



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:49 PM UTC

PDB ID : 8K6I / pdb_00008k6i
Title : LnaB-Actin-PRUb ternary complex
Authors : Chen, T.T.; Ouyang, S.Y.
Deposited on : 2023-07-25
Resolution : 3.19 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:

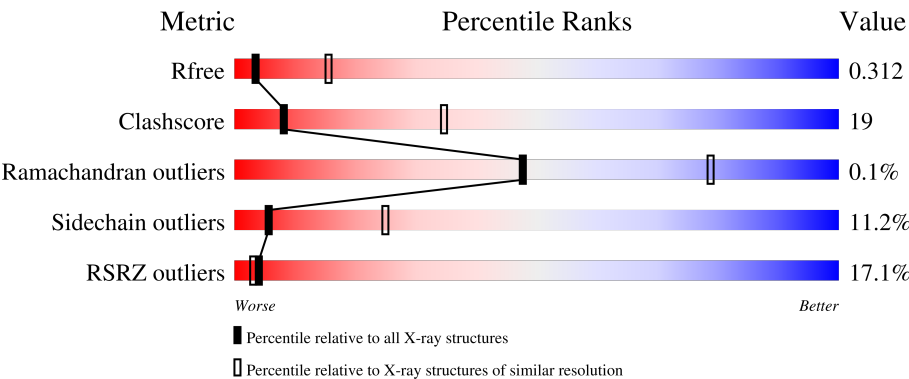
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	375	12% 48% 36% 12% ..
1	B	375	15% 47% 40% 10% ..
2	C	352	20% 41% 38% 14% 6%
2	D	352	26% 41% 42% 14% ..
3	E	78	3% 46% 36% 17% .

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Mol	Chain	Length	Quality of chain
3	F	78	5% 49% 37% 12% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12512 atoms, of which 9 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 Actin gamma 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2855	1812	479	543	21			
1	B	371	Total	C	N	O	S	0	0	0
			2889	1832	486	549	22			

- Molecule 2 is a protein called Legionella effector LnaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	331	Total	C	N	O	S	0	0	0
			2687	1715	440	527	5			
2	D	345	Total	C	N	O	S	0	0	0
			2799	1786	459	549	5			

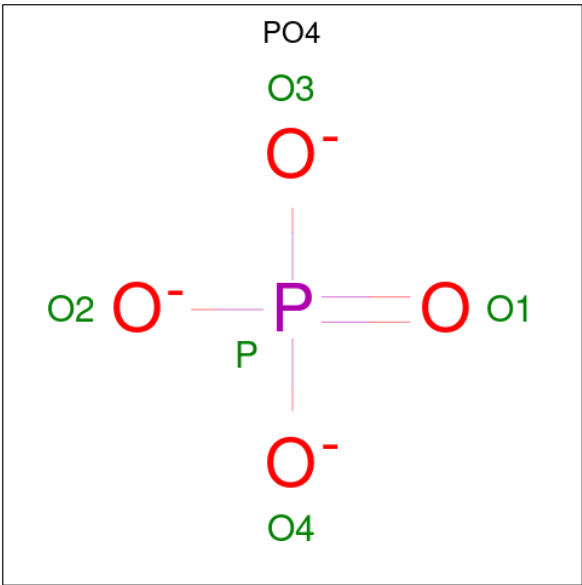
- Molecule 3 is a protein called ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	78	Total	C	N	O	S	0	0	0
			611	383	107	120	1			
3	F	77	Total	C	N	O	S	0	0	0
			608	381	106	120	1			

There are 4 discrepancies between the modelled and reference sequences:

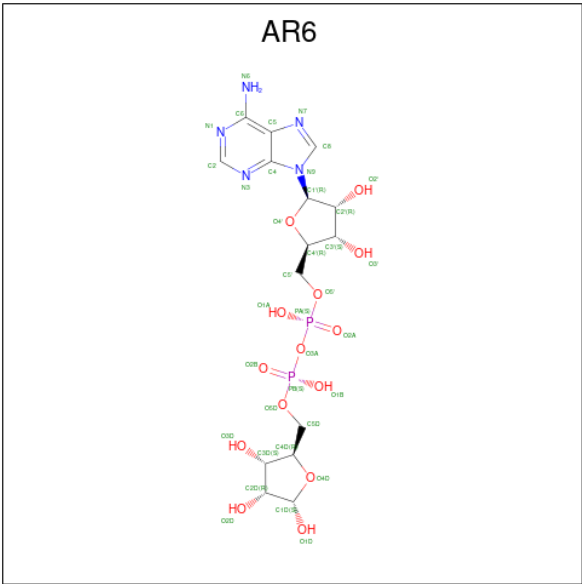
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP P0CG48
E	0	SER	-	expression tag	UNP P0CG48
F	-1	GLY	-	expression tag	UNP P0CG48
F	0	SER	-	expression tag	UNP P0CG48

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-Y L]METHYL[HYDROXY-[[[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOX Y]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	H	O	P	0	0
			23	5	9	8	1		

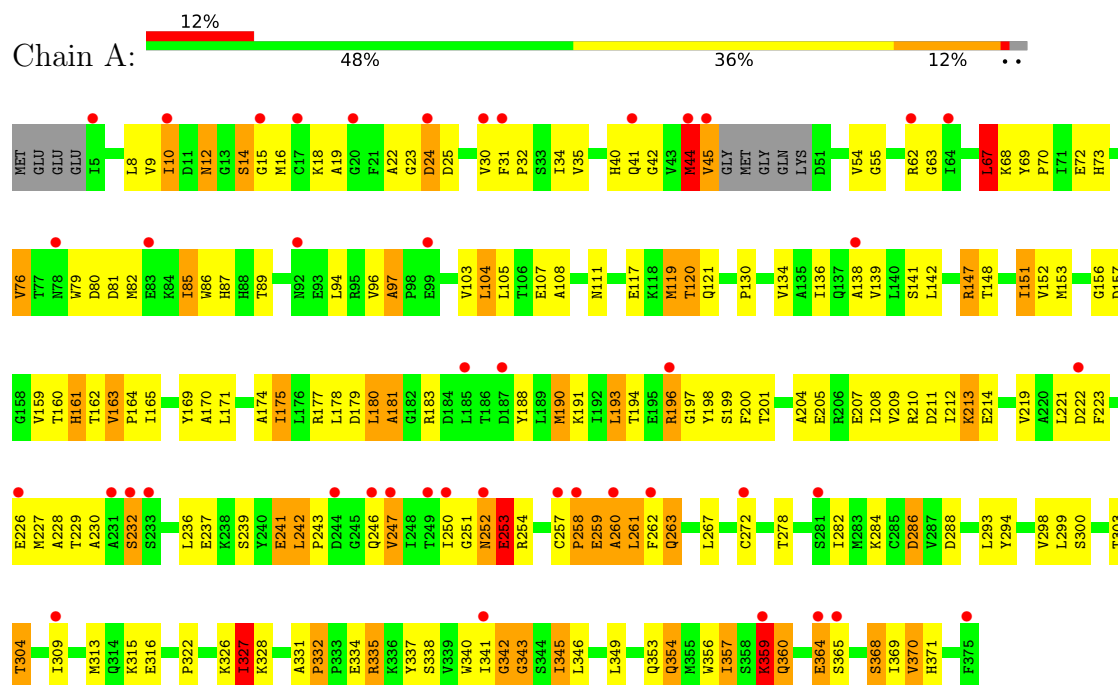
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total 9	O 9	0	0
6	B	10	Total 10	O 10	0	0
6	C	5	Total 5	O 5	0	0
6	D	9	Total 9	O 9	0	0
6	F	2	Total 2	O 2	0	0

