Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 11:51 AM EST

PDB ID	:	1BRL
Title	:	THREE-DIMENSIONAL STRUCTURE OF BACTERIAL LUCIFERASE FROM VIBRIO HARVEYI AT 2.4 ANGSTROMS RESOLUTION
Authors	:	Fisher, A.J.; Rayment, I.
Deposited on	:	1995-03-20
Resolution	:	2.40 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:

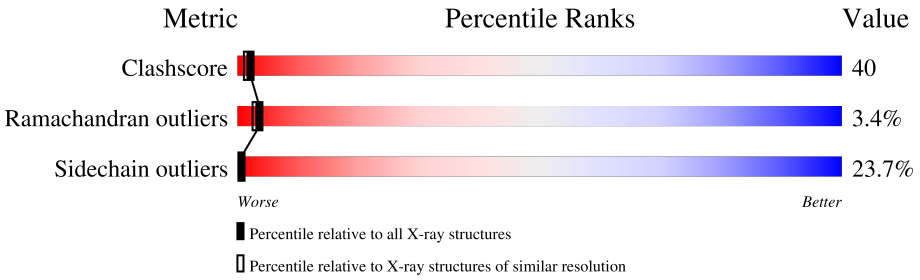
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	355	28% 43% 21%
1	C	355	29% 42% 21%
2	B	324	37% 43% 16%
2	D	324	38% 41% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	356	-	X	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10432 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.

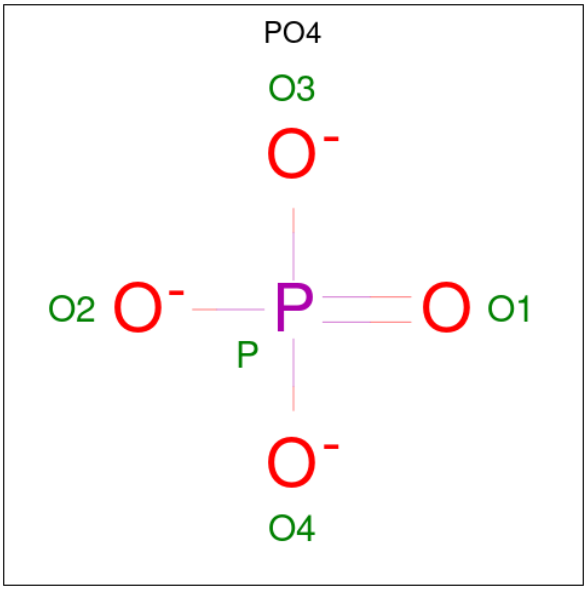
- Molecule 1 is a protein called BACTERIAL LUCIFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2679	1694	447	521	17			
1	C	340	Total	C	N	O	S	0	0	0
			2679	1694	447	521	17			

- Molecule 2 is a protein called BACTERIAL LUCIFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	319	Total	C	N	O	S	0	0	0
			2498	1572	427	484	15			
2	D	319	Total	C	N	O	S	0	0	0
			2498	1572	427	484	15			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	28	Total O 28 28	0	0
4	B	45	Total O 45 45	0	0

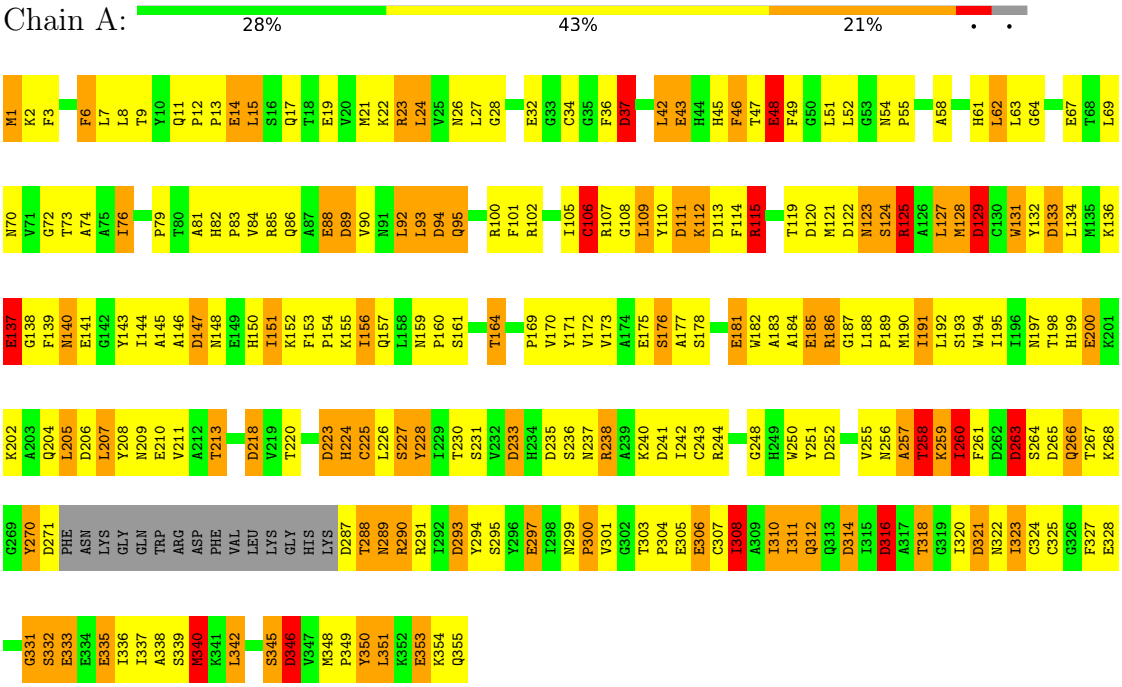
3 Residue-property plots (i)

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

Note EDS was not executed.

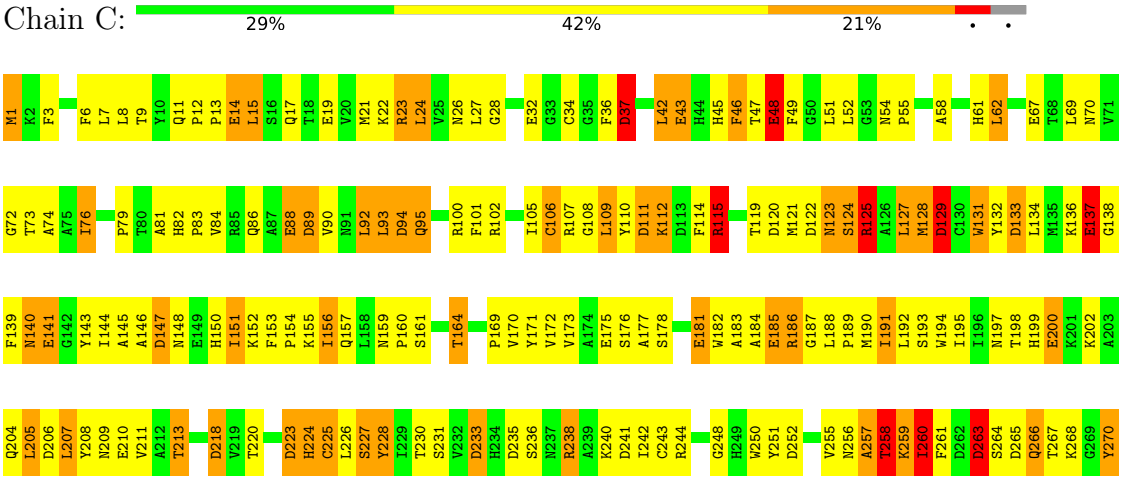
• Molecule 1: BACTERIAL LUCIFERASE

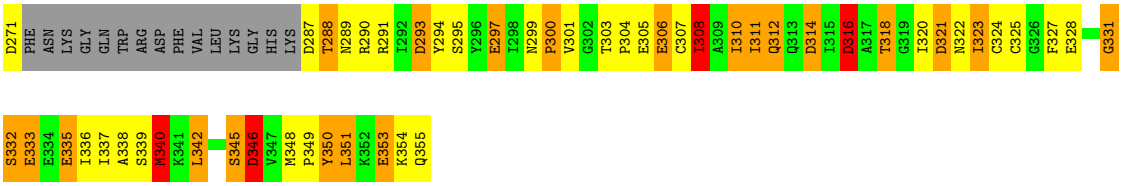
Chain A:



• Molecule 1: BACTERIAL LUCIFERASE

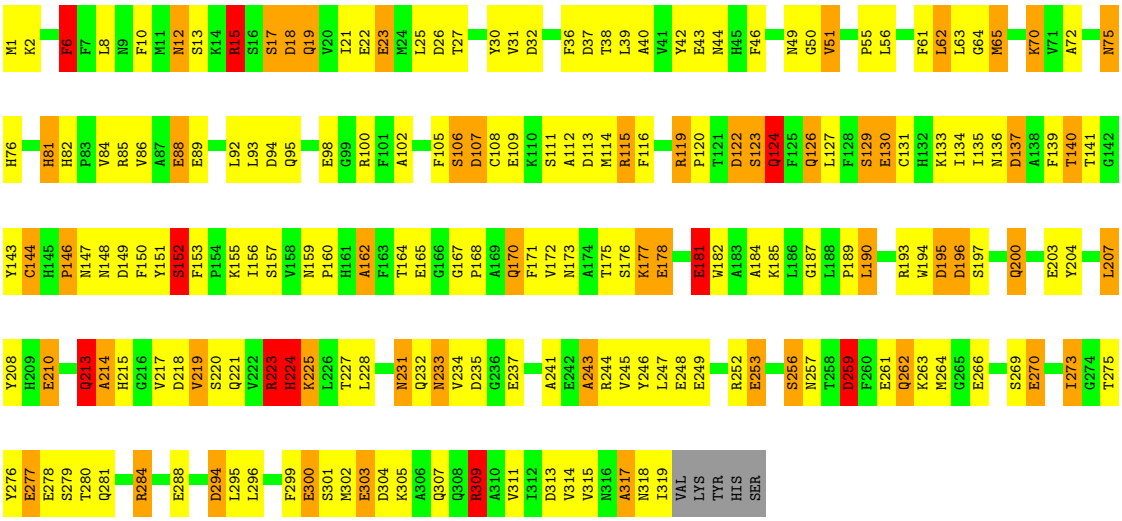
Chain C:





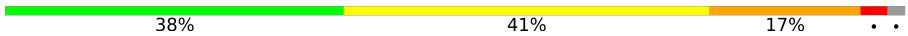
• Molecule 2: BACTERIAL LUCIFERASE

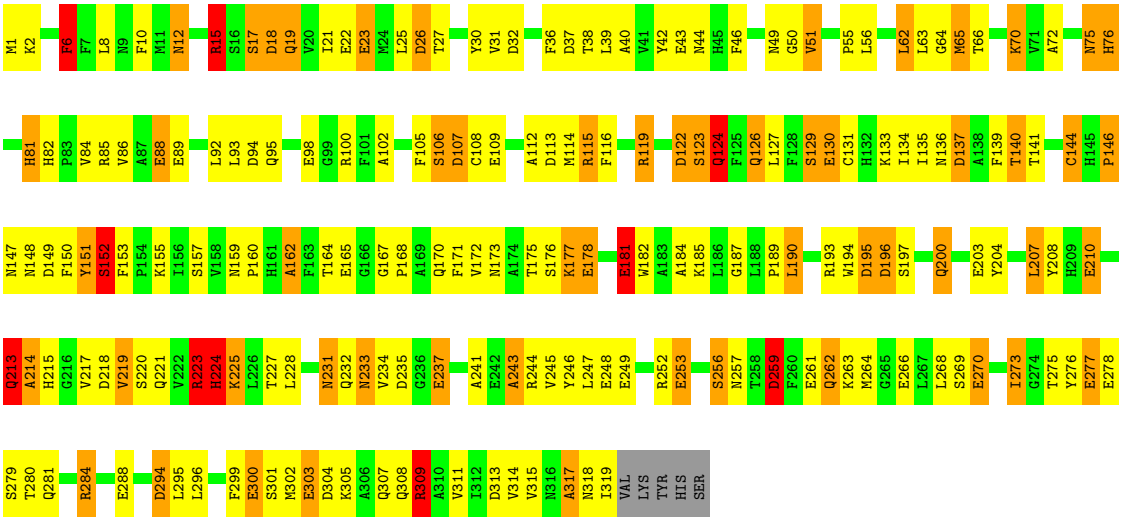
Chain B:



• Molecule 2: BACTERIAL LUCIFERASE

Chain D:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.90Å 112.70Å 301.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.40)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10432	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.12	22/2740 (0.8%)	1.63	52/3716 (1.4%)
1	C	1.12	22/2740 (0.8%)	1.63	51/3716 (1.4%)
2	B	1.12	22/2552 (0.9%)	1.62	44/3457 (1.3%)
2	D	1.12	22/2552 (0.9%)	1.62	45/3457 (1.3%)
All	All	1.12	88/10584 (0.8%)	1.62	192/14346 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	2	0
2	D	2	0
All	All	4	0

