



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:51 AM UTC

PDB ID : 2IXP / pdb_00002ixp
Title : Crystal structure of the Pp2A phosphatase activator Ypa1 PTPA1 in complex with model substrate
Authors : Leulliot, N.; Vicentini, G.; Jordens, J.; Quevillon-Cheruel, S.; Schiltz, M.; Barford, D.; Van Tilbeurgh, H.; Goris, J.
Deposited on : 2006-07-09
Resolution : 2.80 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:

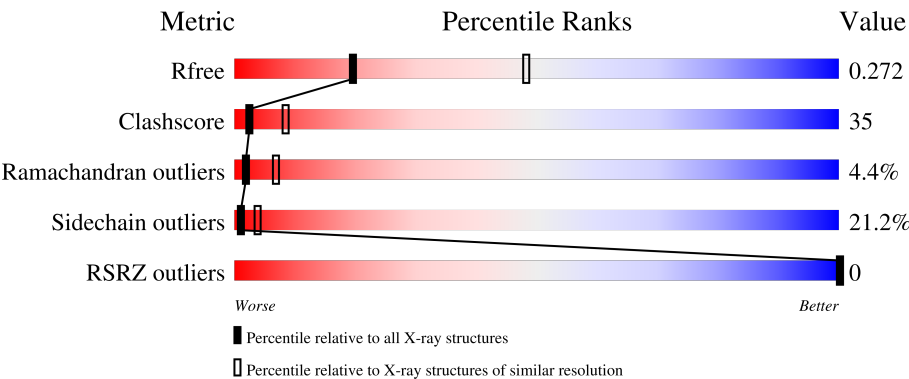
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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.



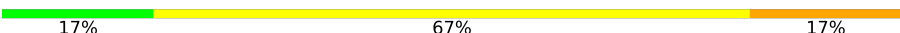
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	323	33%45%15%. .
1	B	323	37%42%14%5%. .
1	C	323	32%46%17%. .
1	D	323	36%44%13%. .
2	F	6	83%17%

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Mol	Chain	Length	Quality of chain
2	G	6	 33% 67%
2	H	6	 50% 33% 17%
2	I	6	 17% 67% 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	SO4	A	1320	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10394 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 SERINE/THREONINE-PROTEIN PHOSPHATASE 2A ACTIVATOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2524	1642	421	447	14			
1	B	316	Total	C	N	O	S	0	0	0
			2576	1675	433	454	14			
1	C	316	Total	C	N	O	S	0	0	0
			2576	1675	433	454	14			
1	D	310	Total	C	N	O	S	0	0	0
			2524	1642	421	447	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	HIS	-	expression tag	UNP P40454
A	319	HIS	-	expression tag	UNP P40454
A	320	HIS	-	expression tag	UNP P40454
A	321	HIS	-	expression tag	UNP P40454
A	322	HIS	-	expression tag	UNP P40454
A	323	HIS	-	expression tag	UNP P40454
B	318	HIS	-	expression tag	UNP P40454
B	319	HIS	-	expression tag	UNP P40454
B	320	HIS	-	expression tag	UNP P40454
B	321	HIS	-	expression tag	UNP P40454
B	322	HIS	-	expression tag	UNP P40454
B	323	HIS	-	expression tag	UNP P40454
C	318	HIS	-	expression tag	UNP P40454
C	319	HIS	-	expression tag	UNP P40454
C	320	HIS	-	expression tag	UNP P40454
C	321	HIS	-	expression tag	UNP P40454
C	322	HIS	-	expression tag	UNP P40454
C	323	HIS	-	expression tag	UNP P40454
D	318	HIS	-	expression tag	UNP P40454
D	319	HIS	-	expression tag	UNP P40454

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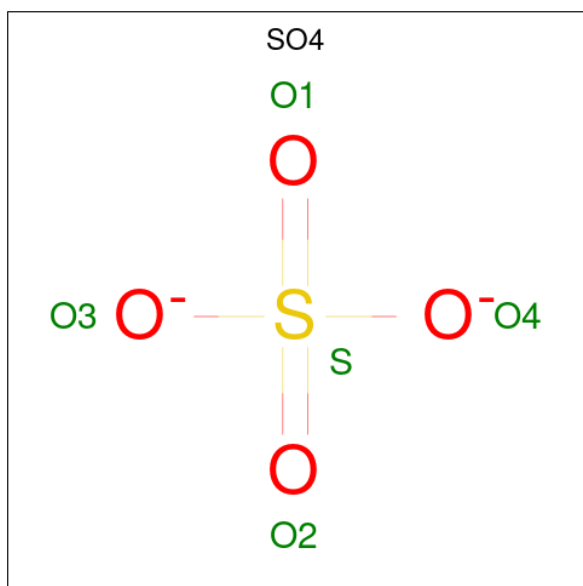
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Chain	Residue	Modelled	Actual	Comment	Reference
D	320	HIS	-	expression tag	UNP P40454
D	321	HIS	-	expression tag	UNP P40454
D	322	HIS	-	expression tag	UNP P40454
D	323	HIS	-	expression tag	UNP P40454

- Molecule 2 is a protein called SIN-ALA-ALA-PRO-LYS-NIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	6	Total	C	N	O	0	0	0
			43	27	7	9			
2	G	6	Total	C	N	O	0	0	0
			43	27	7	9			
2	H	6	Total	C	N	O	0	0	0
			43	27	7	9			
2	I	6	Total	C	N	O	0	0	0
			43	27	7	9			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	1
			5	4	1		

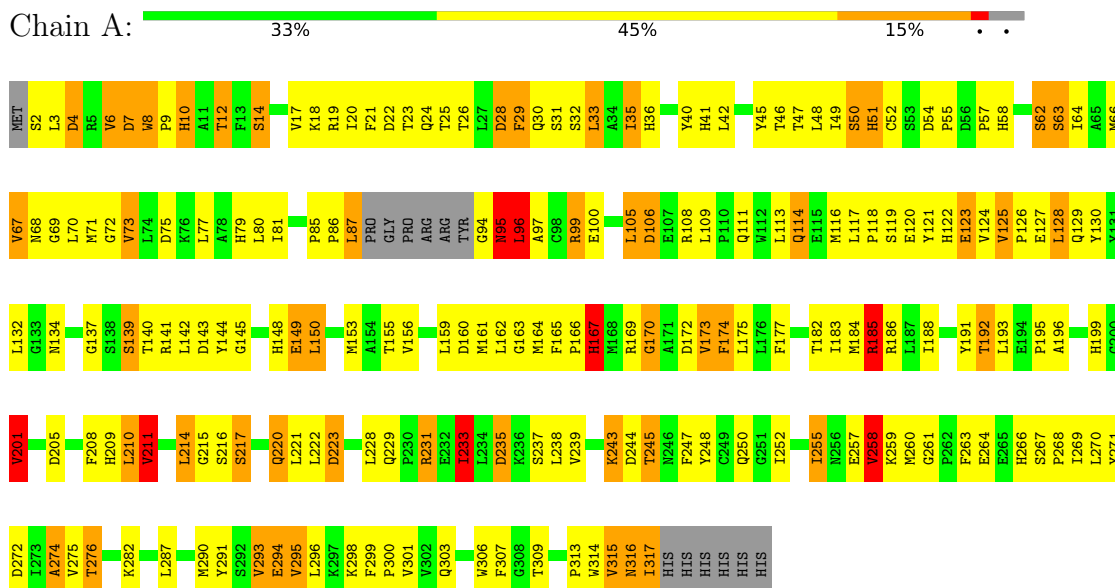
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

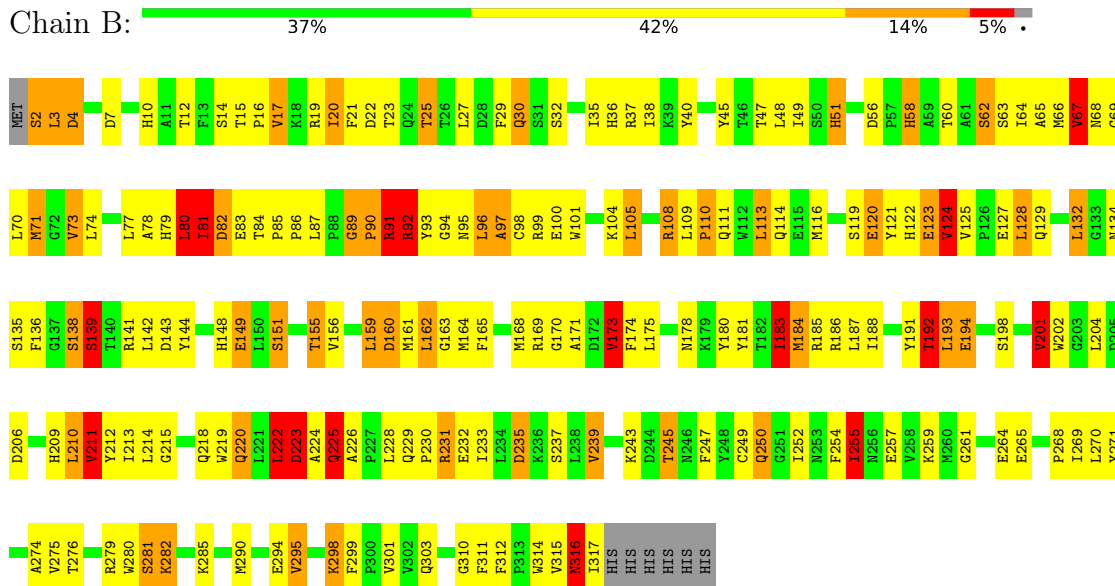
3 Residue-property plots

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.

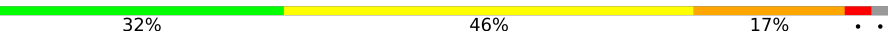
• Molecule 1: SERINE/THREONINE-PROTEIN PHOSPHATASE 2A ACTIVATOR 1

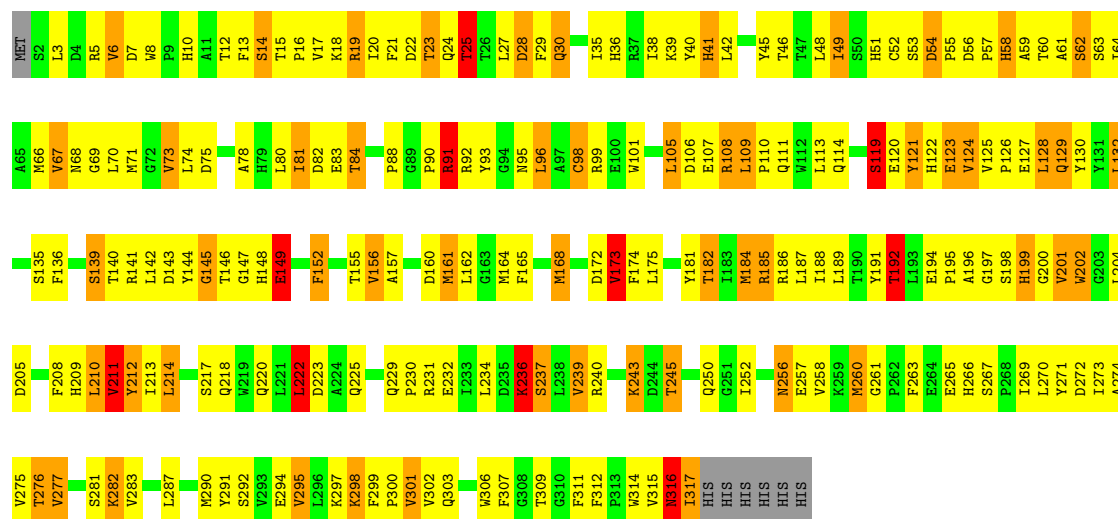


• Molecule 1: SERINE/THREONINE-PROTEIN PHOSPHATASE 2A ACTIVATOR 1

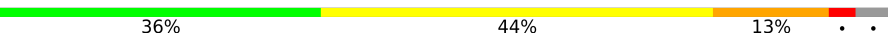


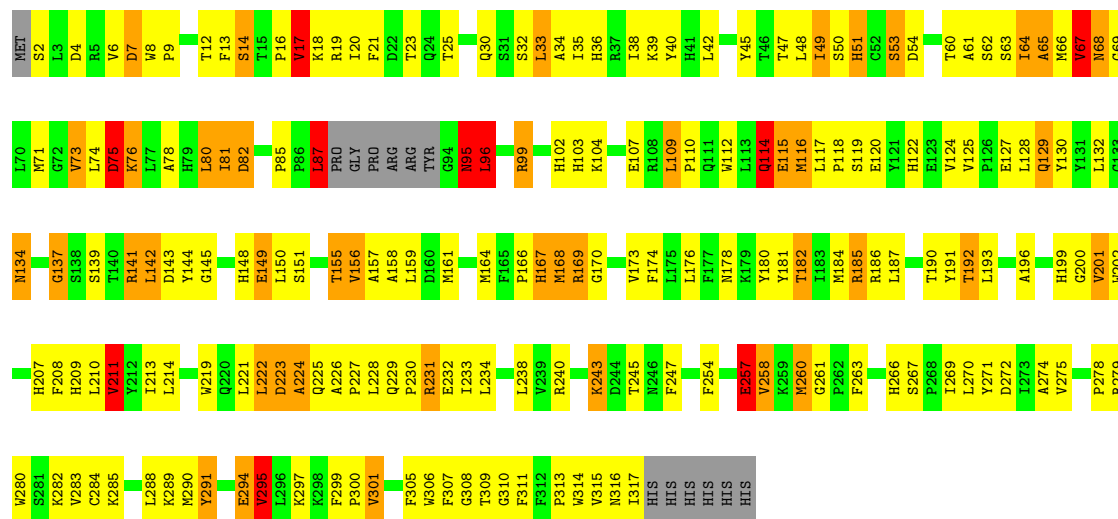
• Molecule 1: SERINE/THREONINE-PROTEIN PHOSPHATASE 2A ACTIVATOR 1

Chain C:  32% 46% 17% . .

