4	D	4006	5/5	0.88	0.13	75,75,76,77	0
2	PO4	C	4003	5/5	0.89	0.09	89,89,90,90	0
3	IPA	A	6001	4/4	0.89	0.12	44,44,45,45	0
2	PO4	D	4004	5/5	0.91	0.08	65,65,66,67	0
2	PO4	B	4002	5/5	0.91	0.09	64,67,67,68	0
2	PO4	B	4007	5/5	0.93	0.15	88,89,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.