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	200	GLU	CD-OE1	7.93	1.34	1.25
1	A	200	GLU	CD-OE1	7.90	1.34	1.25
1	C	48	GLU	CD-OE1	7.78	1.34	1.25
1	A	48	GLU	CD-OE1	7.76	1.34	1.25
1	A	32	GLU	CD-OE2	7.39	1.33	1.25
1	C	32	GLU	CD-OE2	7.35	1.33	1.25
2	D	181	GLU	CD-OE2	7.31	1.33	1.25
2	B	181	GLU	CD-OE2	7.22	1.33	1.25
1	A	333	GLU	CD-OE2	7.20	1.33	1.25
1	C	333	GLU	CD-OE2	7.20	1.33	1.25
1	A	67	GLU	CD-OE2	7.09	1.33	1.25
1	C	67	GLU	CD-OE2	7.08	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	GLU	CD-OE2	6.99	1.33	1.25
1	C	210	GLU	CD-OE2	6.95	1.33	1.25
2	D	130	GLU	CD-OE1	6.86	1.33	1.25
2	B	130	GLU	CD-OE1	6.85	1.33	1.25
1	C	175	GLU	CD-OE2	6.75	1.33	1.25
1	A	175	GLU	CD-OE2	6.74	1.33	1.25
2	B	165	GLU	CD-OE1	6.69	1.33	1.25
2	D	165	GLU	CD-OE1	6.65	1.32	1.25
1	A	181	GLU	CD-OE1	6.65	1.32	1.25
1	C	181	GLU	CD-OE1	6.61	1.32	1.25
2	B	23	GLU	CD-OE2	6.60	1.32	1.25
2	D	23	GLU	CD-OE2	6.57	1.32	1.25
2	D	288	GLU	CD-OE1	6.50	1.32	1.25
2	B	288	GLU	CD-OE1	6.45	1.32	1.25
1	C	297	GLU	CD-OE2	6.44	1.32	1.25
1	A	305	GLU	CD-OE1	6.43	1.32	1.25
2	B	98	GLU	CD-OE1	6.43	1.32	1.25
1	A	297	GLU	CD-OE2	6.43	1.32	1.25
1	C	305	GLU	CD-OE1	6.42	1.32	1.25
2	D	98	GLU	CD-OE1	6.41	1.32	1.25
1	A	141	GLU	CD-OE2	6.37	1.32	1.25
2	B	277	GLU	CD-OE2	6.36	1.32	1.25
2	D	277	GLU	CD-OE2	6.34	1.32	1.25
1	C	141	GLU	CD-OE2	6.34	1.32	1.25
1	C	14	GLU	CD-OE1	6.31	1.32	1.25
1	A	14	GLU	CD-OE1	6.26	1.32	1.25
2	D	22	GLU	CD-OE1	6.26	1.32	1.25
2	B	22	GLU	CD-OE1	6.26	1.32	1.25
2	B	303	GLU	CD-OE2	6.21	1.32	1.25
2	D	303	GLU	CD-OE2	6.17	1.32	1.25
2	D	109	GLU	CD-OE1	6.16	1.32	1.25
2	D	178	GLU	CD-OE1	6.15	1.32	1.25
2	B	109	GLU	CD-OE1	6.12	1.32	1.25
1	C	353	GLU	CD-OE2	6.11	1.32	1.25
2	B	178	GLU	CD-OE1	6.11	1.32	1.25
1	A	328	GLU	CD-OE2	6.07	1.32	1.25
1	C	328	GLU	CD-OE2	6.07	1.32	1.25
2	D	210	GLU	CD-OE2	6.04	1.32	1.25
1	A	306	GLU	CD-OE2	6.04	1.32	1.25
1	C	306	GLU	CD-OE2	6.03	1.32	1.25
2	B	210	GLU	CD-OE2	6.03	1.32	1.25
1	A	353	GLU	CD-OE2	6.02	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	88	GLU	CD-OE1	5.99	1.32	1.25
1	A	88	GLU	CD-OE1	5.96	1.32	1.25
1	A	185	GLU	CD-OE2	5.87	1.32	1.25
1	A	115	ARG	NE-CZ	5.87	1.40	1.33
2	D	203	GLU	CD-OE2	5.86	1.32	1.25
2	B	203	GLU	CD-OE2	5.86	1.32	1.25
1	C	185	GLU	CD-OE2	5.86	1.32	1.25
1	C	115	ARG	NE-CZ	5.84	1.40	1.33
2	B	249	GLU	CD-OE1	5.81	1.32	1.25
2	D	249	GLU	CD-OE1	5.79	1.32	1.25
2	B	237	GLU	CD-OE1	5.71	1.31	1.25
2	D	237	GLU	CD-OE1	5.69	1.31	1.25
2	B	88	GLU	CD-OE1	5.63	1.31	1.25
2	D	88	GLU	CD-OE1	5.62	1.31	1.25
2	D	248	GLU	CD-OE1	5.57	1.31	1.25
1	C	43	GLU	CD-OE1	5.51	1.31	1.25
1	C	137	GLU	CD-OE2	5.51	1.31	1.25
2	B	248	GLU	CD-OE1	5.48	1.31	1.25
1	A	137	GLU	CD-OE2	5.47	1.31	1.25
2	B	270	GLU	CD-OE2	5.47	1.31	1.25
1	A	43	GLU	CD-OE1	5.47	1.31	1.25
2	D	270	GLU	CD-OE2	5.44	1.31	1.25
1	C	335	GLU	CD-OE2	5.35	1.31	1.25
2	D	266	GLU	CD-OE1	5.34	1.31	1.25
2	B	266	GLU	CD-OE1	5.33	1.31	1.25
1	C	19	GLU	CD-OE2	5.32	1.31	1.25
1	A	19	GLU	CD-OE2	5.30	1.31	1.25
1	A	335	GLU	CD-OE2	5.29	1.31	1.25
2	B	278	GLU	CD-OE2	5.29	1.31	1.25
2	D	278	GLU	CD-OE2	5.26	1.31	1.25
2	B	300	GLU	CD-OE1	5.12	1.31	1.25
2	B	253	GLU	CD-OE1	5.05	1.31	1.25
2	D	300	GLU	CD-OE1	5.05	1.31	1.25
2	D	253	GLU	CD-OE1	5.03	1.31	1.25

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	294	ASP	CB-CG-OD1	-10.15	109.16	118.30
2	D	294	ASP	CB-CG-OD1	-10.13	109.18	118.30
1	A	252	ASP	CB-CG-OD1	-8.74	110.43	118.30
1	C	252	ASP	CB-CG-OD1	-8.72	110.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	313	ASP	CB-CG-OD1	-8.54	110.61	118.30
2	D	313	ASP	CB-CG-OD1	-8.53	110.62	118.30
2	D	152	SER	N-CA-CB	8.11	122.66	110.50
2	B	152	SER	N-CA-CB	8.09	122.64	110.50
2	B	317	ALA	N-CA-CB	8.02	121.33	110.10
2	D	317	ALA	N-CA-CB	7.98	121.27	110.10
1	C	235	ASP	CB-CG-OD1	-7.88	111.21	118.30
1	A	235	ASP	CB-CG-OD1	-7.85	111.24	118.30
1	A	111	ASP	CB-CG-OD2	-7.67	111.39	118.30
1	C	111	ASP	CB-CG-OD2	-7.67	111.39	118.30
1	C	235	ASP	CB-CG-OD2	7.54	125.09	118.30
2	D	259	ASP	N-CA-CB	7.52	124.14	110.60
1	A	235	ASP	CB-CG-OD2	7.51	125.06	118.30
2	B	259	ASP	N-CA-CB	7.51	124.11	110.60
1	A	206	ASP	CB-CG-OD1	-7.44	111.61	118.30
2	B	26	ASP	CB-CG-OD1	-7.43	111.61	118.30
2	D	26	ASP	CB-CG-OD1	-7.42	111.63	118.30
1	C	206	ASP	CB-CG-OD1	-7.39	111.65	118.30
2	B	32	ASP	CB-CG-OD1	-7.37	111.67	118.30
2	D	32	ASP	CB-CG-OD1	-7.36	111.68	118.30
2	B	235	ASP	CB-CG-OD2	-7.29	111.74	118.30
2	D	235	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	C	293	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	A	293	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	314	ASP	CB-CG-OD2	-7.17	111.84	118.30
2	B	122	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	233	ASP	CB-CG-OD1	7.17	124.75	118.30
1	C	100	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	C	233	ASP	CB-CG-OD1	7.16	124.75	118.30
1	A	100	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	C	314	ASP	CB-CG-OD2	-7.14	111.87	118.30
2	D	122	ASP	CB-CG-OD1	7.12	124.71	118.30
1	C	218	ASP	CB-CG-OD1	-7.10	111.91	118.30
1	A	233	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	218	ASP	CB-CG-OD1	-7.07	111.94	118.30
1	C	233	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	C	346	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	A	74	ALA	C-N-CA	-7.01	104.19	121.70
1	A	346	ASP	CB-CG-OD1	-7.01	112.00	118.30
2	D	294	ASP	CB-CG-OD2	6.99	124.59	118.30
1	C	74	ALA	C-N-CA	-6.99	104.24	121.70
2	B	294	ASP	CB-CG-OD2	6.98	124.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	228	TYR	CB-CA-C	-6.98	96.44	110.40
1	C	228	TYR	CB-CA-C	-6.95	96.50	110.40
1	A	198	THR	CA-CB-CG2	-6.95	102.68	112.40
1	C	198	THR	CA-CB-CG2	-6.95	102.68	112.40
2	D	195	ASP	CB-CG-OD2	6.94	124.54	118.30
2	B	195	ASP	CB-CG-OD2	6.93	124.54	118.30
2	D	195	ASP	CB-CG-OD1	-6.89	112.10	118.30
2	B	195	ASP	CB-CG-OD1	-6.87	112.12	118.30
2	D	252	ARG	NE-CZ-NH1	6.84	123.72	120.30
2	D	196	ASP	CB-CG-OD2	-6.82	112.16	118.30
2	B	252	ARG	NE-CZ-NH1	6.81	123.70	120.30
2	B	196	ASP	CB-CG-OD2	-6.81	112.17	118.30
2	D	284	ARG	CB-CA-C	6.76	123.93	110.40
2	B	284	ARG	CB-CA-C	6.76	123.92	110.40
1	A	316	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	C	316	ASP	CB-CG-OD2	-6.74	112.23	118.30
2	D	122	ASP	CB-CG-OD2	-6.66	112.31	118.30
2	B	122	ASP	CB-CG-OD2	-6.64	112.32	118.30
2	B	15	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	D	15	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	B	162	ALA	N-CA-CB	6.45	119.13	110.10
2	D	162	ALA	N-CA-CB	6.45	119.12	110.10
1	C	346	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	346	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	238	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	C	238	ARG	NE-CZ-NH1	6.39	123.50	120.30
2	D	304	ASP	CB-CG-OD2	-6.33	112.61	118.30
2	D	94	ASP	CB-CG-OD1	-6.32	112.61	118.30
2	B	94	ASP	CB-CG-OD1	-6.30	112.63	118.30
2	B	235	ASP	CB-CG-OD1	6.29	123.96	118.30
2	B	75	ASN	N-CA-CB	-6.28	99.29	110.60
2	B	304	ASP	CB-CG-OD2	-6.28	112.64	118.30
2	D	75	ASN	N-CA-CB	-6.28	99.30	110.60
2	D	235	ASP	CB-CG-OD1	6.26	123.94	118.30
1	C	321	ASP	CB-CG-OD1	-6.26	112.66	118.30
1	A	321	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	A	146	ALA	CB-CA-C	6.08	119.22	110.10
2	B	107	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	C	146	ALA	CB-CA-C	6.08	119.22	110.10
1	C	258	THR	CB-CA-C	6.07	127.98	111.60
2	D	107	ASP	CB-CG-OD1	-6.06	112.84	118.30
1	C	89	ASP	CB-CG-OD2	-6.06	112.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	THR	CB-CA-C	6.05	127.94	111.60
1	A	89	ASP	CB-CG-OD2	-6.04	112.87	118.30
2	D	224	HIS	C-N-CA	-6.03	106.62	121.70
2	B	224	HIS	C-N-CA	-6.01	106.67	121.70
1	A	206	ASP	CB-CG-OD2	6.00	123.69	118.30
1	C	206	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	100	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	94	ASP	CB-CG-OD1	-5.94	112.95	118.30
2	D	304	ASP	CB-CG-OD1	5.93	123.63	118.30
2	B	304	ASP	CB-CG-OD1	5.92	123.63	118.30
1	C	94	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	C	129	ASP	CB-CG-OD1	-5.90	112.99	118.30
2	B	113	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	100	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	129	ASP	CB-CG-OD1	-5.87	113.02	118.30
2	B	171	PHE	N-CA-CB	5.87	121.16	110.60
2	D	171	PHE	N-CA-CB	5.86	121.14	110.60
1	C	223	ASP	CB-CG-OD2	-5.82	113.06	118.30
2	D	113	ASP	CB-CG-OD2	-5.82	113.07	118.30
1	A	223	ASP	CB-CG-OD2	-5.79	113.09	118.30
2	B	317	ALA	CB-CA-C	5.77	118.76	110.10
2	D	317	ALA	CB-CA-C	5.77	118.75	110.10
1	C	263	ASP	N-CA-C	5.75	126.54	111.00
1	A	263	ASP	N-CA-C	5.74	126.51	111.00
1	C	271	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	A	133	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	A	271	ASP	CB-CG-OD1	-5.66	113.20	118.30
1	A	115	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	271	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	133	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	C	115	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	271	ASP	CB-CG-OD2	5.59	123.33	118.30
2	D	309	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	125	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	B	81	HIS	CA-CB-CG	5.56	123.06	113.60
2	B	309	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	D	81	HIS	CA-CB-CG	5.54	123.01	113.60
1	C	125	ARG	NE-CZ-NH1	5.53	123.06	120.30
2	D	15	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	321	ASP	CB-CG-OD2	5.50	123.25	118.30
2	B	15	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	218	ASP	CB-CG-OD2	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	218	ASP	CB-CG-OD2	5.48	123.23	118.30
2	D	107	ASP	CB-CG-OD2	5.47	123.22	118.30
2	B	137	ASP	CB-CG-OD2	-5.47	113.38	118.30
2	D	137	ASP	CB-CG-OD2	-5.47	113.38	118.30
2	B	107	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	321	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	258	THR	CA-CB-CG2	-5.44	104.79	112.40
1	C	37	ASP	CB-CG-OD2	-5.44	113.41	118.30
2	B	223	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	258	THR	CA-CB-CG2	-5.43	104.80	112.40
2	D	223	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	263	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	37	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	A	263	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	252	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	316	ASP	CB-CG-OD1	5.37	123.13	118.30
2	B	141	THR	N-CA-CB	-5.36	100.12	110.30
1	C	316	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	248	GLY	N-CA-C	-5.35	99.73	113.10
2	D	141	THR	N-CA-CB	-5.34	100.15	110.30
1	C	248	GLY	N-CA-C	-5.34	99.76	113.10
1	C	257	ALA	CB-CA-C	5.33	118.10	110.10
2	B	313	ASP	CB-CG-OD2	5.33	123.09	118.30
1	C	252	ASP	CB-CG-OD2	5.33	123.09	118.30
2	D	313	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	257	ALA	CB-CA-C	5.30	118.06	110.10
1	A	223	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	223	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	340	MET	N-CA-CB	5.29	120.12	110.60
2	B	18	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	A	308	ILE	CB-CA-C	-5.28	101.03	111.60
2	D	18	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	C	308	ILE	CB-CA-C	-5.28	101.04	111.60
1	A	340	MET	N-CA-CB	5.28	120.10	110.60
1	A	122	ASP	CB-CG-OD1	-5.21	113.61	118.30
2	D	237	GLU	N-CA-CB	5.18	119.93	110.60
2	B	76	HIS	CA-CB-CG	-5.18	104.80	113.60
2	D	243	ALA	N-CA-CB	-5.17	102.86	110.10
2	B	237	GLU	N-CA-CB	5.17	119.91	110.60
1	C	264	SER	N-CA-CB	5.17	118.26	110.50
2	D	76	HIS	CA-CB-CG	-5.17	104.81	113.60
2	B	243	ALA	N-CA-CB	-5.17	102.86	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	86	VAL	CA-CB-CG1	-5.16	103.16	110.90
1	C	122	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	D	86	VAL	CA-CB-CG1	-5.14	103.18	110.90
1	A	264	SER	N-CA-CB	5.14	118.21	110.50
1	A	147	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	C	147	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	A	314	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	34	CYS	CA-CB-SG	-5.09	104.83	114.00
1	C	314	ASP	CB-CG-OD1	5.07	122.87	118.30
1	A	34	CYS	CA-CB-SG	-5.07	104.87	114.00
1	A	133	ASP	CB-CG-OD2	5.07	122.86	118.30
2	B	170	GLN	CB-CA-C	-5.05	100.29	110.40
2	D	81	HIS	N-CA-CB	-5.04	101.53	110.60
2	B	6	PHE	CB-CA-C	5.03	120.47	110.40
2	D	170	GLN	CB-CA-C	-5.03	100.33	110.40
1	C	133	ASP	CB-CG-OD2	5.03	122.82	118.30
2	D	6	PHE	CB-CA-C	5.02	120.45	110.40
2	B	81	HIS	N-CA-CB	-5.01	101.58	110.60
2	D	151	TYR	CA-CB-CG	5.00	122.91	113.40
1	A	106	CYS	CB-CA-C	5.00	120.40	110.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	284	ARG	CA
2	B	317	ALA	CA
2	D	284	ARG	CA
2	D	317	ALA	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2679	0	2552	252	2
1	C	2679	0	2552	244	15