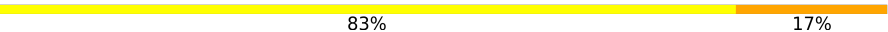


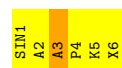
• Molecule 1: SERINE/THREONINE-PROTEIN PHOSPHATASE 2A ACTIVATOR 1

Chain D:  36% 44% 13% . .



• Molecule 2: SIN-ALA-ALA-PRO-LYS-NIT

Chain F:  83% 17%



• Molecule 2: SIN-ALA-ALA-PRO-LYS-NIT

Chain G:  33% 67%



- Molecule 2: SIN-ALA-ALA-PRO-LYS-NIT



- Molecule 2: SIN-ALA-ALA-PRO-LYS-NIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	86.89Å 86.89Å 410.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.12 – 2.80 29.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.12-2.80) 99.9 (29.12-2.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.302 0.238 , 0.272	Depositor DCC
R_{free} test set	2158 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.715	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 13.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.439 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10394	wwPDB-VP
Average B, all atoms (Å ²)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4694e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NIT, SO4, SIN, CL

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	1.40	13/2604 (0.5%)	1.53	33/3543 (0.9%)
1	B	1.34	5/2660 (0.2%)	1.56	50/3621 (1.4%)
1	C	1.36	12/2660 (0.5%)	1.60	44/3621 (1.2%)
1	D	1.33	7/2604 (0.3%)	1.59	48/3543 (1.4%)
2	F	1.54	0/26	2.02	2/34 (5.9%)
2	G	2.42	1/26 (3.8%)	1.73	2/34 (5.9%)
2	H	2.12	1/26 (3.8%)	1.62	0/34
2	I	2.87	2/26 (7.7%)	2.54	3/34 (8.8%)
All	All	1.37	41/10632 (0.4%)	1.57	182/14464 (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
1	B	0	1
1	D	0	3
All	All	0	4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	5	LYS	C-O	11.03	1.45	1.23
2	G	5	LYS	C-O	10.50	1.44	1.23
2	H	5	LYS	C-O	8.48	1.40	1.23
1	A	85	PRO	CA-C	8.02	1.59	1.52
1	A	185	ARG	CB-CG	7.47	1.74	1.52
1	B	194	GLU	N-CA	-7.43	1.39	1.45
2	I	5	LYS	CA-C	7.21	1.68	1.52
1	D	96	LEU	CA-C	7.12	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	PRO	CA-C	6.92	1.60	1.52
1	C	145	GLY	C-O	6.63	1.30	1.23
1	A	233	ILE	CG1-CD1	6.49	1.77	1.51
1	C	98	CYS	N-CA	-6.26	1.38	1.46
1	C	174	PHE	CA-C	-6.20	1.44	1.52
1	A	20	ILE	CA-CB	-6.12	1.46	1.54
1	C	38	ILE	CA-CB	-6.07	1.47	1.54
1	A	96	LEU	CA-C	5.85	1.60	1.52
1	A	188	ILE	CA-CB	-5.75	1.48	1.54
1	D	142	LEU	CA-C	5.70	1.60	1.52
1	A	201	VAL	CA-CB	-5.61	1.46	1.54
1	C	155	THR	CA-CB	5.59	1.62	1.53
1	B	17	VAL	CA-C	5.56	1.58	1.52
1	C	25	THR	CA-C	5.54	1.60	1.52
1	B	139	SER	CA-C	5.51	1.60	1.52
1	A	106	ASP	CA-C	-5.49	1.45	1.52
1	C	194	GLU	CG-CD	5.43	1.65	1.52
1	C	35	ILE	CA-CB	5.42	1.61	1.54
1	A	239	VAL	CA-CB	-5.39	1.47	1.54
1	C	315	VAL	CA-CB	5.35	1.62	1.54
1	C	41	HIS	CA-C	-5.33	1.45	1.52
1	B	255	ILE	CA-CB	5.26	1.61	1.54
1	A	211	VAL	CA-C	-5.17	1.46	1.52
1	C	52	CYS	N-CA	-5.17	1.40	1.46
1	D	180	TYR	N-CA	-5.15	1.40	1.46
1	D	185	ARG	CB-CG	5.12	1.67	1.52
1	B	180	TYR	N-CA	-5.10	1.40	1.46
1	D	33	LEU	CA-C	-5.05	1.46	1.52
1	D	85	PRO	CA-C	5.05	1.56	1.52
1	A	75	ASP	N-CA	-5.03	1.39	1.46
1	A	274	ALA	N-CA	-5.01	1.40	1.46
1	C	205	ASP	N-CA	5.01	1.52	1.46
1	D	95	ASN	N-CA	5.00	1.52	1.46

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	VAL	N-CA-C	-12.33	98.04	110.62
1	D	95	ASN	N-CA-C	10.80	127.10	107.99
1	B	89	GLY	CA-C-N	10.61	133.11	119.84
1	B	89	GLY	C-N-CA	10.61	133.11	119.84
1	C	258	VAL	N-CA-C	9.64	120.46	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	GLN	CA-C-N	-9.33	109.30	119.19
1	A	229	GLN	C-N-CA	-9.33	109.30	119.19
1	D	295	VAL	N-CA-C	9.10	119.38	111.56
1	B	173	VAL	N-CA-C	-8.98	101.65	110.72
1	D	109	LEU	CA-C-N	-8.78	109.31	119.32
1	D	109	LEU	C-N-CA	-8.78	109.31	119.32
1	A	95	ASN	N-CA-C	8.76	122.94	108.49
1	C	237	SER	N-CA-C	8.75	121.92	111.33
1	B	149	GLU	N-CA-C	-8.70	101.73	111.82
1	B	71	MET	N-CA-C	-8.46	102.00	111.14
1	D	125	VAL	CA-C-N	-8.44	110.95	119.56
1	D	125	VAL	C-N-CA	-8.44	110.95	119.56
1	B	132	LEU	N-CA-C	-8.43	102.06	111.07
1	A	99	ARG	N-CA-C	-8.34	102.15	111.82
1	B	51	HIS	N-CA-C	-8.23	103.38	113.50
1	C	147	GLY	N-CA-C	8.06	122.66	112.83
1	C	51	HIS	N-CA-C	-8.02	103.63	113.41
1	B	108	ARG	N-CA-C	8.01	120.01	111.28
2	I	5	LYS	CB-CA-C	7.98	125.26	110.10
1	C	311	PHE	N-CA-C	7.98	119.75	111.14
1	A	33	LEU	N-CA-C	-7.90	102.67	111.28
1	C	245	THR	N-CA-C	-7.85	103.84	113.50
1	C	155	THR	N-CA-C	-7.79	102.74	111.07
1	A	209	HIS	N-CA-C	-7.61	105.16	114.75
1	A	245	THR	CB-CA-C	7.49	121.55	109.27
1	C	298	LYS	CA-C-N	7.48	129.06	119.78
1	C	298	LYS	C-N-CA	7.48	129.06	119.78
1	B	170	GLY	N-CA-C	-7.40	106.53	114.67
1	D	54	ASP	CA-C-N	7.39	127.83	119.92
1	D	54	ASP	C-N-CA	7.39	127.83	119.92
1	C	136	PHE	N-CA-C	7.37	120.90	112.57
1	B	99	ARG	N-CA-C	-7.32	103.30	111.71
1	D	150	LEU	N-CA-C	-7.21	103.36	111.14
1	C	211	VAL	CB-CA-C	-7.21	99.47	111.29
1	D	211	VAL	CB-CA-C	-7.20	102.49	111.70
1	D	78	ALA	N-CA-C	-7.04	102.67	111.11
1	B	92	ARG	N-CA-C	6.92	119.85	111.82
1	C	73	VAL	N-CA-C	-6.92	104.25	111.58
1	C	316	ASN	N-CA-C	6.87	119.84	110.35
1	A	86	PRO	N-CA-C	6.86	122.02	111.11
1	C	173	VAL	N-CA-CB	6.78	118.95	110.47
2	F	3	ALA	CA-C-N	-6.64	112.82	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	ALA	C-N-CA	-6.64	112.82	119.99
2	I	3	ALA	CA-C-N	-6.58	112.88	119.99
2	I	3	ALA	C-N-CA	-6.58	112.88	119.99
1	C	54	ASP	CA-C-N	6.58	126.96	119.92
1	C	54	ASP	C-N-CA	6.58	126.96	119.92
1	B	294	GLU	CA-C-N	-6.53	116.32	122.66
1	B	294	GLU	C-N-CA	-6.53	116.32	122.66
1	D	291	TYR	CA-C-N	-6.48	111.96	122.26
1	D	291	TYR	C-N-CA	-6.48	111.96	122.26
1	D	284	CYS	N-CA-C	6.48	118.00	111.07
1	C	202	TRP	N-CA-C	-6.45	103.53	112.30
1	A	54	ASP	CA-C-N	6.43	126.35	119.85
1	A	54	ASP	C-N-CA	6.43	126.35	119.85
1	A	260	MET	N-CA-C	6.42	121.32	112.90
1	B	226	ALA	CA-C-N	-6.42	113.07	119.56
1	B	226	ALA	C-N-CA	-6.42	113.07	119.56
1	A	237	SER	N-CA-C	6.41	119.26	111.82
1	D	192	THR	N-CA-C	-6.40	97.18	110.80
1	C	309	THR	N-CA-C	-6.36	105.28	114.12
1	D	149	GLU	N-CA-C	-6.32	104.49	111.82
1	C	182	THR	N-CA-C	-6.32	103.92	111.69
1	C	199	HIS	N-CA-C	-6.32	104.89	112.59
1	D	158	ALA	N-CA-C	-6.30	104.10	110.97
1	A	125	VAL	CA-C-N	-6.29	111.98	119.84
1	A	125	VAL	C-N-CA	-6.29	111.98	119.84
1	C	106	ASP	N-CA-C	-6.28	105.58	113.18
1	D	211	VAL	N-CA-CB	6.27	117.20	110.62
1	C	132	LEU	N-CA-C	-6.27	104.37	111.07
1	D	247	PHE	N-CA-C	6.26	119.08	111.82
1	B	155	THR	N-CA-C	-6.25	104.46	111.28
1	A	150	LEU	N-CA-C	-6.23	104.74	112.90
1	B	4	ASP	N-CA-C	6.18	117.69	111.07
1	C	236	LYS	CD-CE-NZ	6.15	131.58	111.90
1	C	192	THR	CB-CA-C	6.14	120.08	111.86
1	B	295	VAL	N-CA-C	6.12	116.86	111.90
1	C	146	THR	CA-C-N	6.10	126.87	120.03
1	C	146	THR	C-N-CA	6.10	126.87	120.03
1	B	56	ASP	CA-C-N	-6.10	113.35	120.12
1	B	56	ASP	C-N-CA	-6.10	113.35	120.12
1	B	183	ILE	N-CA-C	-6.06	104.60	110.72
1	D	33	LEU	N-CA-C	-6.03	104.63	111.14
1	A	85	PRO	CA-C-N	5.96	125.97	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	PRO	C-N-CA	5.96	125.97	119.89
1	B	125	VAL	CA-C-N	-5.91	113.53	119.56
1	B	125	VAL	C-N-CA	-5.91	113.53	119.56
1	D	116	MET	N-CA-C	5.88	118.47	111.71
1	C	236	LYS	CB-CG-CD	5.87	124.81	111.30
1	A	211	VAL	CB-CA-C	-5.87	104.21	112.14
1	D	294	GLU	CA-C-N	-5.87	117.15	123.08
1	D	294	GLU	C-N-CA	-5.87	117.15	123.08
1	D	51	HIS	N-CA-C	-5.85	105.98	113.23
1	D	309	THR	N-CA-C	-5.80	106.05	114.12
1	D	75	ASP	N-CA-C	-5.75	106.40	113.41
1	A	96	LEU	N-CA-C	5.73	123.00	110.80
1	B	211	VAL	CB-CA-C	-5.71	101.92	111.29
1	D	68	ASN	N-CA-C	5.71	117.19	111.07
1	D	67	VAL	N-CA-CB	5.67	120.02	110.56
1	A	274	ALA	N-CA-C	-5.64	105.21	111.36
1	C	38	ILE	CB-CA-C	-5.63	104.77	111.97
1	B	160	ASP	N-CA-C	-5.62	105.07	111.14
1	C	222	LEU	N-CA-C	5.62	120.00	113.20
1	C	257	GLU	CA-C-N	5.61	128.14	120.46
1	C	257	GLU	C-N-CA	5.61	128.14	120.46
1	C	149	GLU	N-CA-C	-5.55	104.62	111.33
1	A	73	VAL	N-CA-C	-5.53	105.46	110.82
1	B	175	LEU	N-CA-C	-5.51	104.91	111.69
1	C	277	VAL	CA-C-N	-5.50	114.00	119.56
1	C	277	VAL	C-N-CA	-5.50	114.00	119.56
1	B	222	LEU	N-CA-C	5.47	119.94	113.16
1	A	72	GLY	N-CA-C	-5.46	107.89	114.66
1	A	162	LEU	N-CA-C	-5.45	106.82	112.93
1	C	28	ASP	N-CA-CB	5.44	118.23	110.06
1	B	91	ARG	CA-CB-CG	5.44	124.98	114.10
1	C	312	PHE	CA-C-N	5.44	125.34	119.85
1	C	312	PHE	C-N-CA	5.44	125.34	119.85
1	A	50	SER	N-CA-C	-5.43	106.63	113.20
1	B	124	VAL	N-CA-C	-5.42	108.56	113.71
1	B	225	GLN	N-CA-C	5.40	118.69	112.97
1	B	89	GLY	N-CA-C	5.39	123.34	112.34
1	C	197	GLY	N-CA-C	-5.39	107.89	115.32
1	D	229	GLN	CA-C-N	-5.38	113.36	119.28
1	D	229	GLN	C-N-CA	-5.38	113.36	119.28
1	A	149	GLU	N-CA-C	-5.37	105.46	112.23
1	A	243	LYS	N-CA-C	5.37	119.32	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	HIS	N-CA-C	-5.36	106.74	113.28
1	D	112	TRP	N-CA-C	5.36	117.82	111.33
1	D	151	SER	N-CA-C	5.35	117.81	111.33
1	B	20	ILE	N-CA-C	5.34	115.89	108.84
1	B	245	THR	N-CA-CB	-5.34	103.26	110.95
1	C	121	TYR	N-CA-C	5.31	120.03	113.50
1	D	137	GLY	CA-C-O	-5.30	117.21	121.77
1	B	223	ASP	N-CA-CB	5.29	119.43	110.49
1	C	152	PHE	N-CA-C	-5.27	105.12	112.45
1	D	20	ILE	N-CA-C	5.26	115.94	107.73
1	B	295	VAL	CB-CA-C	5.24	116.33	111.30
1	C	212	TYR	N-CA-C	5.23	116.98	111.28
1	D	285	LYS	N-CA-C	-5.21	105.60	111.28
1	B	60	THR	CB-CA-C	5.18	118.11	109.56
1	D	7	ASP	N-CA-C	5.18	121.84	110.80
1	D	156	VAL	N-CA-CB	5.18	118.35	110.58
1	B	213	ILE	N-CA-C	-5.18	105.36	111.00
1	B	299	PHE	N-CA-C	5.17	119.98	113.25
1	A	245	THR	N-CA-C	-5.17	106.90	114.39
1	B	222	LEU	CA-CB-CG	5.16	134.35	116.30
1	D	156	VAL	CB-CA-C	5.15	119.33	112.22
1	B	316	ASN	N-CA-C	5.14	121.75	110.80
1	B	134	ASN	N-CA-C	-5.13	106.42	113.30
2	G	3	ALA	CA-C-N	-5.13	114.70	120.14
2	G	3	ALA	C-N-CA	-5.13	114.70	120.14
1	D	155	THR	CA-C-N	-5.13	113.14	120.42
1	D	155	THR	C-N-CA	-5.13	113.14	120.42
1	B	113	LEU	N-CA-C	-5.13	105.87	111.82
1	B	38	ILE	CB-CA-C	-5.12	105.42	111.97
1	B	162	LEU	N-CA-C	-5.12	106.88	113.02
1	B	171	ALA	N-CA-C	-5.12	106.54	112.89
1	D	301	VAL	CB-CA-C	-5.12	105.38	112.24
1	D	53	SER	CA-C-N	-5.11	117.17	122.89
1	D	53	SER	C-N-CA	-5.11	117.17	122.89
1	A	294	GLU	CA-C-N	-5.09	116.57	122.63
1	A	294	GLU	C-N-CA	-5.09	116.57	122.63
1	C	213	ILE	CB-CA-C	-5.09	104.02	112.26
1	B	193	LEU	N-CA-C	-5.08	103.78	110.33
1	C	294	GLU	CA-C-N	-5.08	117.95	123.08
1	C	294	GLU	C-N-CA	-5.08	117.95	123.08
1	A	8	TRP	N-CA-C	5.05	116.25	109.24
1	A	258	VAL	N-CA-CB	-5.04	105.86	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	285	LYS	CA-C-N	5.04	125.55	120.00
1	D	285	LYS	C-N-CA	5.04	125.55	120.00
1	D	40	TYR	N-CA-C	5.04	117.43	111.33
1	D	87	LEU	CA-CB-CG	5.03	133.90	116.30
1	D	81	ILE	N-CA-CB	5.03	116.09	110.51
1	B	67	VAL	N-CA-CB	5.03	119.86	110.77
1	B	192	THR	CB-CA-C	-5.01	104.77	111.89
1	B	73	VAL	N-CA-C	-5.01	105.66	110.72
1	B	80	LEU	N-CA-C	5.01	116.43	110.97