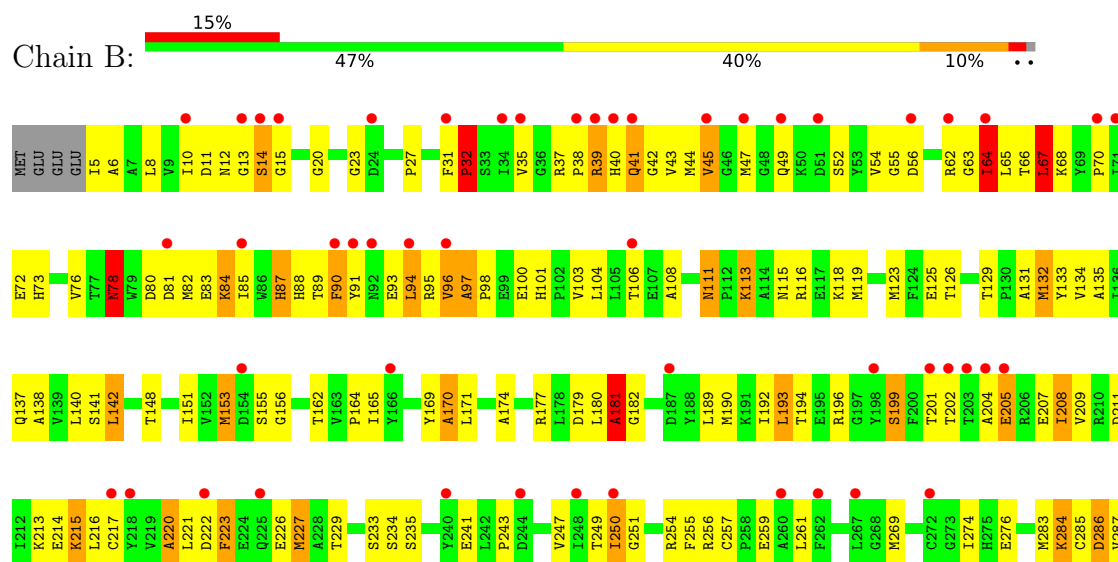
3 Residue-property plots [i](#)

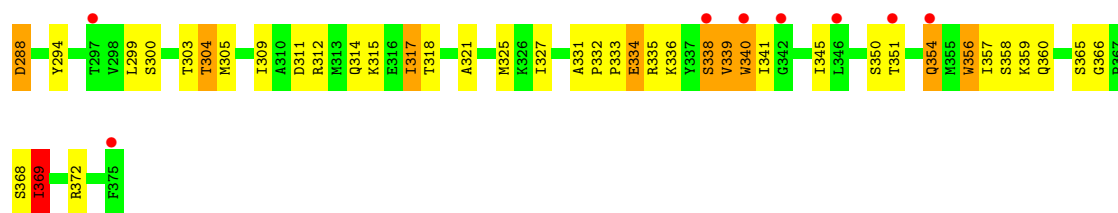
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Actin gamma 1

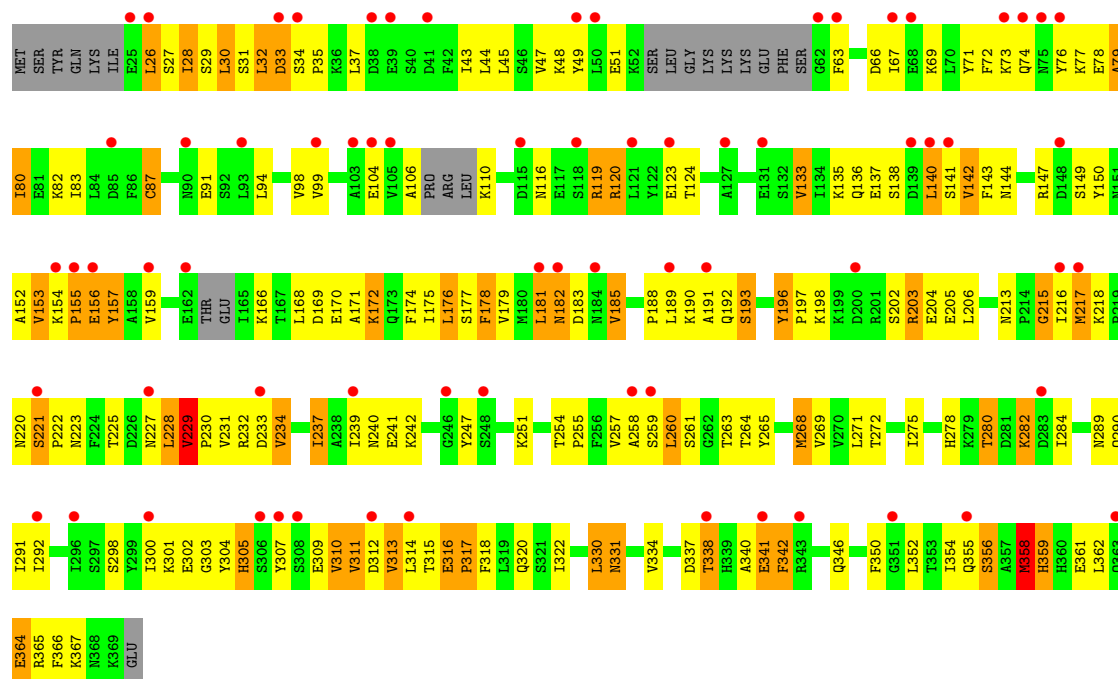


• Molecule 1: Actin gamma 1

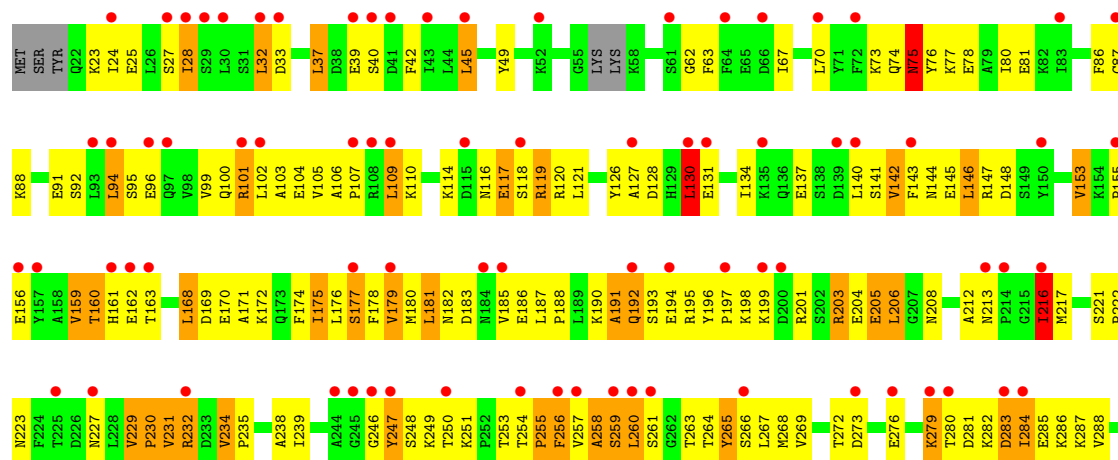


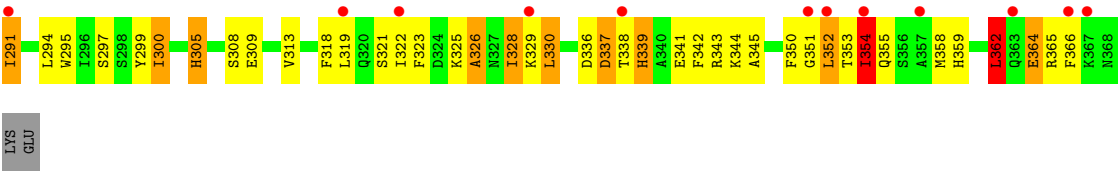


• Molecule 2: Legionella effector LnaB

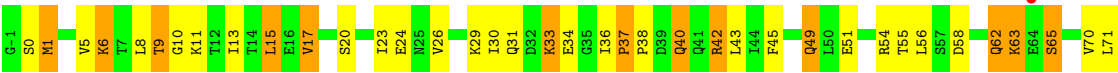


• Molecule 2: Legionella effector LnaB

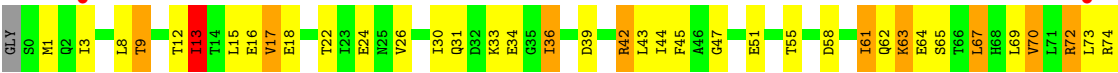




• Molecule 3: ubiquitin



• Molecule 3: ubiquitin



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	57.38Å 165.31Å 224.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.33 – 3.19 41.33 – 3.19	Depositor EDS
% Data completeness (in resolution range)	91.2 (41.33-3.19) 91.3 (41.33-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.292 , 0.315 0.291 , 0.312	Depositor DCC
R_{free} test set	1669 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	12512	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 52.07 % 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 5.1223e-05. 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: AR6, 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	1.85	40/2917 (1.4%)	1.59	74/3952 (1.9%)
1	B	1.78	36/2952 (1.2%)	1.65	84/3998 (2.1%)
2	C	1.66	28/2737 (1.0%)	1.70	96/3692 (2.6%)
2	D	1.62	29/2853 (1.0%)	1.66	87/3851 (2.3%)
3	E	1.84	9/617 (1.5%)	1.47	10/829 (1.2%)
3	F	1.67	8/614 (1.3%)	1.47	16/824 (1.9%)
All	All	1.73	150/12690 (1.2%)	1.63	367/17146 (2.1%)