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2498	0	2362	165	0
2	D	2498	0	2362	161	11
3	A	5	0	0	2	0
4	A	28	0	0	3	0
4	B	45	0	0	1	2
All	All	10432	0	9828	799	15

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 40.

All (799) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLN:HG3	1:A:268:LYS:HB3	1.50	0.94
1:C:266:GLN:HG3	1:C:268:LYS:HB3	1.50	0.94
2:D:181:GLU:HG3	2:D:182:TRP:H	1.33	0.94
1:A:106:CYS:HB2	1:A:173:VAL:HG22	1.51	0.92
1:C:106:CYS:HB2	1:C:173:VAL:HG22	1.51	0.91
2:D:43:GLU:HB2	2:D:55:PRO:HG3	1.52	0.91
2:B:181:GLU:HG3	2:B:182:TRP:H	1.33	0.90
1:A:47:THR:HG22	1:A:49:PHE:H	1.36	0.90
1:C:157:GLN:NE2	1:C:159:ASN:HD21	1.68	0.90
2:D:82:HIS:HD2	2:D:84:VAL:H	1.18	0.90
1:A:157:GLN:NE2	1:A:159:ASN:HD21	1.68	0.90
1:C:47:THR:HG22	1:C:49:PHE:H	1.36	0.89
2:B:82:HIS:HD2	2:B:84:VAL:H	1.18	0.89
1:A:156:ILE:HD13	2:B:46:PHE:CE1	2.07	0.89
1:A:157:GLN:HE21	1:A:159:ASN:HD21	1.18	0.89
1:C:157:GLN:HE21	1:C:159:ASN:HD21	1.18	0.89
2:B:43:GLU:HB2	2:B:55:PRO:HG3	1.52	0.88
1:C:156:ILE:HD13	2:D:46:PHE:CE1	2.07	0.88
1:C:129:ASP:HA	1:C:182:TRP:CZ2	2.09	0.88
1:A:129:ASP:HA	1:A:182:TRP:CZ2	2.09	0.87
2:B:146:PRO:HG3	2:B:153:PHE:CZ	2.10	0.87
1:C:73:THR:HB	1:C:76:ILE:HD12	1.56	0.87
1:A:106:CYS:HB2	1:A:173:VAL:CG2	2.04	0.87
1:A:226:LEU:HB2	1:A:323:ILE:HG22	1.55	0.87
1:C:106:CYS:HB2	1:C:173:VAL:CG2	2.04	0.87
2:D:146:PRO:HG3	2:D:153:PHE:CZ	2.09	0.87
1:C:354:LYS:HE2	1:C:355:GLN:HB3	1.57	0.87
1:A:73:THR:HB	1:A:76:ILE:HD12	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LYS:HE2	1:A:355:GLN:HB3	1.57	0.86
1:A:205:LEU:HD13	1:A:318:THR:HG22	1.57	0.86
1:C:226:LEU:HB2	1:C:323:ILE:HG22	1.55	0.86
1:C:205:LEU:HD13	1:C:318:THR:HG22	1.57	0.85
1:A:226:LEU:HD12	1:A:323:ILE:CG2	2.07	0.85
1:C:226:LEU:HD12	1:C:323:ILE:CG2	2.07	0.84
2:D:146:PRO:HG3	2:D:153:PHE:CE1	2.14	0.82
2:B:184:ALA:HB2	2:B:208:TYR:CD1	2.15	0.82
2:B:146:PRO:HG3	2:B:153:PHE:CE1	2.14	0.81
2:D:184:ALA:HB2	2:D:208:TYR:CD1	2.15	0.81
1:A:226:LEU:HD12	1:A:323:ILE:HG22	1.63	0.81
2:B:106:SER:HB2	2:B:173:ASN:HB3	1.64	0.80
1:C:251:TYR:O	1:C:255:VAL:HG23	1.82	0.80
2:D:106:SER:HB2	2:D:173:ASN:HB3	1.64	0.80
1:C:153:PHE:HB2	2:D:116:PHE:CE2	2.17	0.79
1:A:153:PHE:HB2	2:B:116:PHE:CE2	2.17	0.79
2:B:114:MET:HE3	2:B:119:ARG:HB3	1.64	0.79
1:A:251:TYR:O	1:A:255:VAL:HG23	1.82	0.79
1:C:92:LEU:HD13	1:C:160:PRO:HD3	1.65	0.79
2:B:85:ARG:O	2:B:89:GLU:HG3	1.83	0.78
1:C:226:LEU:HD12	1:C:323:ILE:HG22	1.63	0.78
2:D:85:ARG:O	2:D:89:GLU:HG3	1.83	0.78
2:D:181:GLU:HG3	2:D:182:TRP:N	1.98	0.78
1:A:92:LEU:HD13	1:A:160:PRO:HD3	1.65	0.78
1:C:156:ILE:HD13	2:D:46:PHE:HE1	1.49	0.77
2:D:139:PHE:CE2	2:D:168:PRO:HD2	2.19	0.77
2:B:139:PHE:CE2	2:B:168:PRO:HD2	2.19	0.77
2:B:181:GLU:HG3	2:B:182:TRP:N	1.98	0.77
1:A:156:ILE:HD13	2:B:46:PHE:HE1	1.49	0.76
2:D:17:SER:O	2:D:21:ILE:HD12	1.86	0.76
1:C:208:TYR:CE2	1:C:224:HIS:HE1	2.04	0.75
2:D:217:VAL:HG23	2:D:219:VAL:HG13	1.66	0.75
1:A:73:THR:CB	1:A:76:ILE:HD12	2.17	0.75
1:A:208:TYR:CE2	1:A:224:HIS:HE1	2.04	0.75
1:C:134:LEU:HA	1:C:137:GLU:OE1	1.87	0.75
2:D:114:MET:HE3	2:D:119:ARG:HB3	1.68	0.75
1:C:191:ILE:HG23	1:C:225:CYS:HB3	1.69	0.75
1:A:134:LEU:HA	1:A:137:GLU:OE1	1.87	0.75
2:B:217:VAL:HG23	2:B:219:VAL:HG13	1.66	0.74
1:C:123:ASN:HB2	1:C:127:LEU:CD1	2.17	0.74
1:A:191:ILE:HG23	1:A:225:CYS:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:SER:HA	2:B:126:GLN:NE2	2.03	0.74
1:A:123:ASN:HB2	1:A:127:LEU:CD1	2.17	0.74
1:C:73:THR:CB	1:C:76:ILE:HD12	2.17	0.74
2:B:207:LEU:HD12	2:B:207:LEU:O	1.88	0.74
1:A:157:GLN:HE21	1:A:159:ASN:ND2	1.87	0.73
2:D:207:LEU:HD12	2:D:207:LEU:O	1.88	0.73
2:B:17:SER:O	2:B:21:ILE:HD12	1.86	0.73
1:C:129:ASP:HA	1:C:182:TRP:HZ2	1.51	0.73
2:D:123:SER:HA	2:D:126:GLN:NE2	2.03	0.73
1:C:27:LEU:N	1:C:27:LEU:HD23	2.03	0.72
2:D:119:ARG:HG2	2:D:127:LEU:HD21	1.71	0.72
1:A:184:ALA:HB2	1:A:208:TYR:CD1	2.25	0.72
1:C:157:GLN:HE21	1:C:159:ASN:ND2	1.87	0.72
1:A:89:ASP:O	1:A:93:LEU:HB2	1.89	0.72
1:C:336:ILE:O	1:C:340:MET:HG2	1.89	0.71
2:B:184:ALA:HA	2:B:208:TYR:CE1	2.25	0.71
1:C:89:ASP:O	1:C:93:LEU:HB2	1.89	0.71
2:B:119:ARG:HG2	2:B:127:LEU:HD21	1.71	0.71
1:C:184:ALA:HB2	1:C:208:TYR:CD1	2.25	0.71
1:A:1:MET:HB2	1:A:321:ASP:O	1.90	0.71
1:A:108:GLY:C	1:A:109:LEU:HD23	2.11	0.71
1:A:336:ILE:O	1:A:340:MET:HG2	1.89	0.71
1:C:108:GLY:C	1:C:109:LEU:HD23	2.11	0.71
2:D:82:HIS:CD2	2:D:84:VAL:HG23	2.26	0.71
1:A:27:LEU:N	1:A:27:LEU:HD23	2.03	0.71
1:A:205:LEU:CD1	1:A:318:THR:HG22	2.21	0.71
2:D:184:ALA:HA	2:D:208:TYR:CE1	2.25	0.71
1:C:1:MET:HB2	1:C:321:ASP:O	1.90	0.71
1:A:129:ASP:HA	1:A:182:TRP:HZ2	1.51	0.70
1:A:129:ASP:HB2	1:A:182:TRP:NE1	2.07	0.70
1:C:45:HIS:HB3	1:C:46:PHE:CE1	2.27	0.70
1:C:184:ALA:HA	1:C:208:TYR:CE1	2.26	0.70
1:A:23:ARG:O	1:A:27:LEU:HG	1.92	0.70
1:A:45:HIS:HB3	1:A:46:PHE:CE1	2.27	0.70
1:C:259:LYS:HG3	1:C:260:ILE:N	2.07	0.70
1:A:259:LYS:HG3	1:A:260:ILE:N	2.07	0.70
1:C:129:ASP:HB2	1:C:182:TRP:NE1	2.07	0.70
1:C:205:LEU:CD1	1:C:318:THR:HG22	2.21	0.70
1:A:184:ALA:HA	1:A:208:TYR:CE1	2.26	0.69
2:B:82:HIS:CD2	2:B:84:VAL:HG23	2.26	0.69
2:D:241:ALA:O	2:D:245:VAL:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:225:LYS:CG	2:D:294:ASP:HB2	2.22	0.69
2:D:276:TYR:O	2:D:280:THR:HG22	1.92	0.69
2:B:225:LYS:CG	2:B:294:ASP:HB2	2.22	0.69
2:B:241:ALA:O	2:B:245:VAL:HG23	1.92	0.69
2:B:276:TYR:O	2:B:280:THR:HG22	1.92	0.69
1:C:184:ALA:HB1	1:C:211:VAL:HB	1.75	0.68
1:C:95:GLN:NE2	1:C:161:SER:O	2.27	0.68
1:A:354:LYS:HG2	1:A:355:GLN:N	2.09	0.68
1:A:184:ALA:HB1	1:A:211:VAL:HB	1.75	0.68
1:C:23:ARG:O	1:C:27:LEU:HG	1.92	0.68
1:C:354:LYS:HG2	1:C:355:GLN:H	1.59	0.68
1:A:123:ASN:HB2	1:A:127:LEU:HD11	1.76	0.68
1:C:123:ASN:HB2	1:C:127:LEU:HD11	1.76	0.68
1:C:354:LYS:HG2	1:C:355:GLN:N	2.09	0.68
1:C:82:HIS:HD2	1:C:84:VAL:H	1.42	0.68
1:C:133:ASP:O	1:C:136:LYS:HB3	1.94	0.67
1:A:82:HIS:HD2	1:A:84:VAL:H	1.42	0.67
1:A:133:ASP:O	1:A:136:LYS:HB3	1.94	0.67
1:C:193:SER:OG	1:C:195:ILE:HB	1.95	0.67
1:A:354:LYS:HG2	1:A:355:GLN:H	1.59	0.67
2:B:82:HIS:CD2	2:B:84:VAL:H	2.09	0.67
1:C:295:SER:O	1:C:299:ASN:ND2	2.28	0.66
1:A:295:SER:O	1:A:299:ASN:ND2	2.28	0.66
1:A:95:GLN:NE2	1:A:161:SER:O	2.27	0.66
1:A:193:SER:OG	1:A:195:ILE:HB	1.95	0.66
1:C:12:PRO:HG2	1:C:15:LEU:HG	1.77	0.66
1:C:69:LEU:HG	1:C:70:ASN:N	2.10	0.66
1:C:42:LEU:HG	1:C:43:GLU:N	2.11	0.66
1:C:323:ILE:HD13	1:C:323:ILE:N	2.11	0.66
1:C:136:LYS:O	1:C:139:PHE:HB2	1.96	0.66
1:C:36:PHE:CE2	1:C:340:MET:HE3	2.31	0.65
2:D:12:ASN:OD1	2:D:15:ARG:N	2.28	0.65
1:C:129:ASP:HB2	1:C:182:TRP:HE1	1.61	0.65
1:A:12:PRO:HG2	1:A:15:LEU:HG	1.77	0.65
2:D:112:ALA:O	2:D:115:ARG:N	2.29	0.65
2:B:112:ALA:O	2:B:115:ARG:N	2.29	0.65
1:A:266:GLN:HG3	1:A:268:LYS:CB	2.26	0.65
2:B:12:ASN:OD1	2:B:15:ARG:N	2.28	0.65
1:A:69:LEU:HG	1:A:70:ASN:N	2.10	0.65
1:A:42:LEU:HG	1:A:43:GLU:N	2.11	0.64
1:A:136:LYS:O	1:A:139:PHE:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:HIS:O	1:C:86:GLN:HG3	1.98	0.64
1:A:266:GLN:O	1:A:266:GLN:HG2	1.97	0.64
1:C:17:GLN:O	1:C:21:MET:HG2	1.96	0.64
1:A:17:GLN:O	1:A:21:MET:HG2	1.96	0.64
2:B:146:PRO:HB2	2:B:151:TYR:O	1.98	0.64
1:A:323:ILE:HD13	1:A:323:ILE:N	2.11	0.64
1:A:129:ASP:HB2	1:A:182:TRP:HE1	1.61	0.64
1:A:36:PHE:CE2	1:A:340:MET:HE3	2.33	0.64
1:A:82:HIS:O	1:A:86:GLN:HG3	1.98	0.64
2:B:107:ASP:OD1	2:B:108:CYS:N	2.29	0.64
1:C:300:PRO:HG3	1:C:311:ILE:CD1	2.28	0.64
2:B:75:ASN:OD1	2:B:75:ASN:N	2.30	0.63
1:C:226:LEU:CB	1:C:323:ILE:HG22	2.27	0.63
2:D:146:PRO:HB2	2:D:151:TYR:O	1.98	0.63
2:D:15:ARG:NH2	2:D:300:GLU:O	2.29	0.63
1:A:300:PRO:HG3	1:A:311:ILE:CD1	2.28	0.63
2:D:27:THR:O	2:D:31:VAL:HG23	1.99	0.63
2:D:193:ARG:NH2	2:D:196:ASP:OD1	2.29	0.63
1:C:47:THR:CG2	1:C:49:PHE:H	2.11	0.63
2:B:15:ARG:NH2	2:B:300:GLU:O	2.29	0.63
2:B:27:THR:O	2:B:31:VAL:HG23	1.99	0.63
2:D:75:ASN:OD1	2:D:75:ASN:N	2.30	0.63
2:D:10:PHE:CD1	2:D:49:ASN:HA	2.34	0.63
1:A:300:PRO:HG3	1:A:311:ILE:HD11	1.81	0.63
1:C:156:ILE:HB	2:D:46:PHE:CD1	2.34	0.63
1:A:81:ALA:HB3	1:A:86:GLN:NE2	2.14	0.62
1:C:81:ALA:HB3	1:C:86:GLN:NE2	2.14	0.62
2:D:82:HIS:CD2	2:D:84:VAL:H	2.09	0.62
1:A:226:LEU:CB	1:A:323:ILE:HG22	2.27	0.62
2:B:233:ASN:HD22	2:B:234:VAL:N	1.98	0.62
1:C:300:PRO:HG3	1:C:311:ILE:HD11	1.81	0.62
1:C:323:ILE:O	1:C:323:ILE:HG12	1.99	0.62
2:D:107:ASP:OD1	2:D:108:CYS:N	2.29	0.62
1:C:346:ASP:OD1	1:C:346:ASP:N	2.31	0.62
1:A:52:LEU:HD11	1:A:58:ALA:HB2	1.82	0.62
1:A:156:ILE:HB	2:B:46:PHE:CD1	2.34	0.62
1:A:83:PRO:HD3	1:A:131:TRP:CE2	2.35	0.62
2:B:10:PHE:CD1	2:B:49:ASN:HA	2.34	0.62
2:B:193:ARG:NH2	2:B:196:ASP:OD1	2.29	0.62
1:C:83:PRO:HD3	1:C:131:TRP:CE2	2.35	0.62
1:A:323:ILE:HG12	1:A:323:ILE:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:ASN:HD22	2:D:234:VAL:N	1.98	0.61
1:C:266:GLN:HG3	1:C:268:LYS:CB	2.26	0.61