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	138	SER	Peptide
1	D	17	VAL	Peptide
1	D	257	GLU	Peptide
1	D	261	GLY	Peptide

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	2524	0	2466	175	0
1	B	2576	0	2519	190	0
1	C	2576	0	2519	189	0
1	D	2524	0	2466	166	0
2	F	43	0	39	17	0
2	G	43	0	38	3	0
2	H	43	0	38	5	0
2	I	43	0	39	4	0
3	A	10	0	0	4	0
3	B	5	0	0	1	0
3	D	5	0	0	1	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
All	All	10394	0	10124	717	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (717) 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:185:ARG:CG	1:A:185:ARG:CB	1.74	1.65
1:A:233:ILE:CD1	1:A:233:ILE:CG1	1.77	1.61
2:F:5:LYS:C	2:F:6:NIT:HN12	1.18	1.47
2:F:5:LYS:C	2:F:6:NIT:N1	1.88	1.31
1:B:20:ILE:HA	1:B:25:THR:CG2	1.61	1.29
1:B:45:TYR:HE2	1:B:168:MET:HE1	1.05	1.14
1:C:298:LYS:HE2	2:G:1:SIN:O3	1.48	1.13
1:B:92:ARG:HH11	1:B:92:ARG:HG2	1.13	1.11
1:D:260:MET:HE2	1:D:260:MET:HA	1.13	1.11
1:C:21:PHE:H	1:C:25:THR:CG2	1.64	1.10
1:B:20:ILE:HA	1:B:25:THR:HG21	1.17	1.09
1:D:260:MET:HA	1:D:260:MET:CE	1.80	1.08
1:C:21:PHE:N	1:C:25:THR:HG21	1.69	1.07
1:C:21:PHE:H	1:C:25:THR:HG21	1.00	1.06
1:B:45:TYR:CE2	1:B:168:MET:HE1	1.89	1.06
1:C:184:MET:HA	1:C:184:MET:CE	1.84	1.05
1:D:114:GLN:HE21	1:D:114:GLN:HA	1.20	1.03
1:C:184:MET:HA	1:C:184:MET:HE2	1.40	1.03
1:D:21:PHE:H	1:D:25:THR:HG21	1.21	1.01
1:B:298:LYS:HE2	2:H:1:SIN:O3	1.63	0.99
1:A:22:ASP:OD2	1:A:25:THR:HG22	1.60	0.98
1:A:316:ASN:O	1:A:317:ILE:HG12	1.63	0.97
1:D:66:MET:HG2	1:D:164:MET:HB3	1.47	0.97
1:B:81:ILE:HD12	1:B:81:ILE:H	1.26	0.97
1:B:91:ARG:O	1:B:192:THR:HG21	1.66	0.96
1:A:231:ARG:HG3	1:A:231:ARG:HH11	1.27	0.95
1:D:45:TYR:CE2	1:D:168:MET:CE	2.50	0.94
1:B:316:ASN:HD22	1:B:317:ILE:H	1.15	0.93
1:B:20:ILE:CA	1:B:25:THR:HG21	1.98	0.93
1:B:45:TYR:HE2	1:B:168:MET:CE	1.83	0.92
1:D:231:ARG:HG3	1:D:231:ARG:HH11	1.34	0.91
1:D:191:TYR:O	1:D:192:THR:HB	1.69	0.91
1:A:62:SER:HB3	1:A:67:VAL:HG22	1.52	0.91
1:C:272:ASP:O	1:C:276:THR:HB	1.71	0.89
1:D:45:TYR:CE2	1:D:168:MET:HE1	2.08	0.89
1:B:298:LYS:CE	2:H:1:SIN:O3	2.22	0.88
1:A:316:ASN:HD22	1:A:317:ILE:H	1.22	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:HH11	1:A:231:ARG:CG	1.88	0.84
1:A:125:VAL:O	1:A:126:PRO:C	2.18	0.84
1:A:231:ARG:H	1:A:231:ARG:HD3	1.42	0.84
1:B:231:ARG:HG3	1:B:231:ARG:HH11	1.42	0.84
1:A:19:ARG:HG2	1:A:314:TRP:CD2	2.12	0.84
2:F:5:LYS:CA	2:F:6:NIT:HN12	1.92	0.83
1:B:92:ARG:HG2	1:B:92:ARG:NH1	1.89	0.82
1:B:3:LEU:HD23	1:B:40:TYR:HB2	1.60	0.82
1:A:114:GLN:HA	1:A:114:GLN:HE21	1.44	0.81
2:F:5:LYS:CA	2:F:6:NIT:N1	2.43	0.81
1:C:45:TYR:CE2	1:C:168:MET:HE2	2.16	0.81
1:B:159:LEU:HD13	1:B:165:PHE:CZ	2.16	0.81
1:A:95:ASN:HB2	1:A:191:TYR:O	1.82	0.80
1:D:21:PHE:H	1:D:25:THR:CG2	1.94	0.80
1:A:29:PHE:CZ	1:A:35:ILE:HG12	2.17	0.80
1:D:99:ARG:HG3	1:D:99:ARG:HH11	1.48	0.79
1:B:184:MET:HE3	1:B:184:MET:HA	1.63	0.79
1:C:316:ASN:HD22	1:C:317:ILE:H	1.27	0.79
1:B:62:SER:HB3	1:B:67:VAL:HG22	1.64	0.78
1:A:42:LEU:HD11	1:A:210:LEU:HD21	1.65	0.78
1:C:184:MET:HE2	1:C:184:MET:CA	2.13	0.78
1:D:114:GLN:HE21	1:D:114:GLN:CA	1.96	0.77
1:C:298:LYS:CE	2:G:1:SIN:O3	2.29	0.77
2:I:5:LYS:O	2:I:6:NIT:H6	1.84	0.77
1:D:62:SER:HB2	1:D:67:VAL:HG22	1.66	0.77
1:C:81:ILE:HD12	1:C:81:ILE:H	1.50	0.77
1:B:19:ARG:HG2	1:B:314:TRP:CD2	2.20	0.76
1:C:3:LEU:HD21	1:C:36:HIS:HB3	1.65	0.76
1:D:62:SER:HB2	1:D:67:VAL:CG2	2.17	0.75
1:A:272:ASP:O	1:A:276:THR:HB	1.87	0.75
1:A:233:ILE:HD11	1:A:274:ALA:HB2	1.69	0.74
1:D:45:TYR:HE2	1:D:168:MET:CE	2.00	0.74
1:B:268:PRO:HG2	2:I:4:PRO:HG2	1.68	0.73
1:C:20:ILE:HA	1:C:25:THR:HG23	1.70	0.73
1:D:30:GLN:NE2	1:D:297:LYS:HD3	2.03	0.73
1:A:266:HIS:HD2	1:A:267:SER:OG	1.70	0.73
1:D:222:LEU:HD12	1:D:226:ALA:HA	1.70	0.73
1:A:95:ASN:O	1:A:97:ALA:N	2.22	0.73
1:D:174:PHE:O	1:D:178:ASN:HB2	1.87	0.72
1:A:3:LEU:HD11	1:A:36:HIS:HB3	1.69	0.72
1:D:291:TYR:O	1:D:295:VAL:HG13	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ASN:O	1:B:317:ILE:HG12	1.89	0.72
1:D:266:HIS:HD2	1:D:267:SER:OG	1.72	0.72
1:D:257:GLU:HA	1:D:257:GLU:OE1	1.90	0.72
1:B:113:LEU:HD22	1:B:128:LEU:HD13	1.70	0.72
1:D:64:ILE:HB	1:D:67:VAL:HG13	1.72	0.72
1:D:181:TYR:CZ	1:D:211:VAL:HG13	2.25	0.72
1:A:191:TYR:O	1:A:192:THR:HB	1.89	0.71
1:C:49:ILE:HD13	1:C:218:GLN:HG3	1.71	0.71
1:C:184:MET:HA	1:C:184:MET:HE3	1.72	0.71
1:D:260:MET:HE2	1:D:260:MET:CA	2.08	0.70
1:C:61:ALA:HA	1:C:68:ASN:HD21	1.55	0.70
1:C:3:LEU:CD2	1:C:36:HIS:HB3	2.21	0.70
1:B:316:ASN:HD22	1:B:317:ILE:N	1.87	0.70
1:C:45:TYR:CE2	1:C:168:MET:CE	2.75	0.70
1:C:277:VAL:CG1	1:C:282:LYS:HB3	2.21	0.70
1:B:149:GLU:CD	1:B:210:LEU:HB2	2.17	0.70
1:D:61:ALA:HA	1:D:68:ASN:HD21	1.57	0.70
1:D:87:LEU:HD23	1:D:95:ASN:OD1	1.91	0.69
1:B:19:ARG:HG2	1:B:314:TRP:CG	2.28	0.69
1:C:141:ARG:NH1	1:C:143:ASP:OD1	2.25	0.69
1:C:22:ASP:OD2	1:C:25:THR:HB	1.93	0.69
1:C:110:PRO:O	1:C:114:GLN:HG2	1.92	0.69
1:B:316:ASN:ND2	1:B:317:ILE:H	1.89	0.69
1:C:99:ARG:HG3	1:C:99:ARG:HH11	1.58	0.69
1:B:96:LEU:O	1:B:98:CYS:N	2.26	0.68
1:B:235:ASP:C	1:B:235:ASP:OD1	2.36	0.68
1:D:21:PHE:N	1:D:25:THR:HG21	2.04	0.68
1:B:81:ILE:HD12	1:B:101:TRP:HE1	1.58	0.68
1:B:45:TYR:CE2	1:B:168:MET:CE	2.66	0.68
1:D:13:PHE:CD2	1:D:310:GLY:HA3	2.28	0.68
1:A:21:PHE:H	1:A:25:THR:HG23	1.57	0.68
1:B:101:TRP:CZ3	1:B:105:LEU:HD12	2.29	0.68
1:B:104:LYS:O	1:B:108:ARG:HD2	1.93	0.68
1:D:19:ARG:HG2	1:D:314:TRP:CE2	2.28	0.68
1:B:21:PHE:N	1:B:25:THR:HG21	2.08	0.68
1:D:62:SER:CB	1:D:67:VAL:HG22	2.23	0.68
1:A:111:GLN:O	1:A:114:GLN:HB2	1.95	0.67
1:D:109:LEU:HD11	1:D:132:LEU:HD23	1.77	0.67
1:B:92:ARG:HD2	1:D:193:LEU:O	1.95	0.67
2:F:5:LYS:O	2:F:6:NIT:H6	1.94	0.67
1:B:81:ILE:HD12	1:B:81:ILE:N	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:PRO:HG2	1:C:58:HIS:HD2	1.60	0.66
1:B:58:HIS:N	1:B:58:HIS:CD2	2.61	0.66
1:B:220:GLN:HG3	1:B:281:SER:HB3	1.75	0.66
2:F:5:LYS:O	2:F:6:NIT:N1	2.08	0.66
1:B:231:ARG:HH11	1:B:231:ARG:CG	2.08	0.66
1:D:191:TYR:O	1:D:192:THR:CB	2.42	0.66
1:A:109:LEU:HD11	1:A:132:LEU:HD23	1.76	0.66
1:A:195:PRO:HG3	1:C:92:ARG:HH22	1.61	0.66
1:D:8:TRP:CH2	1:D:120:GLU:O	2.48	0.66
1:B:62:SER:OG	1:B:63:SER:N	2.29	0.65
1:B:21:PHE:H	1:B:25:THR:HG21	1.61	0.65
1:C:92:ARG:O	1:C:92:ARG:HD3	1.96	0.65
1:C:211:VAL:HG23	1:C:212:TYR:H	1.62	0.65
1:B:22:ASP:OD2	1:B:25:THR:HB	1.95	0.65
1:B:20:ILE:HA	1:B:25:THR:HG22	1.73	0.65
1:D:181:TYR:O	1:D:182:THR:C	2.39	0.65
1:B:92:ARG:HH11	1:B:92:ARG:CG	2.02	0.64
1:C:99:ARG:HE	1:C:140:THR:HA	1.62	0.64
1:A:118:PRO:HA	1:B:96:LEU:HD12	1.79	0.64
1:D:143:ASP:HB2	1:D:196:ALA:HB2	1.77	0.64
1:B:184:MET:HA	1:B:184:MET:CE	2.27	0.64
1:A:185:ARG:CB	1:A:185:ARG:HH11	2.11	0.64
1:B:96:LEU:C	1:B:98:CYS:H	2.06	0.64
1:D:200:GLY:C	1:D:202:TRP:H	2.04	0.64
1:C:121:TYR:O	1:C:124:VAL:HB	1.98	0.64
1:B:81:ILE:H	1:B:81:ILE:CD1	2.07	0.63
1:D:231:ARG:HH11	1:D:231:ARG:CG	2.08	0.63
1:A:97:ALA:O	1:A:100:GLU:HB3	1.98	0.63
1:B:159:LEU:CD1	1:B:165:PHE:CZ	2.82	0.63
1:A:185:ARG:HB3	1:A:185:ARG:NH1	2.13	0.63
1:B:269:ILE:O	1:B:270:LEU:C	2.40	0.63
1:C:54:ASP:N	1:C:55:PRO:CD	2.62	0.63
1:C:95:ASN:CB	1:C:192:THR:HG22	2.29	0.63
1:C:110:PRO:HG3	1:C:129:GLN:NE2	2.13	0.63
1:C:184:MET:HE3	1:C:187:LEU:HD12	1.81	0.63
1:C:145:GLY:H	1:C:148:HIS:HD2	1.46	0.63
1:D:260:MET:CE	1:D:260:MET:CA	2.70	0.63
1:A:145:GLY:H	1:A:148:HIS:HD2	1.47	0.63
1:C:119:SER:O	1:C:121:TYR:N	2.32	0.63
2:F:1:SIN:O3	2:F:2:ALA:C	2.42	0.63
1:C:57:PRO:HG2	1:C:58:HIS:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD22	1:A:105:LEU:HD21	1.82	0.62
1:C:93:TYR:O	1:C:192:THR:HG23	2.00	0.62
1:C:64:ILE:HB	1:C:67:VAL:HG13	1.82	0.62
1:C:210:LEU:O	1:C:211:VAL:C	2.41	0.62
1:A:141:ARG:HD2	1:A:143:ASP:OD1	2.00	0.62
1:B:2:SER:O	1:B:3:LEU:C	2.41	0.62
1:B:185:ARG:HH12	1:B:250:GLN:HE21	1.48	0.62
1:D:19:ARG:HG2	1:D:314:TRP:CD2	2.33	0.62
1:D:45:TYR:CE2	1:D:168:MET:HE3	2.34	0.62
1:A:70:LEU:HD12	1:A:70:LEU:O	1.99	0.61
1:B:62:SER:OG	1:B:64:ILE:N	2.27	0.61
1:B:204:LEU:HD13	1:B:290:MET:HE1	1.82	0.61
1:C:195:PRO:HB2	1:C:198:SER:HB2	1.81	0.61