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	114	LYS	CA-C	-9.53	1.44	1.52
2	C	133	VAL	C-O	-8.62	1.14	1.24
3	F	63	LYS	CA-C	-7.81	1.46	1.53
1	B	332	PRO	C-O	-7.80	1.18	1.24
1	A	22	ALA	C-O	-7.79	1.15	1.24
1	B	108	ALA	CA-C	-7.69	1.42	1.52
2	C	217	MET	CA-C	-7.68	1.43	1.52
1	A	359	LYS	CA-C	-7.65	1.42	1.52
3	E	37	PRO	CA-C	-7.42	1.47	1.51
1	A	169	TYR	CA-C	-7.39	1.43	1.52
1	A	284	LYS	CA-C	-7.27	1.44	1.53
1	B	314	GLN	CA-C	-7.23	1.45	1.52
1	A	199	SER	CA-C	-7.20	1.44	1.52
2	C	331	ASN	CA-C	-7.20	1.43	1.52
3	E	11	LYS	CA-C	-7.19	1.43	1.52
1	A	313	MET	C-O	-7.17	1.15	1.24
1	A	338	SER	CA-C	-7.01	1.43	1.52
1	A	286	ASP	CA-C	-6.99	1.44	1.52
1	A	300	SER	CA-C	-6.87	1.44	1.52
2	D	230	PRO	N-CD	-6.83	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	SER	CA-C	-6.81	1.44	1.52
3	F	65	SER	CA-C	-6.80	1.44	1.52
1	A	263	GLN	CA-C	-6.79	1.45	1.52
1	A	253	GLU	CA-C	-6.75	1.43	1.52
2	C	307	TYR	CA-C	-6.71	1.44	1.52
3	F	62	GLN	CA-C	-6.70	1.44	1.52
1	A	69	TYR	CA-C	-6.67	1.46	1.52
1	A	262	PHE	CA-C	-6.65	1.44	1.52
2	C	316	GLU	CA-C	-6.57	1.44	1.52
2	C	190	LYS	CA-C	-6.56	1.43	1.52
2	D	127	ALA	CA-C	-6.44	1.43	1.52
3	E	36	ILE	CA-C	-6.43	1.47	1.53
2	C	157	TYR	CA-C	-6.38	1.45	1.52
1	B	169	TYR	CA-C	-6.37	1.45	1.52
2	D	172	LYS	CA-C	-6.37	1.44	1.52
3	E	62	GLN	CA-C	-6.34	1.46	1.53
1	A	252	ASN	CA-C	-6.34	1.43	1.52
2	D	193	SER	CA-C	-6.33	1.45	1.52
2	C	247	TYR	CA-C	-6.30	1.44	1.52
1	B	300	SER	CA-C	-6.28	1.45	1.52
1	A	171	LEU	CA-C	-6.26	1.44	1.52
2	D	248	SER	CA-C	-6.23	1.44	1.52
2	D	258	ALA	CA-C	-6.22	1.45	1.52
3	E	42	ARG	CA-C	-6.22	1.46	1.52
1	A	328	LYS	CA-C	-6.18	1.45	1.52
1	A	175	ILE	CA-C	-6.18	1.44	1.52
1	A	181	ALA	CA-CB	-6.18	1.46	1.54
1	A	223	PHE	CA-C	-6.13	1.45	1.52
2	D	326	ALA	CA-C	-6.11	1.45	1.52
2	D	160	THR	CA-C	-6.10	1.46	1.53
1	B	284	LYS	CA-C	-6.10	1.44	1.52
3	E	55	THR	CA-C	-6.10	1.45	1.53
1	A	332	PRO	CA-C	-6.09	1.46	1.52
1	A	55	GLY	C-O	-6.08	1.20	1.24
1	B	334	GLU	CA-C	-6.05	1.44	1.52
1	B	181	ALA	CA-C	-6.03	1.44	1.52
2	D	75	ASN	CA-C	-6.03	1.47	1.53
1	B	171	LEU	CA-C	-6.01	1.45	1.52
2	D	172	LYS	C-O	-5.97	1.16	1.24
2	D	130	LEU	CA-C	-5.95	1.44	1.52
1	B	325	MET	CA-C	-5.94	1.45	1.52
1	A	108	ALA	CA-C	-5.94	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	150	TYR	CA-C	-5.88	1.45	1.52
1	A	170	ALA	CA-C	-5.88	1.45	1.52
1	A	180	LEU	CA-C	-5.87	1.45	1.52
1	B	259	GLU	CA-C	-5.87	1.45	1.52
2	D	171	ALA	CA-C	-5.85	1.44	1.52
1	A	41	GLN	CA-C	-5.82	1.47	1.53
1	B	312	ARG	C-O	-5.81	1.16	1.23
1	A	25	ASP	CA-C	-5.79	1.45	1.52
2	C	171	ALA	CA-C	-5.79	1.44	1.52
2	D	119	ARG	CA-C	-5.79	1.45	1.52
2	C	172	LYS	CA-C	-5.78	1.45	1.52
1	B	170	ALA	CA-C	-5.77	1.45	1.52
2	C	251	LYS	CA-C	-5.77	1.46	1.52
1	B	14	SER	CA-C	-5.76	1.45	1.52
3	F	51	GLU	CA-C	-5.75	1.45	1.52
2	D	217	MET	CA-C	-5.74	1.45	1.52
1	B	85	ILE	CA-C	-5.70	1.45	1.52
3	F	42	ARG	CA-C	-5.70	1.45	1.52
2	C	172	LYS	C-O	-5.69	1.17	1.24
1	B	317	ILE	C-O	-5.68	1.17	1.24
1	B	180	LEU	CA-C	-5.67	1.45	1.52
1	A	97	ALA	CA-C	-5.63	1.45	1.52
2	D	216	ILE	CA-C	-5.63	1.46	1.52
2	D	40	SER	CA-C	-5.62	1.45	1.52
2	D	110	LYS	CA-C	-5.62	1.45	1.52
1	B	47	MET	N-CA	-5.61	1.39	1.45
1	A	343	GLY	C-O	-5.61	1.17	1.24
2	C	202	SER	CA-C	-5.61	1.45	1.53
2	C	342	PHE	CA-C	-5.60	1.45	1.52
2	D	203	ARG	CA-C	-5.58	1.46	1.52
1	A	315	LYS	CA-C	-5.58	1.45	1.52
1	B	286	ASP	CA-C	-5.56	1.45	1.52
1	B	332	PRO	CA-C	-5.56	1.48	1.52
2	D	142	VAL	C-O	-5.55	1.17	1.24
2	D	221	SER	CA-C	-5.53	1.46	1.52
1	B	174	ALA	CA-C	-5.51	1.45	1.53
1	B	314	GLN	C-O	-5.50	1.16	1.23
1	A	12	ASN	CA-C	-5.49	1.45	1.52
2	D	297	SER	C-O	-5.48	1.17	1.24
1	B	220	ALA	CA-C	-5.48	1.46	1.52
1	B	182	GLY	CA-C	-5.48	1.45	1.52
1	B	340	TRP	CA-C	-5.46	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	VAL	CA-C	-5.44	1.45	1.52
1	A	121	GLN	C-O	-5.43	1.17	1.24
2	C	234	VAL	N-CA	-5.43	1.39	1.46
2	C	232	ARG	CA-C	-5.43	1.46	1.52
1	A	345	ILE	C-O	-5.42	1.18	1.23
1	A	111	ASN	CA-C	-5.39	1.46	1.53
1	A	261	LEU	CA-C	-5.39	1.45	1.52
1	B	6	ALA	CA-C	-5.39	1.45	1.53
2	C	157	TYR	C-N	-5.36	1.26	1.33
2	C	205	GLU	CA-C	-5.36	1.46	1.52
2	C	261	SER	CA-C	-5.33	1.46	1.52
2	C	71	TYR	CA-C	-5.33	1.46	1.52
1	B	35	VAL	CA-C	-5.33	1.45	1.52
2	C	120	ARG	CA-C	-5.32	1.46	1.52
2	C	182	ASN	CA-C	-5.32	1.46	1.52
3	F	64	GLU	CA-C	-5.31	1.45	1.53
3	E	65	SER	CA-C	-5.30	1.46	1.52
2	C	216	ILE	CA-C	-5.30	1.46	1.52
2	C	313	VAL	CA-C	-5.27	1.46	1.53
1	B	360	GLN	CA-C	-5.27	1.45	1.52
1	B	111	ASN	CA-C	-5.26	1.47	1.53
1	B	52	SER	CA-C	-5.25	1.46	1.52
2	C	290	GLN	C-O	-5.24	1.17	1.24
2	D	255	PRO	CA-C	-5.22	1.45	1.52
2	D	251	LYS	CA-C	-5.21	1.47	1.52
3	E	74	ARG	CA-C	-5.20	1.46	1.52
1	B	311	ASP	CA-C	-5.19	1.45	1.52
2	C	66	ASP	CA-C	-5.17	1.46	1.52
2	D	141	SER	CA-C	-5.17	1.45	1.52
1	A	174	ALA	CA-CB	-5.15	1.46	1.54
1	B	151	ILE	C-O	-5.14	1.18	1.24
1	B	294	TYR	CA-C	-5.14	1.45	1.52
2	D	231	VAL	CA-C	-5.14	1.47	1.52
1	B	223	PHE	CA-C	-5.13	1.45	1.52
3	E	51	GLU	CA-C	-5.09	1.46	1.52
3	F	72	ARG	CA-C	-5.08	1.46	1.52
2	D	232	ARG	CA-C	-5.07	1.46	1.52
2	D	181	LEU	CA-C	-5.07	1.46	1.53
1	A	360	GLN	CA-C	-5.06	1.46	1.52
1	A	19	ALA	CA-C	-5.05	1.46	1.52
1	B	78	ASN	CA-C	-5.05	1.46	1.52
2	C	231	VAL	CA-C	-5.03	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	24	GLU	CA-C	-5.03	1.46	1.52
2	D	40	SER	CA-CB	-5.03	1.45	1.53
1	A	332	PRO	C-O	-5.01	1.18	1.24
1	A	342	GLY	CA-C	-5.00	1.44	1.51