2:B:147:ASN:HA	2:B:152:SER:OG	2.01	0.61
1:A:86:GLN:O	1:A:90:VAL:HG23	2.00	0.61
1:C:23:ARG:NH2	1:C:331:GLY:O	2.27	0.61
1:C:52:LEU:HD11	1:C:58:ALA:HB2	1.82	0.61
2:D:63:LEU:HD12	2:D:93:LEU:HD22	1.82	0.61
1:A:233:ASP:O	1:A:303:THR:HA	2.00	0.61
1:C:86:GLN:O	1:C:90:VAL:HG23	2.00	0.61
1:C:233:ASP:O	1:C:303:THR:HA	2.00	0.61
2:D:119:ARG:HG2	2:D:127:LEU:CD2	2.30	0.61
2:D:172:VAL:HG22	2:D:173:ASN:N	2.16	0.61
1:A:47:THR:CG2	1:A:49:PHE:H	2.11	0.61
2:B:84:VAL:O	2:B:88:GLU:HG3	2.00	0.61
1:C:355:GLN:HG2	1:C:355:GLN:OXT	2.01	0.61
2:D:204:TYR:O	2:D:207:LEU:HB3	2.01	0.61
1:C:13:PRO:HD2	1:C:14:GLU:OE1	2.01	0.60
1:C:105:ILE:CD1	1:C:128:MET:HE2	2.31	0.60
2:B:204:TYR:O	2:B:207:LEU:HB3	2.01	0.60
2:B:2:LYS:HB2	2:B:294:ASP:OD1	2.02	0.60
2:D:63:LEU:HD12	2:D:93:LEU:CD2	2.32	0.60
2:D:84:VAL:O	2:D:88:GLU:HG3	2.00	0.60
2:B:63:LEU:HD12	2:B:93:LEU:HD22	1.82	0.60
1:C:1:MET:HE1	1:C:351:LEU:HB3	1.81	0.60
2:D:2:LYS:HB2	2:D:294:ASP:OD1	2.02	0.60
1:A:346:ASP:OD1	1:A:346:ASP:N	2.31	0.60
2:B:172:VAL:HG22	2:B:173:ASN:N	2.16	0.60
2:B:119:ARG:HG2	2:B:127:LEU:CD2	2.30	0.60
1:C:197:ASN:OD1	1:C:200:GLU:HG3	2.02	0.60
1:A:79:PRO:HB3	1:A:127:LEU:HD22	1.84	0.60
1:A:205:LEU:O	1:A:208:TYR:N	2.34	0.60
1:C:205:LEU:O	1:C:208:TYR:N	2.34	0.60
2:D:147:ASN:HA	2:D:152:SER:OG	2.01	0.60
1:C:170:VAL:O	1:C:189:PRO:HD2	2.02	0.60
2:D:247:LEU:N	2:D:247:LEU:HD22	2.17	0.60
1:C:231:SER:HB3	1:C:301:VAL:HG13	1.84	0.60
2:B:225:LYS:HG3	2:B:294:ASP:HB2	1.84	0.60
1:A:13:PRO:HD2	1:A:14:GLU:OE1	2.01	0.59
1:A:170:VAL:O	1:A:189:PRO:HD2	2.02	0.59
1:A:197:ASN:OD1	1:A:200:GLU:HG3	2.02	0.59
2:B:25:LEU:HD22	2:B:65:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:PRO:HB3	1:C:127:LEU:HD22	1.84	0.59
2:B:130:GLU:O	2:B:133:LYS:N	2.36	0.59
2:B:63:LEU:HD12	2:B:93:LEU:CD2	2.32	0.59
1:A:345:SER:HB2	1:A:346:ASP:OD1	2.02	0.59
1:C:310:ILE:O	1:C:310:ILE:HD13	2.03	0.59
1:A:1:MET:HE1	1:A:351:LEU:HB3	1.85	0.59
1:A:231:SER:HB3	1:A:301:VAL:HG13	1.84	0.59
1:A:226:LEU:HD12	1:A:323:ILE:HG21	1.85	0.59
1:C:170:VAL:HG12	1:C:171:TYR:N	2.18	0.59
1:A:310:ILE:HD13	1:A:310:ILE:O	2.03	0.59
1:A:355:GLN:OXT	1:A:355:GLN:HG2	2.01	0.59
1:C:345:SER:HB2	1:C:346:ASP:OD1	2.02	0.59
1:A:123:ASN:HB2	1:A:127:LEU:HD12	1.84	0.58
1:C:123:ASN:HB2	1:C:127:LEU:HD12	1.84	0.58
2:D:225:LYS:HG3	2:D:294:ASP:HB2	1.84	0.58
1:A:115:ARG:HD2	1:A:267:THR:HB	1.86	0.58
1:A:176:SER:N	3:A:356:PO4:O2	2.33	0.58
2:B:247:LEU:HD22	2:B:247:LEU:N	2.17	0.58
2:B:44:ASN:HB3	2:B:50:GLY:HA3	1.85	0.58
1:C:115:ARG:HD2	1:C:267:THR:HB	1.86	0.58
1:C:92:LEU:HD13	1:C:160:PRO:CD	2.33	0.58
1:A:240:LYS:O	1:A:244:ARG:HG3	2.04	0.58
2:B:6:PHE:HE1	2:B:8:LEU:HD21	1.69	0.58
1:C:140:ASN:N	1:C:140:ASN:OD1	2.37	0.58
2:D:6:PHE:HE1	2:D:8:LEU:HD21	1.69	0.58
2:D:130:GLU:O	2:D:133:LYS:N	2.36	0.58
1:A:92:LEU:HD13	1:A:160:PRO:CD	2.33	0.58
1:A:134:LEU:HD22	1:A:145:ALA:O	2.04	0.58
2:D:65:MET:O	2:D:65:MET:HG2	2.03	0.58
2:B:217:VAL:CG2	2:B:219:VAL:HG13	2.34	0.57
1:C:134:LEU:HD22	1:C:145:ALA:O	2.04	0.57
1:C:207:LEU:O	1:C:211:VAL:HG23	2.05	0.57
1:C:226:LEU:HD12	1:C:323:ILE:HG21	1.85	0.57
2:B:134:ILE:HG22	2:B:135:ILE:N	2.19	0.57
1:A:140:ASN:N	1:A:140:ASN:OD1	2.37	0.57
1:A:207:LEU:O	1:A:211:VAL:HG23	2.05	0.57
1:C:110:TYR:CB	1:C:112:LYS:HE3	2.35	0.57
2:D:25:LEU:HD22	2:D:65:MET:HE1	1.85	0.57
2:D:217:VAL:CG2	2:D:219:VAL:HG13	2.34	0.57
1:A:170:VAL:HG12	1:A:171:TYR:N	2.18	0.57
1:C:54:ASN:HD21	2:D:88:GLU:HB3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LYS:O	1:C:244:ARG:HG3	2.04	0.57
2:B:8:LEU:O	2:B:50:GLY:HA2	2.04	0.57
2:D:44:ASN:HB3	2:D:50:GLY:HA3	1.85	0.57
1:A:54:ASN:HD21	2:B:88:GLU:HB3	1.70	0.57
2:B:65:MET:O	2:B:65:MET:HG2	2.03	0.57
1:C:266:GLN:O	1:C:266:GLN:HG2	1.96	0.57
1:A:23:ARG:NH2	1:A:331:GLY:O	2.27	0.57
1:C:28:GLY:HA3	1:C:62:LEU:HD22	1.87	0.57
1:A:184:ALA:HB2	1:A:208:TYR:HD1	1.69	0.56
1:C:61:HIS:CE1	2:D:64:GLY:HA2	2.40	0.56
1:C:159:ASN:HB3	2:D:51:VAL:HG22	1.87	0.56
1:A:105:ILE:CD1	1:A:128:MET:HE2	2.34	0.56
1:A:110:TYR:CB	1:A:112:LYS:HE3	2.35	0.56
2:D:8:LEU:O	2:D:50:GLY:HA2	2.04	0.56
2:D:134:ILE:HG22	2:D:135:ILE:N	2.19	0.56
2:B:207:LEU:HD12	2:B:207:LEU:C	2.25	0.56
1:A:194:TRP:HB2	1:A:299:ASN:OD1	2.05	0.56
2:B:189:PRO:HB3	2:B:223:ARG:O	2.06	0.56
1:C:318:THR:HB	1:C:320:ILE:HD12	1.88	0.56
1:A:123:ASN:C	1:A:127:LEU:HD12	2.26	0.56
1:C:115:ARG:CD	1:C:267:THR:HB	2.36	0.56
1:A:28:GLY:HA3	1:A:62:LEU:HD22	1.87	0.56
1:A:61:HIS:CE1	2:B:64:GLY:HA2	2.40	0.56
1:C:312:GLN:HA	1:C:312:GLN:NE2	2.20	0.56
1:C:184:ALA:HA	1:C:208:TYR:HE1	1.71	0.56
1:A:303:THR:OG1	1:A:306:GLU:HG3	2.06	0.55
1:A:159:ASN:HB3	2:B:51:VAL:HG22	1.87	0.55
1:C:123:ASN:C	1:C:127:LEU:HD12	2.26	0.55
1:C:194:TRP:HB2	1:C:299:ASN:OD1	2.05	0.55
1:A:312:GLN:HA	1:A:312:GLN:NE2	2.20	0.55
1:C:26:ASN:HD22	1:C:26:ASN:N	2.02	0.55
1:A:226:LEU:CD1	1:A:323:ILE:HG22	2.35	0.55
1:C:226:LEU:CD1	1:C:323:ILE:HG22	2.35	0.55
2:D:243:ALA:O	2:D:247:LEU:HD23	2.07	0.55
1:A:115:ARG:CD	1:A:267:THR:HB	2.36	0.55
2:B:72:ALA:HB2	2:B:102:ALA:HB3	1.89	0.55
2:B:200:GLN:CA	2:B:200:GLN:HE21	2.19	0.55
1:C:186:ARG:HG3	1:C:186:ARG:HH11	1.72	0.55
1:A:110:TYR:CD1	1:A:110:TYR:N	2.75	0.55
2:B:221:GLN:O	2:B:223:ARG:HG2	2.06	0.55
1:C:256:ASN:C	1:C:258:THR:H	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:THR:OG1	1:C:306:GLU:HG3	2.06	0.55
2:B:185:LYS:O	2:B:217:VAL:HG11	2.07	0.55
2:D:189:PRO:HB3	2:D:223:ARG:O	2.06	0.55
2:B:243:ALA:O	2:B:247:LEU:HD23	2.07	0.55
1:C:115:ARG:HH11	1:C:267:THR:CG2	2.20	0.55
2:D:40:ALA:HA	2:D:72:ALA:O	2.06	0.55
1:C:17:GLN:OE1	2:D:160:PRO:HA	2.07	0.55
2:D:207:LEU:HD12	2:D:207:LEU:C	2.25	0.55
1:A:186:ARG:HG3	1:A:186:ARG:HH11	1.72	0.54
1:A:256:ASN:C	1:A:258:THR:H	2.08	0.54
2:D:221:GLN:O	2:D:223:ARG:HG2	2.06	0.54
1:A:171:TYR:N	1:A:171:TYR:CD1	2.75	0.54
1:C:184:ALA:HB2	1:C:208:TYR:HD1	1.69	0.54
1:C:134:LEU:O	1:C:144:ILE:HD13	2.08	0.54
2:D:82:HIS:NE2	2:D:84:VAL:HG23	2.22	0.54
1:A:17:GLN:OE1	2:B:160:PRO:HA	2.07	0.54
1:A:332:SER:HB3	1:A:335:GLU:OE2	2.07	0.54
2:B:40:ALA:HA	2:B:72:ALA:O	2.06	0.54
2:B:82:HIS:NE2	2:B:84:VAL:HG23	2.22	0.54
1:A:115:ARG:HH11	1:A:267:THR:CG2	2.20	0.54
1:A:318:THR:HB	1:A:320:ILE:HD12	1.88	0.54
1:C:171:TYR:N	1:C:171:TYR:CD1	2.75	0.54
2:D:72:ALA:HB2	2:D:102:ALA:HB3	1.89	0.54
1:A:184:ALA:HA	1:A:208:TYR:HE1	1.70	0.54
1:C:1:MET:CE	1:C:351:LEU:HB3	2.38	0.54
2:D:185:LYS:O	2:D:217:VAL:HG11	2.07	0.54
1:A:1:MET:CE	1:A:351:LEU:HB3	2.38	0.54
1:A:333:GLU:O	1:A:337:ILE:HG12	2.08	0.54
1:C:110:TYR:CD1	1:C:110:TYR:N	2.75	0.54
1:A:85:ARG:HG2	4:A:2007:HOH:O	2.08	0.53
1:C:208:TYR:CE2	1:C:224:HIS:CE1	2.92	0.53
1:A:208:TYR:CE2	1:A:224:HIS:CE1	2.92	0.53
2:B:126:GLN:HA	2:B:129:SER:OG	2.08	0.53
2:B:193:ARG:HH21	2:B:196:ASP:CG	2.11	0.53
1:C:333:GLU:O	1:C:337:ILE:HG12	2.08	0.53
2:D:193:ARG:HH21	2:D:196:ASP:CG	2.11	0.53
1:A:13:PRO:HD2	1:A:14:GLU:CD	2.29	0.53
1:A:134:LEU:O	1:A:144:ILE:HD13	2.08	0.53
1:C:332:SER:HB3	1:C:335:GLU:OE2	2.07	0.53
2:D:200:GLN:HE21	2:D:200:GLN:CA	2.19	0.53
2:D:231:ASN:C	2:D:231:ASN:HD22	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:105:PHE:N	2:D:105:PHE:CD1	2.77	0.53
1:A:350:TYR:CD1	1:A:350:TYR:N	2.77	0.53
1:C:88:GLU:O	1:C:92:LEU:HD22	2.09	0.53
1:C:13:PRO:HD2	1:C:14:GLU:CD	2.29	0.53
1:C:123:ASN:CB	1:C:127:LEU:HD12	2.39	0.53
2:D:126:GLN:HA	2:D:129:SER:OG	2.08	0.53
1:C:224:HIS:CD2	1:C:224:HIS:N	2.77	0.52
1:A:181:GLU:O	1:A:185:GLU:HG3	2.09	0.52
2:B:105:PHE:CD1	2:B:105:PHE:N	2.77	0.52
1:C:109:LEU:HD23	1:C:109:LEU:N	2.24	0.52
1:C:115:ARG:HH11	1:C:267:THR:HG22	1.74	0.52
1:C:181:GLU:O	1:C:185:GLU:HG3	2.09	0.52
2:B:95:GLN:HE21	2:B:95:GLN:CA	2.23	0.52
1:A:26:ASN:N	1:A:26:ASN:HD22	2.02	0.52
1:A:88:GLU:O	1:A:92:LEU:HD22	2.09	0.52
1:C:230:THR:OG1	1:C:325:CYS:HB3	2.10	0.52
1:A:224:HIS:N	1:A:224:HIS:CD2	2.77	0.52
1:A:287:ASP:O	1:A:288:THR:HG23	2.10	0.52
1:A:109:LEU:HD23	1:A:109:LEU:N	2.24	0.52
1:A:115:ARG:HH11	1:A:267:THR:HG22	1.74	0.52
1:A:143:TYR:HB2	4:A:2014:HOH:O	2.10	0.52
2:B:184:ALA:CA	2:B:208:TYR:CE1	2.93	0.52
1:C:350:TYR:N	1:C:350:TYR:CD1	2.77	0.52
2:D:136:ASN:O	2:D:140:THR:OG1	2.28	0.52
2:B:259:ASP:HB3	2:B:262:GLN:HB3	1.92	0.52
1:C:73:THR:HG23	1:C:101:PHE:CE1	2.45	0.52
2:D:95:GLN:HE21	2:D:95:GLN:CA	2.23	0.52
1:A:123:ASN:CB	1:A:127:LEU:HD12	2.39	0.52
1:C:299:ASN:O	1:C:301:VAL:N	2.41	0.52
2:D:146:PRO:CG	2:D:153:PHE:CE1	2.90	0.52
2:D:184:ALA:HB2	2:D:208:TYR:CE1	2.45	0.52
1:A:73:THR:HG23	1:A:101:PHE:CE1	2.45	0.51
1:A:230:THR:OG1	1:A:325:CYS:HB3	2.10	0.51
2:B:136:ASN:O	2:B:140:THR:OG1	2.28	0.51
2:B:231:ASN:C	2:B:231:ASN:HD22	2.12	0.51
1:C:177:ALA:O	1:C:181:GLU:HG3	2.10	0.51
1:C:287:ASP:O	1:C:288:THR:HG23	2.10	0.51
1:A:151:ILE:HD12	1:A:153:PHE:CE2	2.45	0.51
1:A:177:ALA:O	1:A:181:GLU:HG3	2.10	0.51