1:B:181:TYR:CZ	1:B:211:VAL:HG13	2.36	0.61
1:B:235:ASP:O	1:B:239:VAL:HG23	2.00	0.61
1:B:78:ALA:O	1:B:81:ILE:HD13	2.01	0.61
1:B:111:GLN:HA	1:B:114:GLN:HG2	1.81	0.61
1:A:10:HIS:CE1	1:D:186:ARG:NH1	2.68	0.61
1:C:3:LEU:HD21	1:C:36:HIS:CB	2.31	0.61
1:A:7:ASP:OD1	1:A:10:HIS:HB3	2.00	0.61
1:C:277:VAL:HG13	1:C:282:LYS:HB3	1.82	0.61
1:D:295:VAL:HG23	1:D:301:VAL:HG11	1.83	0.61
1:A:118:PRO:HB2	1:A:121:TYR:HD1	1.66	0.60
1:B:20:ILE:CA	1:B:25:THR:CG2	2.56	0.60
1:B:98:CYS:HB3	1:B:142:LEU:HD21	1.83	0.60
1:C:99:ARG:HG3	1:C:99:ARG:NH1	2.16	0.60
1:A:87:LEU:HD23	1:A:95:ASN:OD1	2.01	0.60
1:A:8:TRP:CH2	1:A:123:GLU:HG2	2.36	0.60
1:C:20:ILE:HA	1:C:25:THR:CG2	2.32	0.60
1:C:316:ASN:O	1:C:317:ILE:HG12	2.02	0.59
1:B:143:ASP:HB2	1:B:194:GLU:O	2.02	0.59
1:B:184:MET:HE3	1:B:187:LEU:HD12	1.84	0.59
1:D:13:PHE:CE2	1:D:310:GLY:HA3	2.37	0.59
1:A:7:ASP:O	1:A:10:HIS:N	2.34	0.59
1:A:137:GLY:HA2	1:A:148:HIS:CE1	2.37	0.59
1:C:202:TRP:CZ3	2:F:1:SIN:O2	2.55	0.59
1:C:208:PHE:HB3	1:C:211:VAL:HG22	1.84	0.59
1:D:223:ASP:O	1:D:224:ALA:C	2.46	0.59
1:A:8:TRP:CZ3	1:A:123:GLU:HG2	2.37	0.59
1:A:21:PHE:H	1:A:25:THR:CG2	2.15	0.59
1:A:99:ARG:HE	1:A:140:THR:HA	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:PHE:HB3	1:B:312:PHE:CD1	2.37	0.59
1:C:62:SER:HB2	1:C:67:VAL:CG2	2.33	0.59
1:A:66:MET:HE3	1:A:164:MET:SD	2.43	0.59
1:C:20:ILE:HB	1:C:303:GLN:HA	1.84	0.59
1:C:144:TYR:CD2	1:C:188:ILE:HD11	2.37	0.59
1:C:70:LEU:O	1:C:74:LEU:HG	2.03	0.58
1:A:142:LEU:HD12	1:C:260:MET:HG2	1.85	0.58
1:A:144:TYR:CE1	1:A:148:HIS:HB2	2.38	0.58
1:A:258:VAL:HG22	1:C:93:TYR:CE1	2.39	0.58
1:B:70:LEU:O	1:B:74:LEU:HG	2.03	0.58
1:D:16:PRO:HA	1:D:307:PHE:O	2.03	0.58
1:B:298:LYS:HE3	2:H:1:SIN:O3	2.01	0.58
1:C:61:ALA:CA	1:C:68:ASN:HD21	2.16	0.58
1:C:95:ASN:HB2	1:C:192:THR:HG22	1.84	0.58
1:C:66:MET:HB3	1:C:165:PHE:CE2	2.38	0.58
2:F:1:SIN:O3	2:F:3:ALA:N	2.37	0.58
1:C:231:ARG:HA	1:C:274:ALA:O	2.03	0.58
1:C:316:ASN:HD22	1:C:317:ILE:N	1.98	0.58
1:C:69:GLY:O	1:C:73:VAL:HG23	2.03	0.58
1:D:50:SER:O	1:D:221:LEU:HD12	2.04	0.58
1:B:268:PRO:CG	2:I:4:PRO:HG2	2.33	0.58
1:C:40:TYR:C	1:C:40:TYR:CD2	2.82	0.58
1:A:62:SER:HB3	1:A:67:VAL:CG2	2.30	0.57
1:A:185:ARG:CB	1:A:185:ARG:NH1	2.67	0.57
1:B:2:SER:OG	1:B:3:LEU:N	2.37	0.57
1:A:28:ASP:OD1	1:A:28:ASP:N	2.37	0.57
1:B:233:ILE:HD12	1:B:233:ILE:C	2.28	0.57
1:B:84:THR:HG23	1:B:100:GLU:HG2	1.87	0.57
1:D:45:TYR:CD2	1:D:168:MET:HE3	2.39	0.57
1:D:109:LEU:O	1:D:110:PRO:C	2.43	0.57
1:A:62:SER:N	1:A:68:ASN:HD21	2.02	0.57
1:A:261:GLY:HA3	1:C:141:ARG:HG3	1.85	0.57
1:D:124:VAL:HG13	1:D:311:PHE:CZ	2.40	0.57
1:B:181:TYR:O	1:B:185:ARG:HG3	2.05	0.57
1:C:13:PHE:CE2	1:C:124:VAL:HG22	2.39	0.57
1:C:81:ILE:H	1:C:81:ILE:CD1	2.17	0.57
1:C:108:ARG:NH1	1:C:108:ARG:HB2	2.20	0.57
1:B:229:GLN:O	1:B:232:GLU:N	2.25	0.57
1:D:143:ASP:CB	1:D:196:ALA:HB2	2.35	0.57
1:B:261:GLY:HA3	1:D:141:ARG:HG3	1.87	0.57
1:D:129:GLN:HG2	1:D:129:GLN:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:TRP:HH2	1:D:120:GLU:O	1.88	0.56
1:A:66:MET:HB3	1:A:165:PHE:CE2	2.41	0.56
1:B:206:ASP:OD2	1:B:259:LYS:NZ	2.34	0.56
1:C:14:SER:O	1:C:127:GLU:HG3	2.05	0.56
1:C:263:PHE:HA	1:C:266:HIS:CE1	2.41	0.56
1:D:66:MET:SD	1:D:116:MET:HE3	2.46	0.56
1:C:109:LEU:HD21	1:C:132:LEU:HD23	1.88	0.56
1:D:233:ILE:HD12	1:D:233:ILE:C	2.30	0.56
1:A:66:MET:SD	1:A:116:MET:HE3	2.45	0.56
1:C:3:LEU:CD2	1:C:36:HIS:CB	2.83	0.56
1:C:222:LEU:O	1:C:225:GLN:N	2.39	0.56
1:B:231:ARG:CG	1:B:231:ARG:NH1	2.68	0.56
1:B:231:ARG:HB3	1:B:274:ALA:O	2.06	0.56
1:B:58:HIS:N	1:B:58:HIS:HD2	2.04	0.55
1:B:113:LEU:HD22	1:B:128:LEU:CD1	2.34	0.55
1:D:263:PHE:HA	1:D:266:HIS:CE1	2.42	0.55
1:D:257:GLU:OE1	1:D:257:GLU:CA	2.54	0.55
1:A:62:SER:H	1:A:68:ASN:HD21	1.55	0.55
1:C:95:ASN:HB2	1:C:192:THR:CG2	2.37	0.55
1:D:210:LEU:HD23	1:D:213:ILE:HD12	1.88	0.55
1:C:99:ARG:NE	1:C:140:THR:HA	2.22	0.55
2:F:5:LYS:O	2:F:6:NIT:C6	2.55	0.55
1:A:19:ARG:HB3	1:A:307:PHE:CE1	2.42	0.55
1:A:258:VAL:HG13	1:C:93:TYR:CE2	2.42	0.55
1:B:211:VAL:HG23	1:B:212:TYR:N	2.22	0.55
1:C:21:PHE:N	1:C:25:THR:CG2	2.46	0.55
1:B:29:PHE:HB2	1:B:314:TRP:HZ3	1.72	0.55
1:B:29:PHE:O	1:B:35:ILE:HG21	2.06	0.55
1:C:67:VAL:O	1:C:71:MET:HB2	2.07	0.55
1:D:209:HIS:HE1	1:D:290:MET:HG2	1.72	0.55
1:B:164:MET:O	1:B:165:PHE:CD2	2.60	0.55
3:A:1320:SO4:O4	2:F:5:LYS:HE3	2.07	0.55
1:B:169:ARG:NH2	3:B:1319:SO4:O1	2.31	0.55
1:D:145:GLY:H	1:D:148:HIS:HD2	1.54	0.54
1:D:228:LEU:HD22	1:D:238:LEU:HD13	1.89	0.54
1:A:149:GLU:CD	1:A:210:LEU:HB2	2.31	0.54
1:B:27:LEU:O	1:B:30:GLN:HB2	2.08	0.54
1:C:53:SER:CB	1:C:222:LEU:HD21	2.38	0.54
1:A:125:VAL:O	1:A:127:GLU:N	2.40	0.54
1:A:169:ARG:NH2	3:A:1318[A]:SO4:O1	2.35	0.54
1:B:69:GLY:O	1:B:73:VAL:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:TYR:O	1:D:274:ALA:HB3	2.06	0.54
1:A:208:PHE:HB3	1:A:211:VAL:CG2	2.37	0.54
1:C:191:TYR:O	1:C:192:THR:HG22	2.07	0.54
1:A:231:ARG:CG	1:A:231:ARG:NH1	2.57	0.54
1:C:99:ARG:HD3	1:C:139:SER:O	2.08	0.54
1:D:32:SER:O	1:D:35:ILE:HG22	2.08	0.54
1:D:272:ASP:OD1	2:H:5:LYS:HB2	2.07	0.54
1:D:181:TYR:CE1	1:D:211:VAL:HG13	2.42	0.54
1:D:128:LEU:HD11	1:D:159:LEU:HD21	1.90	0.54
1:C:18:LYS:O	1:C:19:ARG:HD3	2.08	0.53
1:C:211:VAL:HG23	1:C:212:TYR:N	2.22	0.53
1:A:52:CYS:SG	1:A:55:PRO:HB3	2.48	0.53
1:B:49:ILE:C	1:B:51:HIS:H	2.16	0.53
1:B:91:ARG:HH22	1:D:87:LEU:HD11	1.73	0.53
1:C:105:LEU:CD2	1:C:109:LEU:HG	2.38	0.53
1:A:205:ASP:OD1	1:A:255:ILE:HD11	2.08	0.53
1:C:49:ILE:HG13	1:C:173:VAL:HG22	1.90	0.53
1:A:258:VAL:HG13	1:C:93:TYR:CZ	2.44	0.53
1:B:279:ARG:HB2	1:B:279:ARG:NH1	2.23	0.53
1:C:301:VAL:HG12	1:C:302:VAL:HG13	1.91	0.53
1:D:21:PHE:N	1:D:25:THR:CG2	2.67	0.53
1:A:26:THR:OG1	1:A:299:PHE:HB2	2.09	0.53
1:B:92:ARG:HB2	1:D:192:THR:HA	1.91	0.53
1:C:62:SER:HB2	1:C:67:VAL:HG22	1.91	0.53
1:C:222:LEU:HD12	1:C:225:GLN:O	2.08	0.53
1:B:121:TYR:O	1:B:124:VAL:HB	2.09	0.53
1:B:223:ASP:OD2	1:B:281:SER:OG	2.17	0.53
1:D:208:PHE:HB3	1:D:211:VAL:HG22	1.91	0.53
1:A:174:PHE:O	1:A:177:PHE:N	2.42	0.53
1:B:315:VAL:HG12	1:B:316:ASN:N	2.24	0.53
1:C:29:PHE:HB2	1:C:314:TRP:CZ3	2.43	0.53
1:A:62:SER:HB2	1:A:172:ASP:OD1	2.07	0.53
1:D:61:ALA:HA	1:D:68:ASN:ND2	2.24	0.53
1:C:19:ARG:HG2	1:C:314:TRP:CD2	2.44	0.52
1:A:185:ARG:HH22	1:A:250:GLN:NE2	2.06	0.52
1:A:316:ASN:C	1:A:317:ILE:HG12	2.34	0.52
2:H:5:LYS:O	2:H:6:NIT:H6	2.09	0.52
1:A:144:TYR:HE2	1:A:208:PHE:CE2	2.27	0.52
1:C:143:ASP:CG	1:C:196:ALA:HB2	2.34	0.52
1:A:19:ARG:HG2	1:A:314:TRP:CE2	2.45	0.52
1:B:32:SER:OG	1:B:35:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ILE:HD12	1:D:234:LEU:N	2.24	0.52
1:B:62:SER:HB3	1:B:67:VAL:CG2	2.36	0.52
1:C:81:ILE:HD12	1:C:101:TRP:HE1	1.75	0.52
1:D:99:ARG:HH11	1:D:99:ARG:CG	2.17	0.52
1:A:62:SER:OG	1:A:63:SER:N	2.42	0.52
1:B:211:VAL:HG23	1:B:212:TYR:H	1.75	0.52
1:D:114:GLN:HA	1:D:114:GLN:NE2	2.05	0.52
1:A:49:ILE:C	1:A:51:HIS:H	2.18	0.52
1:D:18:LYS:HB2	1:D:306:TRP:CE2	2.44	0.52
2:F:5:LYS:HA	2:F:6:NIT:N1	2.21	0.52
1:B:66:MET:HE3	1:B:164:MET:HE2	1.92	0.51
1:B:159:LEU:HA	1:B:162:LEU:HD13	1.92	0.51
1:A:3:LEU:CD1	1:A:36:HIS:HB3	2.40	0.51
1:B:223:ASP:O	1:B:224:ALA:C	2.51	0.51
1:C:90:PRO:C	1:C:92:ARG:H	2.18	0.51
1:A:316:ASN:ND2	1:A:317:ILE:H	2.00	0.51
1:B:82:ASP:N	1:B:82:ASP:OD2	2.42	0.51
1:B:92:ARG:HG2	1:B:92:ARG:O	2.10	0.51
1:C:19:ARG:HG2	1:C:314:TRP:CG	2.46	0.51
1:A:291:TYR:CE1	1:A:295:VAL:HG11	2.45	0.51
1:B:219:TRP:HH2	1:B:228:LEU:HD12	1.75	0.51
1:C:144:TYR:CE1	1:C:148:HIS:HB2	2.45	0.51
1:B:84:THR:OG1	1:B:104:LYS:HE3	2.10	0.51
1:B:254:PHE:O	1:B:255:ILE:C	2.53	0.51
1:D:169:ARG:NH2	3:D:1319[B]:SO4:O2	2.37	0.51
1:A:70:LEU:HD22	1:A:159:LEU:CD1	2.40	0.51
1:A:143:ASP:CG	1:A:196:ALA:HB2	2.36	0.51
1:B:74:LEU:O	1:B:183:ILE:HD11	2.10	0.51
1:C:204:LEU:HD22	1:C:290:MET:HE2	1.92	0.51
1:D:61:ALA:CA	1:D:68:ASN:HD21	2.21	0.51
1:A:12:THR:O	1:A:309:THR:OG1	2.27	0.51
1:D:18:LYS:H	1:D:306:TRP:HB3	1.76	0.51
1:B:37:ARG:HD3	1:B:161:MET:SD	2.51	0.51
1:D:30:GLN:CD	1:D:297:LYS:HD3	2.35	0.51
1:A:120:GLU:OE2	1:B:93:TYR:HD1	1.93	0.50