All (367) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	ARG	N-CA-C	16.76	130.98	111.71
2	C	313	VAL	N-CA-C	-14.31	98.65	112.96
1	A	24	ASP	N-CA-C	13.70	129.25	110.35
1	B	76	VAL	N-CA-C	13.33	124.21	110.62
2	C	258	ALA	N-CA-C	-13.26	89.21	108.96
2	D	191	ALA	N-CA-C	-13.18	91.01	110.52
1	A	284	LYS	N-CA-C	-13.15	91.82	112.99
2	D	259	SER	N-CA-C	12.87	127.85	110.35
2	D	146	LEU	N-CA-C	-12.85	96.09	113.30
3	E	58	ASP	N-CA-C	-12.60	94.71	113.61
2	C	263	THR	N-CA-C	-12.53	96.70	114.12
2	D	118	SER	N-CA-C	-12.31	96.77	112.90
2	C	138	SER	N-CA-C	12.23	126.11	110.33
2	C	216	ILE	N-CA-C	-11.94	93.25	109.37
2	C	181	LEU	N-CA-C	-11.92	87.16	108.02
1	A	42	GLY	N-CA-C	-11.85	95.18	115.80
2	D	114	LYS	N-CA-C	-11.69	96.11	112.13
1	B	43	VAL	N-CA-C	-11.59	102.18	113.53
1	B	44	MET	N-CA-C	-11.56	96.39	112.45
1	B	284	LYS	N-CA-C	-11.48	99.60	112.57
2	C	260	LEU	N-CA-C	-11.22	91.09	108.14
2	D	96	GLU	N-CA-C	11.18	123.04	111.07
1	A	14	SER	N-CA-C	-11.15	94.06	110.23
2	D	217	MET	N-CA-C	-10.88	92.54	107.88
2	C	137	GLU	N-CA-C	-10.62	88.19	110.80
1	B	205	GLU	N-CA-C	-10.46	100.00	113.17
1	A	23	GLY	N-CA-C	10.44	125.26	112.73
1	B	67	LEU	N-CA-C	10.34	126.18	109.85
2	D	366	PHE	N-CA-C	-10.26	99.46	112.90
2	D	171	ALA	N-CA-C	-10.24	100.92	113.41
1	B	49	GLN	N-CA-C	-10.16	100.37	113.17
1	A	45	VAL	N-CA-CB	10.15	128.76	111.50
1	A	157	ASP	N-CA-C	9.96	122.21	111.36
1	B	108	ALA	CA-C-N	-9.92	109.54	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	ALA	C-N-CA	-9.92	109.54	119.76
1	B	250	ILE	N-CA-C	9.85	120.74	111.48
1	A	111	ASN	CA-C-N	-9.76	109.71	119.76
1	A	111	ASN	C-N-CA	-9.76	109.71	119.76
2	C	364	GLU	N-CA-C	-9.74	97.31	112.99
2	C	282	LYS	N-CA-C	9.56	122.90	111.33
2	D	248	SER	N-CA-C	-9.55	101.63	113.38
2	C	305	HIS	N-CA-C	9.55	123.66	109.24
2	C	356	SER	N-CA-C	-9.54	100.88	111.28
2	C	28	ILE	N-CA-C	-9.52	101.85	112.80
2	D	208	ASN	N-CA-C	9.51	124.30	110.42
2	D	336	ASP	N-CA-C	9.30	122.74	111.40
3	E	45	PHE	N-CA-C	-9.29	93.26	109.06
3	E	40	GLN	N-CA-C	-9.25	102.13	113.97
3	F	9	THR	N-CA-C	-9.23	102.53	113.88
1	A	22	ALA	N-CA-C	9.22	120.93	111.07
1	B	215	LYS	N-CA-C	9.18	121.37	111.36
2	C	170	GLU	N-CA-C	-9.17	102.11	113.38
1	B	15	GLY	N-CA-C	9.15	124.49	112.77
1	B	354	GLN	N-CA-C	9.13	121.31	111.36
2	D	337	ASP	CB-CA-C	-9.13	98.18	112.05
1	B	97	ALA	N-CA-C	9.11	121.21	109.64
2	C	156	GLU	N-CA-C	9.09	122.37	111.82
1	B	303	THR	N-CA-C	-9.09	101.96	113.23
2	C	32	LEU	N-CA-C	8.99	121.16	111.36
2	D	260	LEU	N-CA-C	8.96	123.72	111.90
2	C	157	TYR	N-CA-C	-8.95	104.42	114.62
2	C	358	MET	N-CA-C	-8.93	101.82	112.89
2	C	367	LYS	N-CA-C	-8.91	101.65	111.36
2	D	177	SER	N-CA-C	-8.91	99.82	113.89
1	B	23	GLY	N-CA-C	-8.87	103.41	113.79
2	D	284	ILE	N-CA-C	-8.86	101.77	110.72
1	B	312	ARG	N-CA-C	-8.83	102.67	113.97
3	E	9	THR	N-CA-C	-8.75	102.77	113.97
2	C	242	LYS	N-CA-C	-8.73	100.52	113.61
1	B	88	HIS	N-CA-C	-8.71	102.78	112.72
2	C	331	ASN	N-CA-C	-8.70	95.03	109.46
2	D	169	ASP	N-CA-C	-8.61	102.80	113.38
2	D	364	GLU	N-CA-C	-8.58	102.87	112.57
2	D	102	LEU	N-CA-C	-8.51	102.09	111.36
1	A	261	LEU	N-CA-C	-8.50	103.09	113.97
1	A	25	ASP	N-CA-C	8.47	120.13	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASP	N-CA-C	-8.47	102.96	113.20
2	C	182	ASN	CB-CA-C	-8.41	98.35	110.62
2	D	235	PRO	N-CA-C	8.38	122.95	111.22
2	D	130	LEU	N-CA-C	-8.38	103.19	113.41
1	A	227	MET	N-CA-C	-8.37	102.08	111.71
2	D	172	LYS	N-CA-C	-8.37	102.12	111.82
1	A	242	LEU	N-CA-C	-8.36	99.22	109.83
3	F	47	GLY	N-CA-C	-8.28	103.76	115.43
2	D	230	PRO	N-CA-C	8.26	123.14	111.33
1	B	321	ALA	N-CA-C	8.26	121.22	110.40
1	B	207	GLU	N-CA-C	-8.21	103.41	113.50
2	C	179	VAL	N-CA-C	-8.20	101.34	113.39
2	D	101	ARG	N-CA-C	8.18	122.53	112.23
2	D	117	GLU	N-CA-C	8.16	122.02	112.72
2	D	78	GLU	N-CA-C	-8.12	102.42	111.28
1	B	83	GLU	N-CA-C	-8.09	102.44	111.82
2	C	362	LEU	N-CA-C	-8.09	103.54	113.41
2	D	282	LYS	N-CA-C	8.08	122.24	112.38
1	A	87	HIS	N-CA-C	-8.06	100.84	111.24
3	E	36	ILE	CA-C-N	-8.04	113.79	119.66
3	E	36	ILE	C-N-CA	-8.04	113.79	119.66
2	C	152	ALA	N-CA-C	7.93	119.71	111.14
2	D	323	PHE	N-CA-C	-7.88	102.28	111.03
2	D	326	ALA	N-CA-C	-7.86	101.86	112.94
2	C	169	ASP	N-CA-C	-7.84	103.03	114.39
1	B	311	ASP	N-CA-C	-7.82	103.24	114.12
2	C	365	ARG	N-CA-C	-7.82	104.63	114.56
2	D	116	ASN	CB-CA-C	-7.81	99.32	111.74
2	D	131	GLU	N-CA-C	-7.78	102.88	111.36
1	A	41	GLN	N-CA-CB	-7.77	101.65	110.35
2	C	26	LEU	N-CA-C	-7.72	101.70	113.89
1	B	64	ILE	N-CA-C	-7.70	105.19	111.81
2	C	140	LEU	N-CA-C	-7.70	102.86	112.72
2	D	33	ASP	N-CA-C	-7.68	103.91	113.20
1	A	148	THR	N-CA-C	-7.66	104.54	114.04
1	B	369	ILE	N-CA-C	-7.65	106.03	113.53
1	A	230	ALA	N-CA-C	7.58	119.62	111.36
2	D	178	PHE	N-CA-C	-7.57	104.45	112.93
1	B	180	LEU	N-CA-C	-7.55	96.22	109.06
1	A	260	ALA	N-CA-C	-7.53	104.19	113.15
1	A	67	LEU	N-CA-C	7.49	122.03	110.20
1	B	103	VAL	N-CA-C	7.48	119.05	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	THR	CB-CA-C	-7.45	102.06	111.22
2	C	316	GLU	N-CA-C	-7.43	98.73	110.10
2	C	280	THR	N-CA-C	-7.41	104.13	113.02
1	B	115	ASN	N-CA-C	-7.39	103.72	112.89
1	A	163	VAL	N-CA-C	7.39	116.15	107.73
1	B	314	GLN	N-CA-C	-7.37	103.12	112.93