2:B:200:GLN:HA	2:B:200:GLN:NE2	2.26	0.51
1:C:205:LEU:O	1:C:208:TYR:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:MET:CE	2:D:119:ARG:HB3	2.40	0.51
1:A:299:ASN:O	1:A:301:VAL:N	2.41	0.51
2:B:31:VAL:HG13	2:B:36:PHE:CD2	2.46	0.51
2:B:146:PRO:CG	2:B:153:PHE:CE1	2.90	0.51
1:A:332:SER:O	1:A:336:ILE:HG13	2.10	0.51
2:D:184:ALA:CA	2:D:208:TYR:CE1	2.93	0.51
1:A:205:LEU:O	1:A:208:TYR:HB3	2.10	0.51
1:C:151:ILE:HD12	1:C:153:PHE:CE2	2.45	0.51
1:C:230:THR:HG23	1:C:300:PRO:HB2	1.93	0.51
2:D:259:ASP:HB3	2:D:262:GLN:HB3	1.92	0.50
2:D:31:VAL:HG13	2:D:36:PHE:CD2	2.46	0.50
2:B:133:LYS:O	2:B:137:ASP:N	2.45	0.50
2:B:184:ALA:HB2	2:B:208:TYR:CE1	2.45	0.50
2:B:193:ARG:O	2:B:196:ASP:HB2	2.11	0.50
1:C:138:GLY:HA2	1:C:143:TYR:O	2.11	0.50
1:C:332:SER:O	1:C:336:ILE:HG13	2.11	0.50
2:D:177:LYS:H	2:D:177:LYS:CD	2.25	0.50
1:C:259:LYS:O	1:C:261:PHE:N	2.45	0.50
1:C:320:ILE:O	1:C:320:ILE:HG22	2.12	0.50
1:C:354:LYS:CE	1:C:355:GLN:HB3	2.37	0.50
2:D:193:ARG:O	2:D:196:ASP:HB2	2.11	0.50
1:A:138:GLY:HA2	1:A:143:TYR:O	2.11	0.50
1:A:307:CYS:O	1:A:311:ILE:HG12	2.11	0.50
2:B:63:LEU:CD1	2:B:93:LEU:HD22	2.41	0.50
2:B:200:GLN:CA	2:B:200:GLN:NE2	2.75	0.50
2:D:187:GLY:HA3	2:D:217:VAL:HG21	1.93	0.50
2:B:218:ASP:C	2:B:220:SER:H	2.15	0.50
1:C:46:PHE:CD1	1:C:46:PHE:N	2.80	0.50
1:C:204:GLN:O	1:C:207:LEU:HB3	2.12	0.50
2:D:63:LEU:CD1	2:D:93:LEU:HD22	2.41	0.50
1:A:354:LYS:CE	1:A:355:GLN:HB3	2.37	0.50
2:D:218:ASP:C	2:D:220:SER:H	2.15	0.50
1:A:226:LEU:HD13	1:A:228:TYR:OH	2.12	0.49
1:A:184:ALA:CB	1:A:211:VAL:HB	2.42	0.49
1:A:230:THR:HG23	1:A:300:PRO:HB2	1.93	0.49
2:B:187:GLY:HA3	2:B:217:VAL:HG21	1.93	0.49
1:C:144:ILE:HG22	1:C:145:ALA:N	2.27	0.49
1:C:307:CYS:O	1:C:311:ILE:HG12	2.11	0.49
1:A:184:ALA:CA	1:A:208:TYR:CE1	2.95	0.49
1:A:209:ASN:O	1:A:213:THR:OG1	2.28	0.49
1:A:259:LYS:O	1:A:261:PHE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASN:O	1:C:127:LEU:HD12	2.12	0.49
1:A:294:TYR:O	1:A:297:GLU:HB2	2.13	0.49
1:C:226:LEU:HD13	1:C:228:TYR:OH	2.12	0.49
2:D:200:GLN:NE2	2:D:200:GLN:HA	2.26	0.49
1:A:143:TYR:CD2	1:A:155:LYS:HE2	2.47	0.49
1:A:144:ILE:HG22	1:A:145:ALA:N	2.27	0.49
2:B:134:ILE:O	2:B:137:ASP:N	2.46	0.49
2:B:177:LYS:CD	2:B:177:LYS:H	2.25	0.49
1:C:73:THR:HG21	1:C:76:ILE:CD1	2.43	0.49
1:C:294:TYR:O	1:C:297:GLU:HB2	2.13	0.49
2:D:133:LYS:O	2:D:137:ASP:N	2.45	0.49
2:B:147:ASN:HA	2:B:152:SER:CB	2.43	0.49
2:D:200:GLN:CA	2:D:200:GLN:NE2	2.75	0.49
2:D:123:SER:O	2:D:126:GLN:HG3	2.13	0.49
1:A:123:ASN:O	1:A:127:LEU:HD12	2.12	0.49
1:A:182:TRP:O	1:A:186:ARG:NH1	2.46	0.49
2:B:197:SER:HA	2:B:270:GLU:OE1	2.13	0.49
2:B:177:LYS:H	2:B:177:LYS:HD2	1.77	0.49
1:C:184:ALA:CA	1:C:208:TYR:CE1	2.95	0.49
1:A:314:ASP:O	1:A:318:THR:OG1	2.29	0.49
2:B:311:VAL:O	2:B:314:VAL:HB	2.13	0.49
2:D:134:ILE:O	2:D:137:ASP:N	2.46	0.49
2:D:172:VAL:HG22	2:D:173:ASN:H	1.77	0.49
1:A:204:GLN:O	1:A:207:LEU:HB3	2.12	0.48
2:B:89:GLU:O	2:B:92:LEU:HB3	2.13	0.48
2:D:89:GLU:O	2:D:92:LEU:HB3	2.13	0.48
2:D:177:LYS:H	2:D:177:LYS:HD2	1.77	0.48
2:D:225:LYS:HB3	2:D:294:ASP:O	2.13	0.48
1:A:46:PHE:CD1	1:A:46:PHE:N	2.80	0.48
1:A:73:THR:HG21	1:A:76:ILE:CD1	2.43	0.48
2:B:123:SER:O	2:B:126:GLN:HG3	2.13	0.48
1:C:143:TYR:CD2	1:C:155:LYS:HE2	2.47	0.48
2:D:305:LYS:O	2:D:309:ARG:HB3	2.13	0.48
1:A:320:ILE:HG22	1:A:320:ILE:O	2.12	0.48
1:A:85:ARG:NH2	4:A:2123:HOH:O	2.46	0.48
1:C:218:ASP:C	1:C:220:THR:H	2.17	0.48
2:D:197:SER:HA	2:D:270:GLU:OE1	2.13	0.48
2:B:95:GLN:CA	2:B:95:GLN:NE2	2.76	0.48
2:B:172:VAL:HG22	2:B:173:ASN:H	1.77	0.48
1:C:314:ASP:O	1:C:318:THR:OG1	2.29	0.48
2:D:147:ASN:HA	2:D:152:SER:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:GLU:OE1	2:B:148:ASN:ND2	2.47	0.48
2:B:305:LYS:O	2:B:309:ARG:HB3	2.13	0.48
1:C:194:TRP:HB3	1:C:228:TYR:HA	1.96	0.48
1:A:123:ASN:N	1:A:123:ASN:ND2	2.62	0.48
1:A:218:ASP:C	1:A:220:THR:H	2.16	0.48
2:B:225:LYS:HB3	2:B:294:ASP:O	2.13	0.48
1:C:119:THR:HG22	1:C:120:ASP:N	2.29	0.47
1:C:182:TRP:O	1:C:186:ARG:NH1	2.46	0.47
2:D:311:VAL:O	2:D:314:VAL:HB	2.13	0.47
1:C:102:ARG:NH1	1:C:169:PRO:HG2	2.30	0.47
1:C:184:ALA:CB	1:C:211:VAL:HB	2.42	0.47
1:C:186:ARG:HH11	1:C:186:ARG:CG	2.27	0.47
2:D:314:VAL:HG12	2:D:315:VAL:N	2.29	0.47
1:A:119:THR:HG22	1:A:120:ASP:N	2.29	0.47
2:B:314:VAL:HG12	2:B:315:VAL:N	2.29	0.47
2:D:213:GLN:O	2:D:215:HIS:N	2.47	0.47
2:B:213:GLN:O	2:B:215:HIS:N	2.47	0.47
2:D:221:GLN:OE1	2:D:221:GLN:HA	2.13	0.47
1:A:69:LEU:CG	1:A:70:ASN:N	2.78	0.47
1:A:291:ARG:HE	1:A:293:ASP:CG	2.18	0.47
2:B:221:GLN:HA	2:B:221:GLN:OE1	2.13	0.47
1:C:190:MET:O	1:C:225:CYS:N	2.40	0.47
1:C:323:ILE:N	1:C:323:ILE:CD1	2.76	0.47
2:D:95:GLN:HG3	2:D:160:PRO:HB2	1.97	0.47
1:A:52:LEU:HG	1:A:52:LEU:O	2.14	0.47
2:B:8:LEU:N	2:B:300:GLU:OE2	2.32	0.47
1:C:123:ASN:N	1:C:123:ASN:HD22	2.13	0.47
1:A:123:ASN:N	1:A:123:ASN:HD22	2.13	0.47
2:B:30:TYR:CZ	2:B:309:ARG:HD2	2.50	0.47
2:B:170:GLN:HG3	4:B:2091:HOH:O	2.15	0.47
1:C:105:ILE:HD12	1:C:128:MET:HE2	1.97	0.47
2:D:130:GLU:OE1	2:D:148:ASN:ND2	2.47	0.47
1:A:173:VAL:HG23	1:A:173:VAL:O	2.16	0.47
1:C:45:HIS:HB3	1:C:46:PHE:CD1	2.49	0.47
1:C:208:TYR:CD2	1:C:224:HIS:HE1	2.33	0.47
1:C:225:CYS:SG	1:C:322:ASN:ND2	2.88	0.47
1:C:312:GLN:NE2	1:C:316:ASP:OD1	2.47	0.47
2:D:299:PHE:CD1	2:D:299:PHE:N	2.83	0.47
2:D:308:GLN:HE21	2:D:308:GLN:HB2	1.47	0.47
1:A:47:THR:HG22	1:A:49:PHE:N	2.17	0.46
1:A:121:MET:HE1	1:A:267:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:NH1	1:A:186:ARG:CG	2.78	0.46
1:A:194:TRP:HB3	1:A:228:TYR:HA	1.96	0.46
1:C:49:PHE:CZ	1:C:250:TRP:CH2	3.03	0.46
1:C:123:ASN:N	1:C:123:ASN:ND2	2.62	0.46
1:C:151:ILE:HD12	1:C:153:PHE:HE2	1.80	0.46
2:B:218:ASP:O	2:B:220:SER:N	2.47	0.46
1:C:170:VAL:CG1	1:C:171:TYR:N	2.78	0.46
1:A:45:HIS:HB3	1:A:46:PHE:CD1	2.49	0.46
1:A:197:ASN:O	1:A:200:GLU:HB2	2.16	0.46
1:A:312:GLN:NE2	1:A:316:ASP:OD1	2.48	0.46
2:D:30:TYR:CZ	2:D:309:ARG:HD2	2.50	0.46
1:A:186:ARG:HH11	1:A:186:ARG:CG	2.27	0.46
1:A:202:LYS:O	1:A:205:LEU:HB2	2.16	0.46
1:A:225:CYS:SG	1:A:322:ASN:ND2	2.88	0.46
2:B:70:LYS:HA	2:B:100:ARG:HG2	1.98	0.46
1:C:72:GLY:HA3	1:C:102:ARG:HB2	1.97	0.46
1:C:173:VAL:HG23	1:C:173:VAL:O	2.15	0.46
2:D:70:LYS:HA	2:D:100:ARG:HG2	1.98	0.46
1:A:49:PHE:CZ	1:A:250:TRP:CH2	3.03	0.46
1:A:102:ARG:NH1	1:A:169:PRO:HG2	2.30	0.46
1:A:176:SER:HB2	3:A:356:PO4:O4	2.15	0.46
2:B:19:GLN:NE2	2:B:23:GLU:OE2	2.49	0.46
1:C:186:ARG:NH1	1:C:186:ARG:CG	2.78	0.46
1:C:202:LYS:O	1:C:205:LEU:HB2	2.16	0.46
1:C:242:ILE:HG22	1:C:243:CYS:N	2.29	0.46
1:A:3:PHE:CD2	1:A:348:MET:CE	2.99	0.46
1:A:54:ASN:HD21	2:B:88:GLU:CB	2.28	0.46
1:C:291:ARG:HE	1:C:293:ASP:CG	2.18	0.46
1:A:170:VAL:CG1	1:A:171:TYR:N	2.78	0.46
1:A:190:MET:O	1:A:225:CYS:N	2.40	0.46
2:B:114:MET:CE	2:B:119:ARG:HB3	2.40	0.46
2:B:299:PHE:N	2:B:299:PHE:CD1	2.83	0.46
1:C:143:TYR:O	1:C:144:ILE:HG12	2.16	0.46
1:C:312:GLN:NE2	1:C:312:GLN:CA	2.79	0.46
2:D:8:LEU:HA	2:D:42:TYR:HB3	1.98	0.46
2:D:30:TYR:CE2	2:D:309:ARG:CD	2.99	0.46
1:A:73:THR:CB	1:A:76:ILE:CD1	2.93	0.46
1:A:105:ILE:HD12	1:A:128:MET:CE	2.46	0.46
2:B:246:TYR:HD2	2:B:247:LEU:HD22	1.81	0.46
1:C:111:ASP:O	1:C:114:PHE:N	2.46	0.46
1:C:250:TRP:CD1	1:C:251:TYR:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:LYS:CG	1:C:355:GLN:N	2.79	0.46
2:D:38:THR:CG2	2:D:39:LEU:N	2.76	0.46
2:D:82:HIS:HD2	2:D:84:VAL:N	2.00	0.46
2:D:95:GLN:CA	2:D:95:GLN:NE2	2.76	0.46
2:D:218:ASP:O	2:D:220:SER:N	2.47	0.46
1:A:242:ILE:HG22	1:A:243:CYS:N	2.29	0.46
1:C:3:PHE:CD2	1:C:348:MET:CE	2.99	0.46
1:C:304:PRO:O	1:C:308:ILE:HG13	2.16	0.46
1:A:24:LEU:O	1:A:24:LEU:HD12	2.16	0.45
1:A:47:THR:CG2	1:A:48:GLU:N	2.79	0.45
1:A:250:TRP:CD1	1:A:251:TYR:N	2.84	0.45
2:B:30:TYR:CE2	2:B:309:ARG:CD	2.99	0.45
2:B:123:SER:HB3	2:B:150:PHE:HZ	1.81	0.45
1:C:52:LEU:O	1:C:52:LEU:HG	2.14	0.45
1:A:11:GLN:HB2	1:A:51:LEU:HD11	1.98	0.45
1:A:52:LEU:CD1	1:A:58:ALA:HB2	2.46	0.45
1:A:159:ASN:HB3	1:A:160:PRO:HA	1.98	0.45
1:A:226:LEU:HG	1:A:320:ILE:HG21	1.98	0.45
1:A:304:PRO:O	1:A:308:ILE:HG13	2.16	0.45
2:B:51:VAL:HG13	2:B:51:VAL:O	2.16	0.45
2:B:95:GLN:HG3	2:B:160:PRO:HB2	1.97	0.45
1:C:47:THR:CG2	1:C:48:GLU:N	2.79	0.45
1:C:54:ASN:HD21	2:D:88:GLU:CB	2.28	0.45
1:C:110:TYR:CG	1:C:112:LYS:HE3	2.51	0.45
1:C:323:ILE:HD13	1:C:323:ILE:H	1.79	0.45
2:D:19:GLN:NE2	2:D:23:GLU:OE2	2.49	0.45
1:C:105:ILE:HD12	1:C:128:MET:CE	2.46	0.45
1:C:143:TYR:CD2	1:C:155:LYS:CE	3.00	0.45
1:C:197:ASN:H	1:C:200:GLU:HB2	1.82	0.45
2:D:30:TYR:CE2	2:D:309:ARG:HD3	2.52	0.45
2:D:76:HIS:HD1	2:D:76:HIS:HA	1.62	0.45
1:A:110:TYR:CG	1:A:112:LYS:HE3	2.51	0.45
2:B:159:ASN:HA	2:B:160:PRO:C	2.36	0.45
2:B:184:ALA:CB	2:B:208:TYR:CE1	2.99	0.45
1:C:188:LEU:HA	1:C:188:LEU:HD23	1.67	0.45
1:C:24:LEU:HD12	1:C:24:LEU:O	2.16	0.45