1:D:137:GLY:HA2	1:D:148:HIS:CE1	2.46	0.50
1:B:20:ILE:C	1:B:25:THR:HG21	2.36	0.50
1:B:162:LEU:HD11	1:B:311:PHE:CE2	2.46	0.50
1:A:191:TYR:CB	1:A:193:LEU:HD21	2.42	0.50
1:A:228:LEU:CD2	1:A:238:LEU:HD12	2.41	0.50
1:B:219:TRP:CH2	1:B:228:LEU:HD12	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:TYR:CD2	1:C:168:MET:HE2	2.46	0.50
1:A:160:ASP:O	1:A:163:GLY:N	2.44	0.50
3:A:1320:SO4:O3	2:F:5:LYS:HE3	2.12	0.50
1:B:20:ILE:HG23	1:B:25:THR:HG22	1.93	0.50
1:C:185:ARG:HH21	1:C:250:GLN:HG3	1.76	0.50
1:C:243:LYS:HD3	1:C:243:LYS:C	2.36	0.50
1:A:28:ASP:O	1:A:29:PHE:C	2.55	0.50
1:A:228:LEU:HD21	1:A:238:LEU:HD12	1.92	0.50
1:B:105:LEU:CD2	1:B:109:LEU:HB2	2.42	0.50
1:C:122:HIS:C	1:C:124:VAL:H	2.18	0.50
1:A:231:ARG:HD3	1:A:231:ARG:N	2.19	0.50
1:C:16:PRO:HD3	1:C:127:GLU:HG2	1.94	0.50
1:C:209:HIS:CE1	1:C:290:MET:HE2	2.46	0.50
1:D:33:LEU:O	1:D:34:ALA:C	2.54	0.50
1:C:45:TYR:HE2	1:C:168:MET:HE2	1.73	0.50
1:C:298:LYS:O	1:C:302:VAL:HG22	2.10	0.50
1:B:191:TYR:CB	1:B:193:LEU:HD21	2.42	0.49
1:D:231:ARG:HG3	1:D:231:ARG:NH1	2.13	0.49
3:A:1320:SO4:S	2:F:5:LYS:HE3	2.52	0.49
1:B:231:ARG:H	1:B:231:ARG:HD3	1.77	0.49
1:D:39:LYS:O	1:D:42:LEU:HB3	2.12	0.49
1:A:63:SER:O	1:B:85:PRO:HG3	2.11	0.49
1:B:135:SER:HA	1:B:151:SER:HB3	1.94	0.49
1:A:266:HIS:CD2	1:A:267:SER:OG	2.59	0.49
1:A:222:LEU:O	1:A:223:ASP:C	2.54	0.49
1:A:263:PHE:HA	1:A:266:HIS:CE1	2.47	0.49
1:A:316:ASN:HD22	1:A:317:ILE:N	2.00	0.49
1:C:3:LEU:HD13	1:C:36:HIS:O	2.13	0.49
1:A:24:GLN:HG3	1:A:25:THR:N	2.27	0.49
1:A:87:LEU:HG	1:C:91:ARG:HH22	1.76	0.49
1:D:102:HIS:O	1:D:103:HIS:C	2.54	0.49
1:D:230:PRO:HA	1:D:280:TRP:CZ2	2.47	0.49
1:C:27:LEU:O	1:C:30:GLN:HB2	2.13	0.49
1:C:283:VAL:O	1:C:287:LEU:N	2.36	0.49
1:D:35:ILE:HG23	1:D:36:HIS:HD2	1.76	0.49
1:A:231:ARG:HG3	1:A:231:ARG:NH1	2.09	0.49
1:C:204:LEU:HB2	1:C:290:MET:HE1	1.93	0.49
1:C:113:LEU:HD22	1:C:128:LEU:HD13	1.93	0.48
1:D:149:GLU:CD	1:D:210:LEU:HB2	2.37	0.48
1:B:64:ILE:HB	1:B:67:VAL:HG13	1.95	0.48
2:F:5:LYS:C	2:F:6:NIT:C1	2.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HG12	1:A:259:LYS:N	2.26	0.48
1:B:132:LEU:HA	1:B:155:THR:OG1	2.13	0.48
1:C:62:SER:CB	1:C:67:VAL:HG22	2.43	0.48
1:C:114:GLN:O	1:C:122:HIS:CE1	2.67	0.48
1:D:8:TRP:HZ2	1:D:120:GLU:HB3	1.78	0.48
1:D:266:HIS:CD2	1:D:267:SER:OG	2.61	0.48
1:A:81:ILE:CG2	1:A:186:ARG:HH21	2.25	0.48
1:B:86:PRO:HA	1:B:97:ALA:CB	2.44	0.48
1:C:168:MET:HE3	1:C:173:VAL:HG12	1.94	0.48
1:A:144:TYR:CD1	1:A:184:MET:HE2	2.49	0.48
1:B:138:SER:O	1:B:139:SER:C	2.56	0.48
1:D:141:ARG:HD2	1:D:143:ASP:OD1	2.13	0.48
1:B:21:PHE:H	1:B:25:THR:CG2	2.27	0.48
1:B:144:TYR:CE1	1:B:148:HIS:HB2	2.49	0.48
1:B:316:ASN:ND2	1:B:317:ILE:N	2.57	0.48
1:C:204:LEU:HB2	1:C:290:MET:CE	2.43	0.48
1:D:181:TYR:O	1:D:184:MET:N	2.46	0.48
1:A:29:PHE:CE2	1:A:35:ILE:HG12	2.48	0.48
1:B:87:LEU:N	1:B:95:ASN:HD21	2.12	0.48
1:C:299:PHE:C	1:C:301:VAL:N	2.70	0.48
1:D:143:ASP:CG	1:D:196:ALA:HB2	2.39	0.48
1:B:193:LEU:N	1:B:193:LEU:HD23	2.29	0.48
1:C:29:PHE:HB2	1:C:314:TRP:CH2	2.48	0.48
1:D:200:GLY:C	1:D:202:TRP:N	2.68	0.48
1:A:19:ARG:HB3	1:A:307:PHE:CD1	2.49	0.48
1:B:204:LEU:HD22	1:B:290:MET:HE2	1.96	0.48
1:C:149:GLU:CD	1:C:210:LEU:HB2	2.39	0.48
1:C:271:TYR:C	1:C:271:TYR:CD2	2.92	0.48
1:D:134:ASN:OD1	1:D:134:ASN:C	2.56	0.48
1:A:291:TYR:O	1:A:295:VAL:HG13	2.14	0.47
1:B:29:PHE:CE1	1:B:35:ILE:HB	2.50	0.47
1:B:249:CYS:O	1:B:250:GLN:C	2.57	0.47
1:A:191:TYR:HB3	1:A:193:LEU:HD21	1.96	0.47
1:B:160:ASP:O	1:B:163:GLY:N	2.45	0.47
1:D:69:GLY:O	1:D:73:VAL:HG23	2.13	0.47
1:A:81:ILE:CG2	1:A:186:ARG:NH2	2.77	0.47
1:D:199:HIS:O	1:D:202:TRP:HB2	2.14	0.47
1:A:185:ARG:HH11	1:A:185:ARG:HB2	1.76	0.47
1:B:159:LEU:HA	1:B:162:LEU:CD1	2.45	0.47
1:D:118:PRO:O	1:D:119:SER:C	2.57	0.47
1:D:201:VAL:HG12	1:D:202:TRP:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:PHE:HA	1:D:257:GLU:HG2	1.96	0.47
1:D:308:GLY:O	1:D:313:PRO:HA	2.15	0.47
1:B:122:HIS:C	1:B:124:VAL:H	2.23	0.47
1:C:19:ARG:HB2	1:C:307:PHE:CD1	2.49	0.47
1:C:66:MET:HB3	1:C:165:PHE:HE2	1.77	0.47
1:C:71:MET:HE1	1:C:175:LEU:O	2.15	0.47
1:A:300:PRO:HG3	2:F:4:PRO:HD3	1.97	0.47
1:B:141:ARG:HD2	1:B:143:ASP:OD1	2.14	0.47
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.69	0.47
1:C:81:ILE:HD12	1:C:81:ILE:N	2.24	0.47
1:C:113:LEU:HD22	1:C:128:LEU:CD1	2.44	0.47
1:C:232:GLU:C	1:C:234:LEU:N	2.72	0.47
1:D:144:TYR:O	1:D:207:HIS:HD2	1.98	0.47
1:C:90:PRO:O	1:C:92:ARG:N	2.38	0.47
1:D:82:ASP:N	1:D:82:ASP:OD2	2.45	0.47
1:D:95:ASN:N	1:D:142:LEU:HD13	2.30	0.47
1:C:130:TYR:CE2	1:C:306:TRP:HB2	2.51	0.46
1:C:84:THR:HB	1:C:191:TYR:OH	2.15	0.46
1:A:14:SER:OG	1:A:309:THR:HG23	2.14	0.46
1:D:74:LEU:HA	1:D:74:LEU:HD23	1.68	0.46
1:A:108:ARG:O	1:A:111:GLN:HB3	2.16	0.46
1:B:109:LEU:O	1:B:110:PRO:C	2.59	0.46
1:B:185:ARG:NH1	1:B:250:GLN:HG2	2.29	0.46
1:C:96:LEU:C	1:C:98:CYS:H	2.22	0.46
1:C:266:HIS:HD2	1:C:267:SER:OG	1.98	0.46
1:D:38:ILE:HD11	1:D:305:PHE:CZ	2.51	0.46
1:C:220:GLN:HG3	1:C:281:SER:HA	1.95	0.46
1:C:229:GLN:O	1:C:230:PRO:C	2.55	0.46
1:B:96:LEU:C	1:B:98:CYS:N	2.70	0.46
1:B:279:ARG:HH12	1:B:282:LYS:HG2	1.81	0.46
1:C:30:GLN:CD	1:C:297:LYS:HG3	2.40	0.46
1:C:152:PHE:O	1:C:156:VAL:HG12	2.15	0.46
1:D:132:LEU:HB2	1:D:155:THR:HG21	1.97	0.46
1:B:210:LEU:HD23	1:B:210:LEU:HA	1.61	0.46
1:B:210:LEU:O	1:B:211:VAL:C	2.59	0.46
1:B:222:LEU:O	1:B:225:GLN:N	2.48	0.46
1:C:210:LEU:HD13	1:C:214:LEU:HD22	1.98	0.46
1:A:81:ILE:HG21	1:A:186:ARG:HH21	1.80	0.46
1:D:157:ALA:O	1:D:161:MET:HG3	2.16	0.46
1:C:185:ARG:HH11	1:C:185:ARG:HB2	1.79	0.46
1:B:3:LEU:HD11	1:B:36:HIS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:THR:OG1	2:G:2:ALA:HB3	2.15	0.46
1:C:64:ILE:HG22	1:C:66:MET:H	1.81	0.46
1:D:115:GLU:H	1:D:115:GLU:HG2	1.44	0.46
1:B:73:VAL:HG21	1:B:116:MET:SD	2.56	0.45
1:C:160:ASP:O	1:C:162:LEU:N	2.49	0.45
1:D:269:ILE:O	1:D:270:LEU:C	2.58	0.45
1:A:64:ILE:HD12	1:A:172:ASP:OD2	2.16	0.45
1:B:279:ARG:HB2	1:B:279:ARG:HH11	1.80	0.45
1:C:95:ASN:OD1	1:C:95:ASN:C	2.59	0.45
1:C:273:ILE:HG12	2:F:6:NIT:C3	2.47	0.45
1:A:118:PRO:O	1:A:121:TYR:HB2	2.17	0.45
1:A:291:TYR:CD1	1:A:295:VAL:HG11	2.51	0.45
1:B:120:GLU:H	1:B:120:GLU:HG3	1.33	0.45
1:D:62:SER:HB2	1:D:67:VAL:HG21	1.96	0.45
1:D:73:VAL:C	1:D:75:ASP:N	2.73	0.45
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.48	0.45
1:B:77:LEU:HD23	1:B:77:LEU:HA	1.70	0.45
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.85	0.45
1:D:53:SER:HB3	1:D:222:LEU:HD21	1.98	0.45
1:D:66:MET:HE1	1:D:116:MET:O	2.16	0.45
1:B:141:ARG:O	1:B:142:LEU:HB2	2.17	0.45
1:C:71:MET:CE	1:C:175:LEU:HG	2.46	0.45
1:A:113:LEU:HD13	1:A:128:LEU:HD13	1.99	0.45
1:A:19:ARG:HG2	1:A:314:TRP:CG	2.51	0.45
1:A:128:LEU:HD22	1:A:155:THR:HG23	1.99	0.45
1:B:89:GLY:HA3	1:B:90:PRO:HD2	1.78	0.45
1:B:204:LEU:HB2	1:B:290:MET:CE	2.47	0.45
1:C:58:HIS:CD2	1:C:58:HIS:N	2.84	0.45
1:C:135:SER:O	1:C:148:HIS:HB3	2.17	0.45
1:A:3:LEU:HD11	1:A:36:HIS:CB	2.42	0.45
1:B:215:GLY:HA2	1:B:247:PHE:HB2	1.98	0.45
1:D:124:VAL:HG13	1:D:311:PHE:HZ	1.80	0.45
1:D:240:ARG:O	1:D:243:LYS:HB3	2.17	0.45
1:A:28:ASP:C	1:A:30:GLN:N	2.75	0.45
1:C:22:ASP:H	1:C:25:THR:HG22	1.82	0.45
1:D:95:ASN:H	1:D:142:LEU:HD13	1.82	0.45
1:A:144:TYR:CE1	1:A:148:HIS:CB	3.01	0.44
1:B:191:TYR:HB3	1:B:193:LEU:HD21	2.00	0.44
1:C:46:THR:HG23	1:C:217:SER:HB2	1.99	0.44
1:C:232:GLU:C	1:C:234:LEU:H	2.25	0.44
1:D:299:PHE:HB3	1:D:300:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:VAL:O	1:C:8:TRP:N	2.47	0.44
1:C:148:HIS:O	1:C:149:GLU:C	2.58	0.44
1:D:234:LEU:HD23	1:D:234:LEU:HA	1.55	0.44
1:A:125:VAL:C	1:A:127:GLU:N	2.75	0.44
1:A:94:GLY:HA2	1:A:192:THR:O	2.17	0.44
1:B:93:TYR:CZ	1:D:258:VAL:HG13	2.52	0.44
1:A:46:THR:O	1:A:217:SER:OG	2.34	0.44
1:C:45:TYR:CE2	1:C:168:MET:HE1	2.51	0.44
1:C:78:ALA:O	1:C:81:ILE:HD13	2.18	0.44
1:A:192:THR:O	1:A:192:THR:HG22	2.17	0.44
1:B:87:LEU:HD12	1:B:96:LEU:CB	2.48	0.44
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.53	0.44
1:D:299:PHE:HB3	2:I:2:ALA:O	2.18	0.44