2	C	196	TYR	CA-C-N	-7.36	111.97	121.91
2	C	196	TYR	C-N-CA	-7.36	111.97	121.91
1	A	213	LYS	N-CA-C	7.34	119.07	111.14
2	C	366	PHE	N-CA-C	-7.34	104.57	113.97
1	A	221	LEU	N-CA-C	-7.33	104.14	113.23
3	F	63	LYS	CB-CA-C	-7.32	108.14	116.63
2	C	33	ASP	N-CA-C	7.29	119.01	111.14
2	D	156	GLU	N-CA-C	7.26	121.19	108.56
2	C	69	LYS	N-CA-C	-7.25	104.04	113.17
1	B	234	SER	N-CA-C	-7.23	104.40	112.57
2	D	338	THR	N-CA-C	-7.23	103.77	112.59
1	A	179	ASP	N-CA-C	-7.22	104.48	112.72
2	C	192	GLN	N-CA-C	-7.20	104.38	113.02
3	E	74	ARG	N-CA-C	-7.19	95.86	108.23
1	A	117	GLU	N-CA-C	-7.19	104.77	113.97
1	A	139	VAL	N-CA-C	-7.17	102.54	112.50
2	D	86	PHE	N-CA-C	-7.16	103.47	111.28
2	C	98	VAL	N-CA-C	7.13	117.92	110.72
1	A	364	GLU	N-CA-C	7.12	118.83	111.14
2	C	359	HIS	N-CA-C	-7.10	102.95	111.69
2	D	247	TYR	N-CA-C	7.10	124.43	113.28
1	B	251	GLY	N-CA-C	7.08	124.43	110.77
2	C	237	ILE	N-CA-C	-7.04	98.52	108.80
3	F	24	GLU	N-CA-C	-7.04	104.72	113.38
2	D	365	ARG	N-CA-C	-7.04	103.94	114.64
2	C	232	ARG	N-CA-C	-7.03	99.05	108.74
2	D	305	HIS	N-CA-C	7.02	117.29	108.45
1	A	76	VAL	N-CA-C	7.01	121.85	112.04
2	C	298	SER	N-CA-C	6.99	121.65	113.20
1	A	316	GLU	N-CA-C	6.98	118.89	111.28
1	B	55	GLY	N-CA-C	6.97	120.03	111.45
2	D	354	ILE	N-CA-C	-6.97	103.52	113.07
1	B	339	VAL	N-CA-C	-6.97	102.11	111.44
2	D	76	TYR	N-CA-C	6.96	118.87	111.28
2	D	265	TYR	N-CA-C	-6.94	104.78	113.18
2	C	155	PRO	CB-CA-C	-6.94	100.11	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	LEU	N-CA-C	-6.93	104.95	113.41
1	A	335	ARG	N-CA-C	6.93	118.92	111.36
2	C	171	ALA	N-CA-C	-6.92	103.52	112.23
1	B	45	VAL	N-CA-C	-6.90	99.69	109.63
3	E	10	GLY	N-CA-C	-6.89	105.58	115.64
1	A	252	ASN	N-CA-C	-6.89	104.35	112.89
1	B	193	LEU	N-CA-C	-6.89	105.01	113.41
2	C	196	TYR	N-CA-C	6.86	122.16	113.25
1	B	123	MET	N-CA-C	6.80	118.77	111.36
1	A	257	CYS	CA-C-N	-6.79	112.81	119.87
1	A	257	CYS	C-N-CA	-6.79	112.81	119.87
2	C	215	GLY	N-CA-C	6.78	124.84	112.37
1	A	12	ASN	N-CA-C	-6.77	98.89	109.25
2	D	212	ALA	N-CA-C	-6.77	106.22	114.75
3	F	13	ILE	N-CA-C	-6.77	98.60	108.89
3	F	61	ILE	N-CA-C	-6.74	98.62	108.87
2	D	119	ARG	N-CA-C	-6.72	105.11	113.38
1	B	331	ALA	CA-C-N	-6.71	114.83	119.66
1	B	331	ALA	C-N-CA	-6.71	114.83	119.66
2	C	259	SER	N-CA-C	6.70	121.74	113.50
1	A	338	SER	N-CA-C	-6.70	105.39	113.97
1	B	87	HIS	N-CA-C	-6.68	105.42	113.97
1	B	204	ALA	N-CA-C	6.68	122.84	113.56
2	D	253	THR	N-CA-C	6.67	118.35	111.14
1	A	191	LYS	N-CA-C	6.67	118.21	111.07
1	B	84	LYS	N-CA-C	6.66	118.62	111.36
2	C	182	ASN	N-CA-C	6.66	119.33	107.80
1	A	85	ILE	N-CA-C	-6.66	105.03	113.22
2	D	160	THR	N-CA-C	6.65	117.84	108.00
2	D	345	ALA	N-CA-C	-6.65	96.64	110.80
2	D	256	PHE	N-CA-C	6.64	119.16	109.07
3	F	36	ILE	CA-C-N	-6.63	113.56	120.38
3	F	36	ILE	C-N-CA	-6.63	113.56	120.38
1	B	336	LYS	N-CA-C	-6.60	104.17	111.36
1	A	359	LYS	N-CA-C	-6.59	104.09	111.28
1	A	197	GLY	N-CA-C	-6.58	105.67	114.95
2	D	203	ARG	N-CA-C	-6.57	103.37	112.30
2	D	353	THR	N-CA-C	6.56	118.51	111.36
1	A	94	LEU	N-CA-C	-6.55	105.10	113.23
2	C	157	TYR	CB-CA-C	6.52	117.95	109.28
2	D	204	GLU	N-CA-C	-6.50	105.21	113.01
1	B	148	THR	N-CA-C	-6.46	105.14	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	352	LEU	N-CA-C	6.40	118.33	111.36
2	C	221	SER	CA-C-N	-6.36	113.23	119.78
2	C	221	SER	C-N-CA	-6.36	113.23	119.78
1	B	100	GLU	N-CA-C	6.34	118.27	111.36
1	B	142	LEU	N-CA-C	-6.34	106.14	114.31
2	C	190	LYS	N-CA-C	-6.33	105.59	113.38
2	D	102	LEU	N-CA-CB	6.33	119.53	110.16
2	C	341	GLU	N-CA-C	6.33	118.26	111.36
1	A	108	ALA	CA-C-N	-6.31	113.26	119.76
1	A	108	ALA	C-N-CA	-6.31	113.26	119.76
2	C	79	ALA	N-CA-C	6.30	118.22	111.36
1	B	345	ILE	N-CA-C	6.30	116.47	110.42
2	C	354	ILE	N-CA-C	6.26	117.01	110.62
1	B	132	MET	N-CA-C	6.25	118.92	109.23
2	D	32	LEU	N-CA-C	-6.23	105.61	113.72
2	C	78	GLU	N-CA-C	-6.22	104.41	111.07
2	C	302	GLU	N-CA-C	-6.21	105.01	112.59
1	A	163	VAL	CB-CA-C	-6.21	103.71	110.85
1	A	205	GLU	N-CA-C	-6.21	105.53	113.23
2	C	143	PHE	N-CA-C	-6.21	106.35	114.04
1	B	182	GLY	N-CA-C	6.20	121.37	113.24
3	F	45	PHE	N-CA-C	-6.20	98.89	109.24
2	D	294	LEU	N-CA-C	-6.19	104.62	111.36
2	C	30	LEU	N-CA-C	-6.17	104.67	111.82
2	D	94	LEU	N-CA-C	6.16	119.19	110.50
2	C	172	LYS	N-CA-C	-6.16	104.20	111.03
1	A	82	MET	N-CA-C	-6.15	105.61	113.23
2	D	109	LEU	N-CA-C	6.13	119.51	109.76
2	C	119	ARG	N-CA-C	-6.12	105.97	113.50
2	D	206	LEU	N-CA-C	-6.12	101.88	110.50
1	B	80	ASP	N-CA-C	-6.12	105.95	113.41
1	B	366	GLY	CA-C-N	-6.11	114.60	120.83
1	B	366	GLY	C-N-CA	-6.11	114.60	120.83
1	B	170	ALA	N-CA-C	-6.09	100.58	110.20
1	B	94	LEU	N-CA-C	-6.07	103.43	111.02
2	D	128	ASP	N-CA-C	-6.06	105.71	113.23
1	B	294	TYR	N-CA-C	-6.04	104.81	111.82
2	C	220	ASN	N-CA-C	-6.03	103.05	110.65
2	D	342	PHE	N-CA-C	-6.03	104.62	111.07
2	D	205	GLU	N-CA-C	6.01	119.69	111.39
1	A	86	TRP	N-CA-C	-6.01	106.11	113.50
1	A	10	ILE	N-CA-C	6.00	116.51	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	MET	N-CA-C	6.00	118.78	111.82
1	A	119	MET	N-CA-C	-5.99	105.05	112.90
1	B	196	ARG	N-CA-C	-5.99	105.95	113.20
2	C	203	ARG	N-CA-C	-5.99	106.02	113.38
2	C	183	ASP	N-CA-C	5.98	119.89	112.24
3	E	31	GLN	N-CA-C	-5.97	106.53	113.88