1:C:226:LEU:HG	1:C:320:ILE:HG21	1.98	0.45
1:C:332:SER:OG	1:C:333:GLU:N	2.49	0.45
1:A:143:TYR:O	1:A:144:ILE:HG12	2.16	0.45
1:A:354:LYS:CG	1:A:355:GLN:N	2.79	0.45
1:C:69:LEU:CG	1:C:70:ASN:N	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ASN:O	1:C:200:GLU:HB2	2.16	0.45
2:D:184:ALA:CB	2:D:208:TYR:CE1	2.99	0.45
2:D:247:LEU:N	2:D:247:LEU:CD2	2.79	0.45
1:A:143:TYR:CD2	1:A:155:LYS:CE	3.00	0.45
1:A:151:ILE:HD12	1:A:153:PHE:HE2	1.81	0.45
1:A:208:TYR:CD2	1:A:224:HIS:HE1	2.33	0.45
2:B:100:ARG:HH11	2:B:100:ARG:HD3	1.61	0.45
1:C:36:PHE:CE2	1:C:340:MET:CE	3.00	0.45
1:A:72:GLY:HA3	1:A:102:ARG:HB2	1.98	0.45
1:A:289:ASN:HB3	1:A:290:ARG:H	1.39	0.45
2:B:172:VAL:CG2	2:B:173:ASN:N	2.80	0.45
1:C:159:ASN:HB3	1:C:160:PRO:HA	1.98	0.45
2:D:51:VAL:O	2:D:51:VAL:HG13	2.16	0.45
1:A:105:ILE:HD12	1:A:128:MET:HE2	1.97	0.45
1:A:323:ILE:HD13	1:A:323:ILE:H	1.79	0.45
2:D:159:ASN:HA	2:D:160:PRO:C	2.36	0.45
2:D:172:VAL:O	2:D:190:LEU:HA	2.17	0.45
1:A:327:PHE:CD1	1:A:327:PHE:N	2.85	0.44
2:B:8:LEU:HA	2:B:42:TYR:HB3	1.98	0.44
2:B:227:THR:HA	2:B:296:LEU:O	2.18	0.44
1:C:52:LEU:CD1	1:C:58:ALA:HB2	2.46	0.44
2:D:246:TYR:HD2	2:D:247:LEU:HD22	1.81	0.44
1:A:241:ASP:O	1:A:244:ARG:N	2.50	0.44
1:A:312:GLN:NE2	1:A:312:GLN:CA	2.79	0.44
1:C:121:MET:HE1	1:C:267:THR:HG21	2.00	0.44
1:C:125:ARG:O	1:C:129:ASP:HB3	2.18	0.44
2:D:123:SER:HB3	2:D:150:PHE:HZ	1.81	0.44
1:A:189:PRO:HB3	1:A:223:ASP:O	2.17	0.44
1:A:207:LEU:O	1:A:207:LEU:HD12	2.18	0.44
2:B:30:TYR:CE2	2:B:309:ARG:HD3	2.52	0.44
2:B:172:VAL:O	2:B:190:LEU:HA	2.17	0.44
1:C:189:PRO:HB3	1:C:223:ASP:O	2.17	0.44
1:C:250:TRP:CD1	1:C:250:TRP:C	2.90	0.44
2:D:299:PHE:HB3	2:D:302:MET:HE3	1.99	0.44
2:B:247:LEU:N	2:B:247:LEU:CD2	2.79	0.44
1:A:197:ASN:H	1:A:200:GLU:HB2	1.82	0.44
2:D:227:THR:HA	2:D:296:LEU:O	2.18	0.44
1:A:72:GLY:CA	1:A:102:ARG:HB2	2.48	0.44
2:B:6:PHE:CE1	2:B:8:LEU:HD21	2.52	0.44
2:B:31:VAL:HG23	2:B:31:VAL:H	1.55	0.44
1:C:236:SER:HB2	1:C:240:LYS:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASP:O	1:A:114:PHE:N	2.46	0.44
1:C:11:GLN:HB2	1:C:51:LEU:HD11	1.98	0.44
1:C:241:ASP:O	1:C:244:ARG:N	2.50	0.44
1:A:36:PHE:CE2	1:A:340:MET:CE	3.00	0.44
1:A:112:LYS:NZ	1:A:113:ASP:OD1	2.44	0.44
2:B:82:HIS:HD2	2:B:84:VAL:N	2.00	0.44
2:B:106:SER:OG	2:B:107:ASP:O	2.36	0.44
1:C:207:LEU:O	1:C:207:LEU:HD12	2.18	0.44
2:D:126:GLN:HG3	2:D:126:GLN:H	1.39	0.44
2:D:195:ASP:O	2:D:263:LYS:NZ	2.47	0.44
1:A:183:ALA:O	1:A:187:GLY:N	2.51	0.43
1:A:194:TRP:HB3	1:A:227:SER:O	2.18	0.43
1:C:72:GLY:CA	1:C:102:ARG:HB2	2.48	0.43
1:C:94:ASP:OD1	1:C:164:THR:OG1	2.36	0.43
1:C:327:PHE:CD1	1:C:327:PHE:N	2.85	0.43
2:D:131:CYS:O	2:D:135:ILE:HG13	2.18	0.43
2:D:213:GLN:HB3	2:D:214:ALA:H	1.53	0.43
2:D:268:LEU:HA	2:D:268:LEU:HD12	1.44	0.43
1:C:194:TRP:HB3	1:C:227:SER:O	2.18	0.43
1:A:236:SER:HB2	1:A:240:LYS:HE3	2.00	0.43
1:C:209:ASN:O	1:C:213:THR:OG1	2.28	0.43
1:C:349:PRO:HB2	1:C:350:TYR:CD1	2.53	0.43
1:A:250:TRP:CD1	1:A:250:TRP:C	2.90	0.43
1:C:300:PRO:HG3	1:C:311:ILE:HD13	1.99	0.43
2:D:100:ARG:HH11	2:D:100:ARG:HD3	1.61	0.43
2:D:190:LEU:HD12	2:D:224:HIS:ND1	2.32	0.43
1:A:293:ASP:OD1	1:A:293:ASP:N	2.52	0.43
1:A:125:ARG:O	1:A:129:ASP:HB3	2.18	0.43
2:B:38:THR:CG2	2:B:39:LEU:N	2.76	0.43
2:B:299:PHE:HB3	2:B:302:MET:HE3	2.00	0.43
1:C:154:PRO:HD2	2:D:116:PHE:CD2	2.54	0.43
2:D:106:SER:OG	2:D:107:ASP:O	2.36	0.43
1:A:3:PHE:CE2	1:A:348:MET:HG2	2.54	0.43
2:B:190:LEU:HD12	2:B:224:HIS:ND1	2.32	0.43
2:B:231:ASN:C	2:B:231:ASN:ND2	2.72	0.43
2:D:164:THR:HG22	2:D:167:GLY:O	2.19	0.43
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.67	0.43
2:B:164:THR:HG22	2:B:167:GLY:O	2.19	0.43
2:B:195:ASP:O	2:B:263:LYS:NZ	2.47	0.43
2:D:231:ASN:C	2:D:231:ASN:ND2	2.72	0.43
1:A:349:PRO:HB2	1:A:350:TYR:CD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLN:HB3	2:B:214:ALA:H	1.53	0.42
1:C:192:LEU:HD12	1:C:225:CYS:O	2.19	0.42
1:A:94:ASP:OD1	1:A:164:THR:OG1	2.36	0.42
1:A:110:TYR:HB2	1:A:112:LYS:HE3	2.01	0.42
1:A:191:ILE:HG23	1:A:225:CYS:CB	2.45	0.42
1:A:192:LEU:HD12	1:A:225:CYS:O	2.19	0.42
2:B:131:CYS:O	2:B:135:ILE:HG13	2.18	0.42
1:A:3:PHE:CE1	1:A:323:ILE:HD11	2.54	0.42
2:B:144:CYS:O	2:B:155:LYS:HA	2.19	0.42
2:B:232:GLN:HG2	2:B:279:SER:CB	2.50	0.42
1:C:48:GLU:H	1:C:48:GLU:HG3	1.56	0.42
1:C:184:ALA:CA	1:C:208:TYR:HE1	2.32	0.42
1:C:259:LYS:CG	1:C:260:ILE:N	2.78	0.42
2:D:12:ASN:HD21	2:D:15:ARG:HD3	1.84	0.42
2:D:231:ASN:HB3	2:D:273:ILE:HG23	2.01	0.42
1:A:3:PHE:CD2	1:A:348:MET:HE2	2.54	0.42
1:A:300:PRO:HG3	1:A:311:ILE:HD13	1.99	0.42
1:C:3:PHE:CE2	1:C:348:MET:HG2	2.54	0.42
1:C:293:ASP:OD1	1:C:293:ASP:N	2.52	0.42
2:D:25:LEU:HA	2:D:25:LEU:HD23	1.70	0.42
2:D:144:CYS:O	2:D:155:LYS:HA	2.19	0.42
1:A:154:PRO:HD2	2:B:116:PHE:CD2	2.54	0.42
1:C:106:CYS:CB	1:C:173:VAL:HG22	2.36	0.42
1:C:183:ALA:O	1:C:187:GLY:N	2.51	0.42
1:C:26:ASN:N	1:C:26:ASN:ND2	2.67	0.42
1:C:121:MET:CE	1:C:267:THR:HG21	2.49	0.42
1:C:129:ASP:O	1:C:132:TYR:HB3	2.20	0.42
1:C:338:ALA:O	1:C:342:LEU:HB2	2.20	0.42
1:A:121:MET:CE	1:A:267:THR:HG21	2.49	0.42
1:A:218:ASP:OD1	1:A:220:THR:OG1	2.28	0.42
1:A:256:ASN:O	1:A:258:THR:N	2.53	0.42
2:B:246:TYR:HD2	2:B:247:LEU:CD2	2.32	0.42
1:C:43:GLU:HB2	1:C:55:PRO:HG3	2.02	0.42
1:C:102:ARG:HH11	1:C:102:ARG:HD3	1.74	0.42
2:D:246:TYR:HD2	2:D:247:LEU:CD2	2.32	0.42
1:A:144:ILE:HG22	1:A:153:PHE:CE1	2.55	0.42
2:D:8:LEU:N	2:D:300:GLU:OE2	2.32	0.42
2:D:232:GLN:HG2	2:D:279:SER:CB	2.50	0.42
2:B:56:LEU:HD23	2:B:56:LEU:HA	1.94	0.42
1:A:1:MET:HB2	1:A:2:LYS:H	1.56	0.41
1:A:129:ASP:O	1:A:132:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:LYS:O	2:B:294:ASP:HA	2.20	0.41
2:B:10:PHE:CD1	2:B:49:ASN:CA	3.02	0.41
2:B:12:ASN:HD21	2:B:15:ARG:HD3	1.84	0.41
1:C:3:PHE:CE1	1:C:323:ILE:HD11	2.54	0.41
1:C:144:ILE:HG22	1:C:153:PHE:CE1	2.55	0.41
1:C:308:ILE:O	1:C:308:ILE:HG22	2.20	0.41
2:D:62:LEU:HA	2:D:65:MET:HE3	2.01	0.41
2:D:178:GLU:O	2:D:181:GLU:HG2	2.20	0.41
1:A:338:ALA:O	1:A:342:LEU:HB2	2.20	0.41
1:A:160:PRO:HB2	2:B:17:SER:HB2	2.02	0.41
2:B:6:PHE:HA	2:B:40:ALA:O	2.20	0.41
2:B:114:MET:CE	2:B:124:GLN:HG3	2.50	0.41
2:B:194:TRP:HB3	2:B:227:THR:O	2.20	0.41
2:D:6:PHE:HA	2:D:40:ALA:O	2.20	0.41
2:B:259:ASP:HB3	2:B:262:GLN:HG2	2.03	0.41
2:D:10:PHE:CD1	2:D:49:ASN:CA	3.02	0.41
1:A:49:PHE:HZ	1:A:250:TRP:CH2	2.39	0.41
1:A:332:SER:OG	1:A:333:GLU:N	2.49	0.41
2:B:62:LEU:HA	2:B:65:MET:HE3	2.02	0.41
2:D:114:MET:CE	2:D:124:GLN:HG3	2.50	0.41
1:A:226:LEU:CG	1:A:323:ILE:HG22	2.51	0.41
2:B:19:GLN:O	2:B:23:GLU:HG3	2.21	0.41
1:C:49:PHE:HZ	1:C:250:TRP:CH2	2.39	0.41
2:D:259:ASP:HB3	2:D:262:GLN:HG2	2.03	0.41
2:B:143:TYR:CD2	2:B:155:LYS:HE3	2.56	0.41
1:C:110:TYR:HB2	1:C:112:LYS:HE3	2.01	0.41
1:A:6:PHE:HD1	1:A:7:LEU:N	2.19	0.41
2:B:178:GLU:O	2:B:181:GLU:HG2	2.20	0.41
2:B:231:ASN:HB3	2:B:273:ILE:HG23	2.01	0.41
1:C:6:PHE:HD1	1:C:7:LEU:N	2.19	0.41
1:C:160:PRO:HB2	2:D:17:SER:HB2	2.02	0.41
1:C:226:LEU:CG	1:C:323:ILE:HG22	2.51	0.41
1:A:81:ALA:O	1:A:131:TRP:NE1	2.48	0.41
1:A:93:LEU:HD12	1:A:93:LEU:HA	1.92	0.41
1:A:308:ILE:O	1:A:308:ILE:HG22	2.20	0.41
2:B:62:LEU:HD12	2:B:65:MET:CE	2.51	0.41
2:B:119:ARG:HA	2:B:120:PRO:HD3	1.94	0.41
2:B:244:ARG:HB2	2:B:264:MET:SD	2.61	0.41
2:B:246:TYR:CD2	2:B:247:LEU:HD22	2.56	0.41
1:C:1:MET:HB3	1:C:321:ASP:HB2	2.03	0.41
1:C:37:ASP:O	1:C:70:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:GLN:O	2:D:23:GLU:HG3	2.21	0.41
2:D:56:LEU:HD23	2:D:56:LEU:HA	1.94	0.41
2:D:62:LEU:HD12	2:D:65:MET:CE	2.51	0.41
2:D:194:TRP:HB3	2:D:227:THR:O	2.20	0.41
1:A:37:ASP:O	1:A:70:ASN:HB2	2.21	0.41
1:A:64:GLY:HA2	2:B:61:PHE:CZ	2.56	0.41
2:B:111:SER:O	2:B:114:MET:HB3	2.21	0.41
1:C:3:PHE:CD2	1:C:348:MET:HE3	2.56	0.41
1:C:256:ASN:O	1:C:258:THR:N	2.53	0.41
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.78	0.40
1:A:156:ILE:H	1:A:156:ILE:HG13	1.59	0.40
1:C:73:THR:CB	1:C:76:ILE:CD1	2.93	0.40
1:C:172:VAL:O	1:C:190:MET:HB2	2.21	0.40
1:C:310:ILE:HG23	1:C:310:ILE:HD12	1.79	0.40
2:D:2:LYS:O	2:D:294:ASP:HA	2.20	0.40
2:D:15:ARG:HB3	2:D:19:GLN:OE1	2.21	0.40
1:A:43:GLU:HB2	1:A:55:PRO:HG3	2.02	0.40
1:A:172:VAL:O	1:A:190:MET:HB2	2.21	0.40
1:A:310:ILE:HG23	1:A:310:ILE:HD12	1.79	0.40
2:B:31:VAL:HG12	2:B:36:PHE:HB2	2.03	0.40
2:B:155:LYS:CG	2:B:156:ILE:N	2.84	0.40
2:B:305:LYS:O	2:B:309:ARG:N	2.48	0.40
2:D:31:VAL:HG12	2:D:36:PHE:HB2	2.03	0.40
2:B:12:ASN:HB2	2:B:13:SER:H	1.59	0.40
1:C:323:ILE:HD13	1:C:323:ILE:HG23	1.77	0.40
1:A:81:ALA:HB3	1:A:86:GLN:CD	2.42	0.40
2:B:10:PHE:CE1	2:B:49:ASN:C	2.95	0.40
2:D:244:ARG:HB2	2:D:264:MET:SD	2.61	0.40
1:A:1:MET:HB3	1:A:321:ASP:HB2	2.03	0.40
1:C:81:ALA:HB3	1:C:86:GLN:CD	2.42	0.40
2:D:30:TYR:CE2	2:D:309:ARG:HD2	2.57	0.40
2:D:66:THR:OG1	2:D:100:ARG:NH2	2.54	0.40
2:D:246:TYR:CD2	2:D:247:LEU:HD22	2.56	0.40