1:A:42:LEU:HD12	1:A:42:LEU:HA	1.71	0.44
1:A:208:PHE:HB3	1:A:211:VAL:HG23	1.99	0.44
1:C:41:HIS:CE1	1:C:161:MET:HE2	2.53	0.44
1:C:200:GLY:C	1:C:202:TRP:H	2.25	0.44
1:C:299:PHE:O	1:C:300:PRO:C	2.59	0.44
1:A:55:PRO:O	1:A:57:PRO:HD3	2.18	0.44
1:A:67:VAL:O	1:A:71:MET:HG2	2.17	0.44
1:A:267:SER:N	1:A:268:PRO:CD	2.81	0.44
1:C:49:ILE:HD13	1:C:218:GLN:CG	2.46	0.44
1:A:233:ILE:HD12	1:A:248:TYR:CE2	2.53	0.43
1:C:24:GLN:O	1:C:27:LEU:N	2.50	0.43
1:A:141:ARG:HG3	1:C:261:GLY:HA3	2.01	0.43
1:B:264:GLU:OE1	1:B:271:TYR:CZ	2.72	0.43
1:B:315:VAL:HG12	1:B:316:ASN:H	1.83	0.43
1:C:24:GLN:HG3	1:C:25:THR:H	1.83	0.43
1:A:6:VAL:O	1:A:8:TRP:N	2.52	0.43
1:A:79:HIS:HD2	1:A:79:HIS:O	2.01	0.43
1:A:192:THR:HA	1:C:92:ARG:HG2	2.00	0.43
1:C:142:LEU:N	1:C:142:LEU:HD23	2.32	0.43
1:C:199:HIS:O	1:C:202:TRP:HB2	2.19	0.43
1:D:42:LEU:CD1	1:D:210:LEU:HD21	2.49	0.43
1:C:62:SER:HB2	1:C:67:VAL:HG21	2.00	0.43
1:C:184:MET:CE	1:C:187:LEU:HB2	2.48	0.43
1:D:19:ARG:HE	1:D:19:ARG:HB2	1.55	0.43
1:D:14:SER:O	1:D:127:GLU:HG3	2.18	0.43
1:A:166:PRO:O	1:A:167:HIS:C	2.62	0.43
1:B:49:ILE:C	1:B:51:HIS:N	2.77	0.43
1:C:252:ILE:CD1	1:C:270:LEU:HD13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:TYR:HB3	1:A:193:LEU:CD2	2.49	0.43
1:A:252:ILE:CD1	1:A:270:LEU:HD13	2.49	0.43
1:C:111:GLN:O	1:C:114:GLN:HB2	2.19	0.43
1:A:33:LEU:HD23	1:A:313:PRO:HG2	2.00	0.43
1:B:71:MET:HE3	1:B:71:MET:HB3	1.45	0.43
1:B:230:PRO:HA	1:B:280:TRP:CZ2	2.53	0.43
1:D:278:PRO:HG2	1:D:279:ARG:HH11	1.83	0.43
1:A:109:LEU:O	1:A:109:LEU:HG	2.16	0.42
1:B:223:ASP:HB2	1:B:279:ARG:HG2	2.00	0.42
1:C:157:ALA:O	1:C:161:MET:HE3	2.19	0.42
1:C:217:SER:O	1:C:220:GLN:HB2	2.20	0.42
1:D:231:ARG:CG	1:D:231:ARG:NH1	2.73	0.42
1:A:45:TYR:N	1:A:45:TYR:CD2	2.86	0.42
1:D:53:SER:CB	1:D:222:LEU:HD21	2.49	0.42
1:D:114:GLN:CA	1:D:114:GLN:NE2	2.73	0.42
1:B:19:ARG:CG	1:B:314:TRP:CD2	2.99	0.42
1:B:201:VAL:HG12	1:B:202:TRP:CD1	2.55	0.42
1:C:15:THR:HA	1:C:16:PRO:HD2	1.85	0.42
1:A:132:LEU:HB2	1:A:155:THR:HG21	2.02	0.42
1:A:299:PHE:C	1:A:301:VAL:N	2.76	0.42
1:B:229:GLN:O	1:B:230:PRO:C	2.62	0.42
1:C:149:GLU:CD	1:C:210:LEU:CB	2.93	0.42
1:C:181:TYR:O	1:C:185:ARG:HD3	2.19	0.42
1:C:236:LYS:HD3	1:C:256:ASN:OD1	2.19	0.42
1:A:2:SER:C	1:A:4:ASP:H	2.28	0.42
1:A:216:SER:O	1:A:217:SER:C	2.61	0.42
1:B:65:ALA:O	1:B:68:ASN:N	2.53	0.42
1:D:64:ILE:O	1:D:65:ALA:C	2.62	0.42
1:D:124:VAL:CG1	1:D:311:PHE:HZ	2.32	0.42
1:D:186:ARG:O	1:D:187:LEU:C	2.62	0.42
1:B:7:ASP:O	1:B:7:ASP:CG	2.62	0.42
1:C:125:VAL:O	1:C:129:GLN:HB2	2.20	0.42
1:D:35:ILE:HG23	1:D:36:HIS:N	2.35	0.42
1:D:80:LEU:O	1:D:81:ILE:C	2.63	0.42
1:D:176:LEU:HD23	1:D:176:LEU:HA	1.85	0.42
1:A:28:ASP:O	1:A:30:GLN:N	2.53	0.42
1:B:191:TYR:HB2	1:B:193:LEU:HD21	2.01	0.42
1:C:16:PRO:HA	1:C:307:PHE:O	2.20	0.42
1:D:141:ARG:HE	1:D:141:ARG:HB2	1.44	0.42
1:A:18:LYS:HA	1:A:306:TRP:CD1	2.55	0.42
1:A:19:ARG:CB	1:A:307:PHE:CD1	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HD11	1:A:296:LEU:HD13	2.01	0.42
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.78	0.42
1:B:97:ALA:O	1:B:100:GLU:HB3	2.19	0.42
1:B:204:LEU:HB2	1:B:290:MET:HE1	2.01	0.42
1:B:235:ASP:OD1	1:B:235:ASP:O	2.37	0.42
1:D:18:LYS:H	1:D:306:TRP:CB	2.32	0.42
1:D:36:HIS:H	1:D:36:HIS:CD2	2.37	0.42
1:A:8:TRP:HZ2	1:A:120:GLU:O	2.03	0.42
1:B:174:PHE:O	1:B:178:ASN:HB2	2.20	0.42
1:A:18:LYS:HG2	1:A:21:PHE:CE2	2.55	0.41
1:A:48:LEU:O	1:A:51:HIS:HB2	2.21	0.41
1:A:64:ILE:HB	1:A:67:VAL:HG13	2.02	0.41
1:A:69:GLY:O	1:A:73:VAL:HG23	2.20	0.41
1:A:96:LEU:H	1:A:96:LEU:HD23	1.84	0.41
1:A:191:TYR:CB	1:A:193:LEU:CD2	2.98	0.41
1:A:217:SER:O	1:A:220:GLN:HB3	2.20	0.41
1:B:136:PHE:N	1:B:136:PHE:CD1	2.87	0.41
1:A:70:LEU:HD22	1:A:159:LEU:HD12	2.03	0.41
1:A:81:ILE:HB	1:A:186:ARG:NH2	2.35	0.41
1:A:199:HIS:CE1	1:A:294:GLU:OE2	2.73	0.41
1:B:270:LEU:HD23	1:B:270:LEU:HA	1.88	0.41
1:C:125:VAL:O	1:C:126:PRO:C	2.60	0.41
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.77	0.41
1:D:49:ILE:C	1:D:51:HIS:H	2.27	0.41
1:D:73:VAL:O	1:D:76:LYS:N	2.53	0.41
1:D:230:PRO:C	1:D:232:GLU:H	2.28	0.41
1:A:264:GLU:HG3	1:A:271:TYR:CZ	2.55	0.41
1:B:162:LEU:HD11	1:B:311:PHE:HE2	1.85	0.41
1:D:48:LEU:O	1:D:170:GLY:HA3	2.20	0.41
1:D:87:LEU:HD21	1:D:96:LEU:HG	2.02	0.41
1:D:87:LEU:CD2	1:D:96:LEU:HG	2.49	0.41
1:A:3:LEU:HD12	1:A:36:HIS:C	2.45	0.41
1:A:79:HIS:O	1:A:79:HIS:CD2	2.73	0.41
1:A:235:ASP:OD1	1:A:235:ASP:C	2.62	0.41
1:C:172:ASP:O	1:C:173:VAL:C	2.62	0.41
1:D:99:ARG:O	1:D:103:HIS:CD2	2.73	0.41
1:D:114:GLN:O	1:D:115:GLU:C	2.63	0.41
1:D:219:TRP:CZ2	1:D:227:PRO:HG2	2.55	0.41
1:A:50:SER:O	1:A:221:LEU:HD12	2.21	0.41
1:A:282:LYS:HB2	1:A:282:LYS:HE2	1.73	0.41
1:B:15:THR:HA	1:B:16:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ILE:HD13	1:B:252:ILE:HD12	2.03	0.41
1:C:125:VAL:HB	1:C:126:PRO:HD3	2.02	0.41
1:C:160:ASP:C	1:C:162:LEU:N	2.79	0.41
1:D:71:MET:O	1:D:75:ASP:HB2	2.21	0.41
1:A:6:VAL:CG2	1:A:161:MET:HB3	2.50	0.41
1:A:32:SER:HA	1:A:315:VAL:O	2.21	0.41
1:B:111:GLN:O	1:B:111:GLN:HG3	2.21	0.41
1:B:185:ARG:O	1:B:186:ARG:C	2.63	0.41
1:B:222:LEU:O	1:B:223:ASP:C	2.64	0.41
1:C:55:PRO:HG3	1:C:245:THR:O	2.21	0.41
1:C:239:VAL:HG12	1:C:240:ARG:N	2.36	0.41
1:A:118:PRO:HB2	1:A:121:TYR:CD1	2.52	0.41
1:A:169:ARG:O	1:A:170:GLY:C	2.64	0.41
1:B:191:TYR:CB	1:B:193:LEU:CD2	2.99	0.41
1:C:234:LEU:HD23	1:C:234:LEU:HA	1.79	0.41
1:D:16:PRO:HA	1:D:307:PHE:C	2.46	0.41
1:D:35:ILE:HG23	1:D:36:HIS:CD2	2.56	0.41
1:D:99:ARG:CG	1:D:99:ARG:NH1	2.82	0.41
1:D:159:LEU:HA	1:D:159:LEU:HD23	1.76	0.41
1:D:174:PHE:CD2	1:D:174:PHE:C	2.99	0.41
1:D:231:ARG:H	1:D:231:ARG:HD3	1.85	0.41
1:A:40:TYR:HD2	1:A:41:HIS:CE1	2.39	0.41
1:A:130:TYR:CD2	1:A:130:TYR:C	2.95	0.41
1:A:170:GLY:HA2	1:A:173:VAL:HG13	2.02	0.41
1:B:19:ARG:CG	1:B:314:TRP:CE2	3.04	0.41
1:B:173:VAL:O	1:B:174:PHE:C	2.62	0.41
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.96	0.41
1:D:128:LEU:CD2	1:D:155:THR:HG23	2.51	0.41
1:D:166:PRO:O	1:D:167:HIS:C	2.63	0.41
1:D:222:LEU:O	1:D:225:GLN:N	2.33	0.41
1:D:282:LYS:O	1:D:283:VAL:C	2.64	0.41
1:D:290:MET:O	1:D:291:TYR:C	2.60	0.41
1:B:127:GLU:O	1:B:128:LEU:C	2.64	0.41
1:B:135:SER:HB2	1:B:136:PHE:CE1	2.56	0.41
1:C:66:MET:O	1:C:67:VAL:C	2.60	0.41
1:C:121:TYR:O	1:C:123:GLU:N	2.54	0.41
1:D:210:LEU:HD23	1:D:210:LEU:HA	1.58	0.41
1:A:119:SER:C	1:A:121:TYR:H	2.29	0.40
1:C:3:LEU:HD22	1:C:36:HIS:CB	2.51	0.40
1:C:269:ILE:O	1:C:270:LEU:C	2.61	0.40
1:D:66:MET:HG2	1:D:164:MET:CB	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:TYR:HB2	1:B:193:LEU:CD2	2.51	0.40
1:B:265:GLU:H	1:B:265:GLU:HG3	1.63	0.40
1:C:121:TYR:HE2	1:C:162:LEU:HD22	1.86	0.40
1:C:295:VAL:HB	1:C:301:VAL:HG11	2.03	0.40
1:B:94:GLY:HA3	1:B:142:LEU:HB3	2.03	0.40
1:B:181:TYR:CE1	1:B:211:VAL:HG13	2.55	0.40
1:B:271:TYR:CD2	1:B:271:TYR:C	3.00	0.40
1:C:56:ASP:HB3	1:C:59:ALA:HB2	2.02	0.40
1:D:230:PRO:C	1:D:232:GLU:N	2.78	0.40
1:A:121:TYR:O	1:A:123:GLU:N	2.54	0.40
1:A:258:VAL:CG1	1:C:93:TYR:CZ	3.03	0.40
1:B:78:ALA:O	1:B:80:LEU:N	2.55	0.40
1:B:143:ASP:HA	1:B:194:GLU:H	1.86	0.40
1:B:209:HIS:CE1	1:B:290:MET:HE2	2.56	0.40
1:C:62:SER:OG	1:C:63:SER:N	2.55	0.40
1:D:104:LYS:HA	1:D:107:GLU:HB2	2.03	0.40
1:A:79:HIS:CD2	1:A:79:HIS:C	3.00	0.40
1:A:247:PHE:O	1:A:248:TYR:C	2.63	0.40
1:B:104:LYS:O	1:B:105:LEU:C	2.64	0.40
1:B:144:TYR:CD2	1:B:188:ILE:HD11	2.56	0.40
1:D:129:GLN:O	1:D:130:TYR:C	2.63	0.40
1:D:209:HIS:CE1	1:D:291:TYR:HA	2.56	0.40
1:D:233:ILE:HD11	1:D:274:ALA:HB2	2.03	0.40
1:D:278:PRO:HG2	1:D:279:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	306/323 (95%)	257 (84%)	30 (10%)	19 (6%)	1 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	314/323 (97%)	257 (82%)	41 (13%)	16 (5%)	1	5
1	C	314/323 (97%)	259 (82%)	45 (14%)	10 (3%)	3	11
1	D	306/323 (95%)	252 (82%)	44 (14%)	10 (3%)	3	11
2	F	2/6 (33%)	2 (100%)	0	0	100	100
2	G	2/6 (33%)	2 (100%)	0	0	100	100
2	H	2/6 (33%)	2 (100%)	0	0	100	100
2	I	2/6 (33%)	2 (100%)	0	0	100	100
All	All	1248/1316 (95%)	1033 (83%)	160 (13%)	55 (4%)	2	7