2	C	182	ASN	N-CA-CB	-5.96	101.61	110.90
3	F	31	GLN	N-CA-C	-5.90	105.17	112.90
1	A	262	PHE	N-CA-C	-5.90	106.42	113.97
2	C	34	SER	N-CA-C	5.90	122.84	109.81
1	A	258	PRO	N-CA-CB	-5.87	97.90	103.41
2	C	330	LEU	N-CA-C	5.86	118.51	109.07
1	A	357	ILE	N-CA-C	-5.86	98.59	107.73
2	D	267	LEU	N-CA-C	-5.84	104.50	111.69
2	C	156	GLU	N-CA-CB	-5.84	101.23	110.28
1	A	326	LYS	N-CA-C	-5.81	101.02	110.20
2	C	340	ALA	N-CA-C	5.79	118.06	111.11
1	B	199	SER	N-CA-C	5.79	119.04	110.48
2	D	229	VAL	CA-C-N	-5.78	113.64	120.11
2	D	229	VAL	C-N-CA	-5.78	113.64	120.11
1	B	125	GLU	N-CA-C	5.78	118.52	111.82
2	C	176	LEU	N-CA-C	-5.78	106.00	113.16
1	B	249	THR	CA-C-N	-5.77	117.31	122.97
1	B	249	THR	C-N-CA	-5.77	117.31	122.97
2	D	159	VAL	N-CA-C	5.77	117.16	109.37
1	A	196	ARG	N-CA-C	-5.75	107.25	114.56
3	F	69	LEU	N-CA-C	5.75	118.48	108.76
1	B	41	GLN	N-CA-C	-5.75	101.54	110.10
2	D	227	ASN	N-CA-C	-5.74	106.62	113.97
2	C	177	SER	N-CA-C	-5.73	106.09	112.57
2	C	337	ASP	N-CA-CB	-5.73	101.95	110.60
1	A	332	PRO	CA-C-N	-5.72	113.73	119.56
1	A	332	PRO	C-N-CA	-5.72	113.73	119.56
1	A	16	MET	N-CA-C	5.70	118.50	110.23
2	D	362	LEU	N-CA-C	-5.70	105.44	112.90
2	C	309	GLU	N-CA-C	-5.67	105.86	112.89
2	D	117	GLU	CB-CA-C	-5.67	101.58	110.94
1	B	8	LEU	N-CA-C	-5.64	100.21	109.40
2	C	193	SER	N-CA-C	5.64	117.92	108.73
2	D	179	VAL	N-CA-C	-5.64	105.10	113.39
1	B	351	THR	N-CA-C	-5.63	106.07	113.17
2	C	35	PRO	N-CA-C	5.62	119.51	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	153	VAL	N-CA-C	5.62	116.35	110.62
3	F	39	ASP	N-CA-C	-5.62	106.97	113.88
2	C	174	PHE	N-CA-C	5.62	117.20	111.14
1	A	304	THR	N-CA-C	-5.61	105.08	112.72
1	A	55	GLY	N-CA-C	5.61	117.04	111.21
2	C	303	GLY	N-CA-C	5.61	123.79	114.48
2	C	338	THR	N-CA-C	-5.58	106.23	113.16
2	D	92	SER	N-CA-C	-5.54	105.15	111.07
2	C	213	ASN	CA-C-N	-5.53	112.93	119.84
2	C	213	ASN	C-N-CA	-5.53	112.93	119.84
1	B	72	GLU	N-CA-C	-5.52	106.59	113.38
2	D	170	GLU	N-CA-C	-5.52	105.76	112.88
1	A	303	THR	CB-CA-C	5.51	119.24	109.65
1	A	243	PRO	N-CA-C	5.51	123.82	112.47
2	D	192	GLN	CB-CA-C	5.51	120.87	110.35
2	D	216	ILE	CB-CA-C	-5.51	104.27	111.81
1	A	63	GLY	N-CA-C	-5.50	100.15	113.18
2	C	27	SER	N-CA-C	-5.50	106.25	113.17
1	B	70	PRO	CA-C-O	-5.49	115.21	121.96
1	B	129	THR	CA-C-N	-5.48	112.99	119.84
1	B	129	THR	C-N-CA	-5.48	112.99	119.84
2	C	104	GLU	N-CA-C	5.46	117.32	111.36
1	B	259	GLU	N-CA-C	-5.46	106.62	113.72
2	D	321	SER	N-CA-C	5.45	120.31	111.37
1	B	35	VAL	CB-CA-C	-5.45	103.07	110.42
2	D	141	SER	N-CA-C	-5.45	104.88	112.45
1	B	256	ARG	N-CA-C	-5.44	106.15	112.89
2	D	144	ASN	N-CA-C	-5.43	106.66	113.28
1	B	276	GLU	N-CA-C	-5.42	105.28	111.14
1	A	44	MET	N-CA-C	-5.42	98.92	108.23
3	F	42	ARG	N-CA-C	-5.40	99.63	108.76
1	A	32	PRO	N-CA-C	5.40	119.51	111.41
2	D	339	HIS	N-CA-C	-5.38	105.57	111.82
2	C	142	VAL	N-CA-C	-5.38	107.50	112.83
1	B	357	ILE	N-CA-C	-5.37	101.91	109.21
1	B	208	ILE	N-CA-C	-5.37	105.30	110.72
1	A	293	LEU	N-CA-C	-5.36	106.80	113.55
2	D	62	GLY	N-CA-C	-5.36	100.49	113.18
1	A	183	ARG	N-CA-C	-5.33	105.47	111.28
1	B	233	SER	N-CA-C	5.33	117.92	109.50
1	A	370	VAL	CB-CA-C	-5.32	104.28	112.05
2	C	205	GLU	N-CA-C	-5.32	100.63	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	ALA	CA-C-N	5.30	124.63	118.85
1	B	97	ALA	C-N-CA	5.30	124.63	118.85
1	B	63	GLY	N-CA-C	-5.28	100.66	113.18
1	B	318	THR	N-CA-C	-5.28	105.99	112.90
2	C	311	VAL	N-CA-C	5.28	119.79	112.35
3	E	49	GLN	N-CA-C	-5.28	101.18	109.25
2	D	155	PRO	N-CA-C	5.27	120.46	113.40
2	D	239	ILE	N-CA-C	5.27	115.55	108.17
1	A	31	PHE	CA-C-N	-5.25	114.83	120.03
1	A	31	PHE	C-N-CA	-5.25	114.83	120.03
2	C	320	GLN	N-CA-C	-5.25	105.64	111.36
3	F	58	ASP	N-CA-C	-5.24	106.89	113.28
1	B	356	TRP	N-CA-C	-5.23	102.31	110.10
2	C	228	LEU	CA-CB-CG	5.23	134.61	116.30
1	A	232	SER	N-CA-C	-5.22	107.56	114.04
2	C	204	GLU	N-CA-C	-5.21	101.64	109.15
1	B	32	PRO	N-CA-C	5.21	123.21	112.47
2	D	283	ASP	CB-CA-C	-5.21	102.38	111.23
2	D	27	SER	N-CA-C	5.20	116.95	111.28
2	C	94	LEU	N-CA-C	-5.19	101.30	109.50
1	A	368	SER	N-CA-C	-5.19	106.72	113.16
2	C	76	TYR	N-CA-C	5.19	119.46	113.18
1	A	15	GLY	N-CA-C	5.19	120.41	110.86
2	C	178	PHE	N-CA-C	-5.16	106.74	112.57
1	B	138	ALA	N-CA-C	5.16	117.80	111.82
2	D	100	GLN	N-CA-C	-5.16	105.55	111.07
3	F	64	GLU	N-CA-C	-5.14	100.01	108.49
2	C	87	CYS	N-CA-C	-5.13	106.85	113.01
1	B	338	SER	N-CA-C	-5.12	107.41	113.97
2	C	229	VAL	N-CA-CB	-5.11	108.31	111.83
2	C	298	SER	N-CA-CB	-5.10	102.16	110.42
3	F	67	LEU	N-CA-C	-5.09	102.36	109.69
2	C	261	SER	CB-CA-C	-5.09	100.40	109.71
1	B	317	ILE	N-CA-C	-5.08	107.90	113.43
2	D	238	ALA	N-CA-C	5.05	117.22	109.95
2	D	234	VAL	CA-C-N	-5.04	115.37	120.21
2	D	234	VAL	C-N-CA	-5.04	115.37	120.21
2	C	206	LEU	N-CA-CB	-5.03	102.68	110.98
1	A	327	ILE	N-CA-C	-5.01	101.09	108.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2855	0	2826	100	0
1	B	2889	0	2863	87	0
2	C	2687	0	2679	112	0
2	D	2799	0	2796	167	0
3	E	611	0	637	16	0
3	F	608	0	634	18	0
4	C	5	0	0	0	0
5	D	14	9	9	0	0
6	A	9	0	0	0	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	D	9	0	0	0	0
6	F	2	0	0	0	0
All	All	12503	9	12444	484	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 19.