All (15) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:SER:O	2:D:237:GLU:CD[4_467]	0.67	1.53
1:C:345:SER:O	2:D:237:GLU:OE2[4_467]	0.78	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:GLU:OE2	2:D:26:ASP:OD2[4_567]	1.08	1.12
1:A:237:ASN:ND2	1:C:291:ARG:CB[2_464]	1.10	1.10
1:C:345:SER:C	2:D:237:GLU:OE2[4_467]	1.38	0.82
1:A:237:ASN:ND2	1:C:291:ARG:CG[2_464]	1.46	0.74
1:C:141:GLU:CD	2:D:26:ASP:OD2[4_567]	1.46	0.74
1:C:345:SER:C	2:D:237:GLU:CD[4_467]	1.57	0.63
1:C:345:SER:O	2:D:237:GLU:CG[4_467]	1.63	0.57
1:C:268:LYS:CB	4:B:2119:HOH:O[4_566]	1.75	0.45
1:C:141:GLU:OE1	2:D:26:ASP:OD2[4_567]	1.84	0.36
1:C:345:SER:O	2:D:237:GLU:OE1[4_467]	1.94	0.26
1:C:268:LYS:N	4:B:2119:HOH:O[4_566]	2.01	0.19
1:C:346:ASP:CG	2:D:237:GLU:OE1[4_467]	2.09	0.11
1:C:346:ASP:N	2:D:237:GLU:OE2[4_467]	2.10	0.10