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	96	LEU
1	A	175	LEU
1	A	223	ASP
1	A	303	GLN
1	B	90	PRO
1	B	91	ARG
1	B	97	ALA
1	B	139	SER
1	B	201	VAL
1	C	62	SER
1	C	91	ARG
1	C	120	GLU
1	D	65	ALA
1	D	223	ASP
1	A	29	PHE
1	A	174	PHE
1	A	201	VAL
1	A	215	GLY
1	B	79	HIS
1	B	81	ILE
1	B	218	GLN
1	B	223	ASP
1	C	88	PRO
1	C	119	SER
1	C	201	VAL
1	D	7	ASP
1	D	17	VAL

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Mol	Chain	Res	Type
1	D	96	LEU
1	D	122	HIS
1	D	224	ALA
1	A	129	GLN
1	A	134	ASN
1	A	139	SER
1	A	170	GLY
1	C	7	ASP
1	C	161	MET
1	A	192	THR
1	A	214	LEU
1	B	250	GLN
1	B	255	ILE
1	B	310	GLY
1	B	316	ASN
1	A	167	HIS
1	B	123	GLU
1	B	243	LYS
1	C	223	ASP
1	A	122	HIS
1	C	291	TYR
1	D	114	GLN
1	D	243	LYS
1	A	293	VAL
1	B	110	PRO
1	A	9	PRO
1	D	9	PRO