All (484) 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:B:354:GLN:CG	2:D:350:PHE:HZ	1.33	1.39
1:B:354:GLN:HG2	2:D:350:PHE:CZ	1.63	1.30
2:D:229:VAL:HG22	2:D:230:PRO:CD	1.67	1.24
1:B:354:GLN:CG	2:D:350:PHE:CZ	2.24	1.19
2:C:182:ASN:ND2	3:F:70:VAL:HG21	1.60	1.15
2:D:272:THR:HG23	2:D:322:ILE:CD1	1.77	1.14
2:D:229:VAL:HG22	2:D:230:PRO:HD2	1.16	1.09
1:B:221:LEU:HD11	1:B:315:LYS:HG3	1.33	1.05
1:B:190:MET:HE1	1:B:202:THR:HG22	1.34	1.05
2:D:160:THR:HG23	2:D:162:GLU:H	1.21	1.05
2:C:182:ASN:HD21	3:F:70:VAL:HG21	0.88	1.03
1:B:354:GLN:HG3	2:D:350:PHE:HZ	1.21	1.03
2:D:153:VAL:CG1	2:D:269:VAL:HG12	1.86	1.03
2:D:272:THR:HG23	2:D:322:ILE:HD12	1.36	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:229:VAL:HG22	2:C:230:PRO:HD2	1.39	1.02
1:A:353:GLN:O	1:A:356:TRP:HD1	1.41	1.02
1:A:332:PRO:O	1:A:335:ARG:HG3	1.60	1.00
2:D:94:LEU:HD21	2:D:99:VAL:HG13	1.40	1.00
1:B:354:GLN:HG2	2:D:350:PHE:HZ	0.99	1.00
2:D:261:SER:OG	2:D:264:THR:HG23	1.62	0.99
1:B:220:ALA:HB1	1:B:226:GLU:HG3	1.44	0.99
2:D:153:VAL:HG11	2:D:269:VAL:HG12	1.47	0.97
2:D:229:VAL:CG2	2:D:230:PRO:CD	2.42	0.97
2:D:213:ASN:ND2	2:D:223:ASN:HB2	1.79	0.95
2:C:28:ILE:HD13	2:C:350:PHE:HE1	1.32	0.94
1:A:250:ILE:HG22	1:A:254:ARG:HG3	1.50	0.92
2:C:172:LYS:HZ2	2:C:301:LYS:HE3	1.36	0.90
2:C:331:ASN:OD1	2:C:331:ASN:O	1.89	0.90
2:C:80:ILE:HD11	2:C:106:ALA:HB1	1.56	0.86
2:D:185:VAL:HG11	2:D:269:VAL:HG11	1.57	0.85
2:C:140:LEU:HD12	2:C:141:SER:OG	1.77	0.85
2:D:185:VAL:CG1	2:D:269:VAL:HG11	2.06	0.85
2:D:199:LYS:NZ	2:D:201:ARG:HB3	1.91	0.85
2:C:172:LYS:NZ	2:C:301:LYS:HE3	1.92	0.84
2:C:313:VAL:HG23	2:C:314:LEU:HD12	1.59	0.84
1:B:354:GLN:HG2	2:D:350:PHE:CE1	2.12	0.84
2:D:186:GLU:HG3	2:D:190:LYS:HE3	1.60	0.83
1:B:286:ASP:OD1	1:B:287:VAL:N	2.12	0.82
2:C:28:ILE:HG21	2:C:49:TYR:HB2	1.61	0.82
2:C:156:GLU:HG2	2:C:157:TYR:N	1.94	0.81
2:D:181:LEU:HD22	2:D:266:SER:HB3	1.61	0.81
2:C:87:CYS:SG	2:C:99:VAL:HG22	2.21	0.81
2:D:87:CYS:O	2:D:91:GLU:HG3	1.81	0.80
2:D:159:VAL:O	2:D:160:THR:HG22	1.82	0.80
2:D:199:LYS:HZ3	2:D:201:ARG:HB3	1.44	0.80
2:D:94:LEU:HD21	2:D:99:VAL:CG1	2.10	0.80
2:D:153:VAL:HG22	2:D:273:ASP:OD2	1.82	0.79
2:C:28:ILE:HD13	2:C:350:PHE:CE1	2.15	0.79
2:D:263:THR:HG22	2:D:263:THR:O	1.80	0.79
1:A:103:VAL:O	1:A:356:TRP:HZ3	1.66	0.78
1:B:213:LYS:HA	1:B:217:CYS:SG	2.24	0.77
1:B:354:GLN:HG3	2:D:350:PHE:CZ	2.08	0.77
1:B:286:ASP:OD1	1:B:287:VAL:HG22	1.84	0.77
1:B:227:MET:SD	1:B:255:PHE:HE1	2.09	0.76
2:D:229:VAL:CG2	2:D:230:PRO:HD3	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:GLN:O	1:A:356:TRP:CD1	2.34	0.76
2:C:182:ASN:CG	2:C:182:ASN:O	2.24	0.76
1:A:44:MET:O	1:A:45:VAL:HG23	1.84	0.75
2:D:87:CYS:O	2:D:91:GLU:CG	2.35	0.75
2:C:140:LEU:CD1	2:C:141:SER:OG	2.35	0.75
2:D:222:PRO:HG2	2:D:352:LEU:HD21	1.68	0.74
2:C:257:VAL:CG2	2:C:305:HIS:HA	2.18	0.74
2:D:213:ASN:HD22	2:D:223:ASN:HB2	1.50	0.74
1:B:250:ILE:HG12	1:B:254:ARG:HG3	1.70	0.73
2:D:229:VAL:CG2	2:D:230:PRO:HD2	2.07	0.73
1:A:151:ILE:HD12	1:A:164:PRO:HG3	1.71	0.72
1:B:10:ILE:HD12	1:B:89:THR:HG21	1.71	0.72
2:C:26:LEU:C	2:C:26:LEU:HD12	2.14	0.72