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	336/355 (95%)	288 (86%)	36 (11%)	12 (4%)	3	3
1	C	336/355 (95%)	288 (86%)	36 (11%)	12 (4%)	3	3
2	B	317/324 (98%)	265 (84%)	42 (13%)	10 (3%)	4	3
2	D	317/324 (98%)	265 (84%)	42 (13%)	10 (3%)	4	3
All	All	1306/1358 (96%)	1106 (85%)	156 (12%)	44 (3%)	3	3

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ASP
1	A	257	ALA
1	A	260	ILE
1	A	263	ASP

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Mol	Chain	Res	Type
1	A	270	TYR
1	A	288	THR
2	B	162	ALA
2	B	214	ALA
2	B	219	VAL
2	B	256	SER
2	B	259	ASP
1	C	147	ASP
1	C	257	ALA
1	C	260	ILE
1	C	263	ASP
1	C	270	TYR
1	C	288	THR
2	D	162	ALA
2	D	214	ALA
2	D	219	VAL
2	D	256	SER
2	D	259	ASP
1	A	124	SER
1	A	331	GLY
1	A	353	GLU
2	B	213	GLN
1	C	124	SER
1	C	331	GLY
1	C	353	GLU
2	D	213	GLN
2	D	317	ALA
1	A	150	HIS
2	B	124	GLN
2	B	146	PRO
2	B	317	ALA
1	C	150	HIS
2	D	124	GLN
2	D	146	PRO
2	B	257	ASN
2	D	257	ASN
1	A	316	ASP
1	C	316	ASP
1	A	300	PRO
1	C	300	PRO

5.3.2 Protein sidechains (i)

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	286/303 (94%)	214 (75%)	72 (25%)	0	0
1	C	286/303 (94%)	215 (75%)	71 (25%)	0	0
2	B	265/274 (97%)	206 (78%)	59 (22%)	1	1
2	D	265/274 (97%)	206 (78%)	59 (22%)	1	1
All	All	1102/1154 (96%)	841 (76%)	261 (24%)	1	1

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	PHE
1	A	8	LEU
1	A	9	THR
1	A	15	LEU
1	A	22	LYS
1	A	23	ARG
1	A	24	LEU
1	A	37	ASP
1	A	42	LEU
1	A	46	PHE
1	A	48	GLU
1	A	62	LEU
1	A	76	ILE
1	A	92	LEU
1	A	93	LEU
1	A	95	GLN
1	A	106	CYS
1	A	107	ARG
1	A	109	LEU
1	A	112	LYS
1	A	115	ARG
1	A	123	ASN
1	A	124	SER

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Mol	Chain	Res	Type
1	A	125	ARG
1	A	127	LEU
1	A	128	MET
1	A	129	ASP
1	A	131	TRP
1	A	137	GLU
1	A	140	ASN
1	A	148	ASN
1	A	151	ILE
1	A	152	LYS
1	A	156	ILE
1	A	164	THR
1	A	176	SER
1	A	178	SER
1	A	186	ARG
1	A	191	ILE
1	A	199	HIS
1	A	205	LEU
1	A	207	LEU
1	A	213	THR
1	A	224	HIS
1	A	225	CYS
1	A	227	SER
1	A	238	ARG
1	A	258	THR
1	A	259	LYS
1	A	260	ILE
1	A	263	ASP
1	A	265	ASP
1	A	266	GLN
1	A	270	TYR
1	A	289	ASN
1	A	290	ARG
1	A	308	ILE
1	A	310	ILE
1	A	311	ILE
1	A	312	GLN
1	A	318	THR
1	A	323	ILE
1	A	324	CYS
1	A	332	SER
1	A	339	SER

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Mol	Chain	Res	Type
1	A	340	MET
1	A	342	LEU
1	A	345	SER
1	A	346	ASP
1	A	350	TYR
1	A	351	LEU
2	B	1	MET
2	B	6	PHE
2	B	12	ASN
2	B	15	ARG
2	B	17	SER
2	B	18	ASP
2	B	19	GLN
2	B	37	ASP
2	B	51	VAL
2	B	62	LEU
2	B	65	MET
2	B	70	LYS
2	B	81	HIS
2	B	106	SER
2	B	115	ARG
2	B	119	ARG
2	B	122	ASP
2	B	123	SER
2	B	124	GLN
2	B	126	GLN
2	B	129	SER
2	B	140	THR
2	B	144	CYS
2	B	149	ASP
2	B	152	SER
2	B	157	SER
2	B	175	THR
2	B	176	SER
2	B	177	LYS
2	B	181	GLU
2	B	190	LEU
2	B	200	GLN
2	B	207	LEU
2	B	210	GLU
2	B	213	GLN
2	B	223	ARG

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Mol	Chain	Res	Type
2	B	224	HIS
2	B	225	LYS
2	B	228	LEU
2	B	231	ASN
2	B	233	ASN
2	B	253	GLU
2	B	256	SER
2	B	259	ASP
2	B	261	GLU
2	B	262	GLN
2	B	269	SER
2	B	273	ILE
2	B	275	THR
2	B	277	GLU
2	B	281	GLN
2	B	284	ARG
2	B	295	LEU
2	B	301	SER
2	B	303	GLU
2	B	307	GLN
2	B	309	ARG
2	B	318	ASN
2	B	319	ILE
1	C	1	MET
1	C	8	LEU
1	C	9	THR
1	C	15	LEU
1	C	22	LYS
1	C	23	ARG
1	C	24	LEU
1	C	37	ASP
1	C	42	LEU
1	C	46	PHE
1	C	48	GLU
1	C	62	LEU
1	C	76	ILE
1	C	92	LEU
1	C	93	LEU
1	C	95	GLN
1	C	106	CYS
1	C	107	ARG
1	C	109	LEU

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Mol	Chain	Res	Type
1	C	112	LYS
1	C	115	ARG
1	C	123	ASN
1	C	124	SER
1	C	125	ARG
1	C	127	LEU
1	C	128	MET
1	C	129	ASP
1	C	131	TRP
1	C	137	GLU
1	C	140	ASN
1	C	148	ASN
1	C	151	ILE
1	C	152	LYS
1	C	156	ILE
1	C	164	THR
1	C	176	SER
1	C	178	SER
1	C	186	ARG
1	C	191	ILE
1	C	199	HIS
1	C	205	LEU
1	C	207	LEU
1	C	213	THR
1	C	224	HIS
1	C	225	CYS
1	C	227	SER
1	C	238	ARG
1	C	258	THR
1	C	259	LYS
1	C	260	ILE
1	C	263	ASP
1	C	265	ASP
1	C	266	GLN
1	C	270	TYR
1	C	289	ASN
1	C	290	ARG
1	C	308	ILE
1	C	310	ILE
1	C	311	ILE
1	C	312	GLN
1	C	318	THR

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Mol	Chain	Res	Type
1	C	323	ILE
1	C	324	CYS
1	C	332	SER
1	C	339	SER
1	C	340	MET
1	C	342	LEU
1	C	345	SER
1	C	346	ASP
1	C	350	TYR
1	C	351	LEU
2	D	1	MET
2	D	6	PHE
2	D	12	ASN
2	D	15	ARG
2	D	17	SER
2	D	18	ASP
2	D	19	GLN
2	D	37	ASP
2	D	51	VAL
2	D	62	LEU
2	D	65	MET
2	D	70	LYS
2	D	81	HIS
2	D	106	SER
2	D	115	ARG
2	D	119	ARG
2	D	122	ASP
2	D	123	SER
2	D	124	GLN
2	D	126	GLN
2	D	129	SER
2	D	140	THR
2	D	144	CYS
2	D	149	ASP
2	D	152	SER
2	D	157	SER
2	D	175	THR
2	D	176	SER
2	D	177	LYS
2	D	181	GLU
2	D	190	LEU
2	D	200	GLN

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Mol	Chain	Res	Type
2	D	207	LEU
2	D	210	GLU
2	D	213	GLN
2	D	223	ARG
2	D	224	HIS
2	D	225	LYS
2	D	228	LEU
2	D	231	ASN
2	D	233	ASN
2	D	253	GLU
2	D	256	SER
2	D	259	ASP
2	D	261	GLU
2	D	262	GLN
2	D	269	SER
2	D	273	ILE
2	D	275	THR
2	D	277	GLU
2	D	281	GLN
2	D	284	ARG
2	D	295	LEU
2	D	301	SER
2	D	303	GLU
2	D	307	GLN
2	D	309	ARG
2	D	318	ASN
2	D	319	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	54	ASN
1	A	61	HIS
1	A	82	HIS
1	A	86	GLN
1	A	95	GLN
1	A	148	ASN
1	A	157	GLN
1	A	165	GLN
1	A	204	GLN
1	A	224	HIS

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Mol	Chain	Res	Type
1	A	256	ASN
1	A	322	ASN
1	A	330	ASN
2	B	9	ASN
2	B	49	ASN
2	B	81	HIS
2	B	82	HIS
2	B	95	GLN
2	B	118	ASN
2	B	145	HIS
2	B	200	GLN
2	B	209	HIS
2	B	215	HIS
2	B	231	ASN
2	B	232	GLN
2	B	233	ASN
2	B	257	ASN
2	B	308	GLN
2	B	318	ASN
1	C	26	ASN
1	C	54	ASN
1	C	61	HIS
1	C	82	HIS
1	C	86	GLN
1	C	95	GLN
1	C	148	ASN
1	C	157	GLN
1	C	165	GLN
1	C	204	GLN
1	C	224	HIS
1	C	256	ASN
1	C	322	ASN
1	C	330	ASN
2	D	49	ASN
2	D	81	HIS
2	D	82	HIS
2	D	95	GLN
2	D	118	ASN
2	D	145	HIS
2	D	200	GLN
2	D	209	HIS
2	D	215	HIS

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Mol	Chain	Res	Type
2	D	231	ASN
2	D	232	GLN
2	D	233	ASN
2	D	257	ASN
2	D	308	GLN
2	D	318	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	PO4	A	356	-	4,4,4	2.71	4 (100%)	6,6,6	0.61	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	356	PO4	P-O2	-3.00	1.45	1.54
3	A	356	PO4	P-O4	-2.99	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	356	PO4	P-O3	-2.65	1.46	1.54
3	A	356	PO4	P-O1	-2.11	1.45	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	356	PO4	2	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.