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	277/289 (96%)	218 (79%)	59 (21%)	1	4
1	B	282/289 (98%)	222 (79%)	60 (21%)	1	4
1	C	282/289 (98%)	217 (77%)	65 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	277/289 (96%)	223 (80%)	54 (20%)	1	5
2	F	2/2 (100%)	2 (100%)	0	100	100
2	G	2/2 (100%)	2 (100%)	0	100	100
2	H	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	I	2/2 (100%)	2 (100%)	0	100	100
All	All	1126/1164 (97%)	887 (79%)	239 (21%)	1	4

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	6	VAL
1	A	10	HIS
1	A	12	THR
1	A	14	SER
1	A	17	VAL
1	A	23	THR
1	A	28	ASP
1	A	31	SER
1	A	35	ILE
1	A	47	THR
1	A	58	HIS
1	A	62	SER
1	A	63	SER
1	A	67	VAL
1	A	80	LEU
1	A	87	LEU
1	A	95	ASN
1	A	105	LEU
1	A	106	ASP
1	A	114	GLN
1	A	117	LEU
1	A	123	GLU
1	A	124	VAL
1	A	128	LEU
1	A	139	SER
1	A	150	LEU
1	A	153	MET
1	A	156	VAL
1	A	167	HIS

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Mol	Chain	Res	Type
1	A	173	VAL
1	A	182	THR
1	A	183	ILE
1	A	185	ARG
1	A	201	VAL
1	A	210	LEU
1	A	211	VAL
1	A	214	LEU
1	A	217	SER
1	A	220	GLN
1	A	231	ARG
1	A	233	ILE
1	A	235	ASP
1	A	243	LYS
1	A	244	ASP
1	A	245	THR
1	A	255	ILE
1	A	257	GLU
1	A	258	VAL
1	A	269	ILE
1	A	275	VAL
1	A	276	THR
1	A	290	MET
1	A	293	VAL
1	A	295	VAL
1	A	298	LYS
1	A	315	VAL
1	A	316	ASN
1	A	317	ILE
1	B	2	SER
1	B	3	LEU
1	B	4	ASP
1	B	10	HIS
1	B	12	THR
1	B	14	SER
1	B	17	VAL
1	B	23	THR
1	B	25	THR
1	B	30	GLN
1	B	47	THR
1	B	58	HIS
1	B	62	SER

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Mol	Chain	Res	Type
1	B	67	VAL
1	B	80	LEU
1	B	81	ILE
1	B	82	ASP
1	B	83	GLU
1	B	92	ARG
1	B	96	LEU
1	B	105	LEU
1	B	119	SER
1	B	120	GLU
1	B	123	GLU
1	B	124	VAL
1	B	128	LEU
1	B	129	GLN
1	B	139	SER
1	B	151	SER
1	B	156	VAL
1	B	159	LEU
1	B	173	VAL
1	B	183	ILE
1	B	184	MET
1	B	192	THR
1	B	198	SER
1	B	201	VAL
1	B	210	LEU
1	B	211	VAL
1	B	214	LEU
1	B	220	GLN
1	B	222	LEU
1	B	223	ASP
1	B	225	GLN
1	B	231	ARG
1	B	235	ASP
1	B	237	SER
1	B	239	VAL
1	B	245	THR
1	B	257	GLU
1	B	275	VAL
1	B	276	THR
1	B	281	SER
1	B	282	LYS
1	B	285	LYS

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Mol	Chain	Res	Type
1	B	295	VAL
1	B	298	LYS
1	B	301	VAL
1	B	303	GLN
1	B	316	ASN
1	C	5	ARG
1	C	6	VAL
1	C	10	HIS
1	C	12	THR
1	C	14	SER
1	C	17	VAL
1	C	19	ARG
1	C	23	THR
1	C	25	THR
1	C	28	ASP
1	C	30	GLN
1	C	39	LYS
1	C	42	LEU
1	C	49	ILE
1	C	58	HIS
1	C	60	THR
1	C	67	VAL
1	C	75	ASP
1	C	80	LEU
1	C	81	ILE
1	C	82	ASP
1	C	83	GLU
1	C	84	THR
1	C	91	ARG
1	C	96	LEU
1	C	105	LEU
1	C	107	GLU
1	C	108	ARG
1	C	109	LEU
1	C	119	SER
1	C	123	GLU
1	C	124	VAL
1	C	128	LEU
1	C	129	GLN
1	C	139	SER
1	C	149	GLU
1	C	156	VAL

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Mol	Chain	Res	Type
1	C	164	MET
1	C	168	MET
1	C	173	VAL
1	C	182	THR
1	C	184	MET
1	C	185	ARG
1	C	186	ARG
1	C	192	THR
1	C	201	VAL
1	C	210	LEU
1	C	211	VAL
1	C	214	LEU
1	C	222	LEU
1	C	236	LYS
1	C	237	SER
1	C	239	VAL
1	C	243	LYS
1	C	256	ASN
1	C	260	MET
1	C	265	GLU
1	C	275	VAL
1	C	276	THR
1	C	282	LYS
1	C	292	SER
1	C	295	VAL
1	C	301	VAL
1	C	316	ASN
1	C	317	ILE
1	D	2	SER
1	D	4	ASP
1	D	6	VAL
1	D	12	THR
1	D	14	SER
1	D	17	VAL
1	D	23	THR
1	D	47	THR
1	D	49	ILE
1	D	60	THR
1	D	63	SER
1	D	64	ILE
1	D	67	VAL
1	D	73	VAL

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Mol	Chain	Res	Type
1	D	75	ASP
1	D	76	LYS
1	D	80	LEU
1	D	82	ASP
1	D	87	LEU
1	D	95	ASN
1	D	96	LEU
1	D	99	ARG
1	D	114	GLN
1	D	115	GLU
1	D	117	LEU
1	D	129	GLN
1	D	134	ASN
1	D	139	SER
1	D	141	ARG
1	D	156	VAL
1	D	167	HIS
1	D	168	MET
1	D	169	ARG
1	D	173	VAL
1	D	182	THR
1	D	185	ARG
1	D	190	THR
1	D	201	VAL
1	D	211	VAL
1	D	214	LEU
1	D	222	LEU
1	D	231	ARG
1	D	245	THR
1	D	257	GLU
1	D	258	VAL
1	D	260	MET
1	D	275	VAL
1	D	288	LEU
1	D	289	LYS
1	D	294	GLU
1	D	295	VAL
1	D	315	VAL
1	D	316	ASN
1	D	317	ILE
2	H	5	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	30	GLN
1	A	68	ASN
1	A	79	HIS
1	A	114	GLN
1	A	122	HIS
1	A	148	HIS
1	A	199	HIS
1	A	207	HIS
1	A	250	GLN
1	A	266	HIS
1	A	316	ASN
1	B	58	HIS
1	B	68	ASN
1	B	111	GLN
1	B	134	ASN
1	B	178	ASN
1	B	207	HIS
1	B	209	HIS
1	B	250	GLN
1	B	266	HIS
1	B	316	ASN
1	C	58	HIS
1	C	68	ASN
1	C	122	HIS
1	C	129	GLN
1	C	148	HIS
1	C	199	HIS
1	C	207	HIS
1	C	209	HIS
1	C	220	GLN
1	C	225	GLN
1	C	250	GLN
1	C	266	HIS
1	C	316	ASN
1	D	36	HIS
1	D	68	ASN
1	D	102	HIS
1	D	103	HIS
1	D	114	GLN
1	D	148	HIS
1	D	207	HIS

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Mol	Chain	Res	Type
1	D	209	HIS
1	D	225	GLN
1	D	250	GLN
1	D	266	HIS
1	D	316	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	1319	-	4,4,4	0.27	0	6,6,6	0.49	0
3	SO4	A	1318[A]	-	4,4,4	0.28	0	6,6,6	0.69	0
3	SO4	D	1319[B]	-	4,4,4	0.37	0	6,6,6	0.61	0
3	SO4	A	1320	-	4,4,4	0.37	0	6,6,6	0.39	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1319	SO4	1	0
3	A	1318[A]	SO4	1	0
3	D	1319[B]	SO4	1	0
3	A	1320	SO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1
2	H	1
2	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	5:LYS	C	6:NIT	N1	1.88
1	H	1:SIN	C4	2:ALA	N	1.20
1	I	1:SIN	C4	2:ALA	N	1.19

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	310/323 (95%)	-1.79	0 100 100	2, 2, 4, 11	0
1	B	316/323 (97%)	-1.79	0 100 100	2, 2, 3, 9	0
1	C	316/323 (97%)	-1.79	0 100 100	2, 2, 4, 9	0
1	D	310/323 (95%)	-1.79	0 100 100	2, 2, 3, 11	0
2	F	4/6 (66%)	-1.82	0 100 100	2, 2, 2, 2	0
2	G	4/6 (66%)	-1.92	0 100 100	2, 2, 2, 2	0
2	H	4/6 (66%)	-1.84	0 100 100	2, 2, 2, 2	0
2	I	4/6 (66%)	-1.80	0 100 100	2, 2, 3, 6	0
All	All	1268/1316 (96%)	-1.79	0 100 100	2, 2, 4, 11	0

There are no RSRZ outliers to report.

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
3	SO4	A	1320	5/5	0.99	0.03	53,54,54,54	0
4	CL	D	1320	1/1	0.99	0.01	7,7,7,7	0
3	SO4	B	1319	5/5	1.00	0.01	2,2,2,2	5
3	SO4	D	1319[B]	5/5	1.00	0.02	2,2,2,2	5
4	CL	A	1321	1/1	1.00	0.01	13,13,13,13	0
3	SO4	A	1318[A]	5/5	1.00	0.04	2,2,2,2	5

6.5 Other polymers [i](#)

There are no such residues in this entry.