2:C:140:LEU:HD12	2:C:141:SER:CB	2.21	0.71
2:C:182:ASN:O	2:C:182:ASN:OD1	2.09	0.71
2:C:257:VAL:HG21	2:C:305:HIS:HA	1.73	0.71
2:D:351:GLY:O	2:D:355:GLN:HB2	1.91	0.70
1:A:190:MET:HG2	1:A:200:PHE:HB3	1.74	0.70
2:C:172:LYS:HZ2	2:C:301:LYS:CE	2.05	0.69
2:D:191:ALA:O	2:D:192:GLN:HG2	1.91	0.69
2:D:160:THR:HG23	2:D:161:HIS:N	2.06	0.68
2:D:199:LYS:HZ3	2:D:201:ARG:CB	2.07	0.68
2:D:140:LEU:HD21	2:D:168:LEU:HD12	1.74	0.68
2:D:283:ASP:HB2	2:D:286:LYS:HB2	1.74	0.67
1:B:131:ALA:HB1	1:B:356:TRP:HB3	1.77	0.66
2:D:160:THR:HG23	2:D:162:GLU:N	2.03	0.66
2:C:182:ASN:HB2	3:F:42:ARG:NH2	2.11	0.66
1:A:353:GLN:HA	1:A:356:TRP:CD1	2.29	0.66
2:C:310:VAL:O	2:C:313:VAL:HG22	1.96	0.66
1:B:222:ASP:O	1:B:226:GLU:HG2	1.96	0.65
2:D:199:LYS:NZ	2:D:201:ARG:CB	2.60	0.65
2:C:154:LYS:NZ	2:C:178:PHE:HA	2.11	0.65
1:B:229:THR:O	1:B:229:THR:HG22	1.95	0.65
2:C:278:HIS:CB	2:C:284:ILE:HD12	2.26	0.65
2:D:23:LYS:HD3	2:D:24:ILE:HG13	1.79	0.65
2:D:140:LEU:HD22	2:D:143:PHE:CD2	2.32	0.64
1:A:353:GLN:HA	1:A:356:TRP:NE1	2.13	0.64
2:D:28:ILE:HG23	2:D:45:LEU:HG	1.79	0.64
1:A:353:GLN:C	1:A:356:TRP:HD1	2.04	0.64
2:C:135:LYS:HG2	2:C:168:LEU:HD22	1.78	0.64
2:D:272:THR:HG23	2:D:322:ILE:HD11	1.77	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:337:ASP:CG	2:D:337:ASP:O	2.36	0.63
2:D:213:ASN:ND2	2:D:223:ASN:CB	2.58	0.63
1:B:20:GLY:HA2	1:B:94:LEU:HD11	1.80	0.63
2:C:26:LEU:HD12	2:C:26:LEU:O	1.98	0.63
2:C:154:LYS:HZ1	2:C:178:PHE:HA	1.63	0.63
1:B:104:LEU:HD12	1:B:133:TYR:HB3	1.80	0.63
2:D:329:LYS:HG2	2:D:330:LEU:N	2.14	0.63
2:C:278:HIS:HB2	2:C:284:ILE:HD12	1.79	0.63
2:C:28:ILE:CD1	2:C:350:PHE:CE1	2.82	0.63
1:A:103:VAL:O	1:A:356:TRP:CZ3	2.51	0.62
1:A:213:LYS:HE3	1:A:214:GLU:HG2	1.80	0.62
2:D:272:THR:CG2	2:D:322:ILE:CD1	2.68	0.62
2:C:31:SER:HB3	2:C:45:LEU:HD21	1.82	0.62
2:D:213:ASN:HD22	2:D:223:ASN:CB	2.11	0.62
1:B:37:ARG:HB3	1:B:38:PRO:HD2	1.82	0.62
2:D:247:TYR:HA	2:D:250:THR:HB	1.81	0.62
2:D:263:THR:O	2:D:263:THR:CG2	2.46	0.62
1:B:89:THR:O	1:B:94:LEU:HB3	1.99	0.61
1:B:201:THR:OG1	1:B:205:GLU:HB2	1.99	0.61
2:D:257:VAL:HG13	2:D:258:ALA:H	1.65	0.61
2:D:272:THR:CG2	2:D:322:ILE:HD12	2.22	0.61
2:C:156:GLU:HG2	2:C:157:TYR:H	1.65	0.60
1:A:353:GLN:HA	1:A:356:TRP:HE1	1.67	0.60
1:A:34:ILE:HD11	1:A:67:LEU:HD13	1.82	0.60
2:D:329:LYS:HG2	2:D:330:LEU:H	1.67	0.60
2:D:232:ARG:HG3	2:D:234:VAL:HG13	1.84	0.60
2:C:361:GLU:HA	2:C:364:GLU:HG2	1.83	0.60
2:D:254:THR:CG2	2:D:308:SER:HB2	2.31	0.59
2:D:254:THR:HG21	2:D:308:SER:HB2	1.82	0.59
3:E:42:ARG:HD2	3:E:72:ARG:HG3	1.83	0.59
1:A:196:ARG:NE	1:A:253:GLU:OE2	2.34	0.59
2:D:216:ILE:HG12	2:D:300:ILE:HG22	1.85	0.59
1:B:39:ARG:HD2	1:B:66:THR:HG21	1.84	0.59
1:A:188:TYR:HD1	1:A:267:LEU:CD2	2.16	0.58
1:A:70:PRO:HG2	1:A:85:ILE:HD11	1.85	0.58
2:D:259:SER:HA	2:D:309:GLU:OE2	2.04	0.58
1:B:221:LEU:HD21	1:B:315:LYS:HZ1	1.67	0.58
1:B:190:MET:HE1	1:B:202:THR:CG2	2.23	0.57
2:C:278:HIS:O	2:C:284:ILE:CD1	2.52	0.57
1:A:44:MET:O	1:A:45:VAL:CG2	2.52	0.57
2:C:74:GLN:HE22	2:C:254:THR:HA	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:256:PHE:HB2	2:D:309:GLU:CD	2.30	0.57
2:C:67:ILE:HD11	2:C:82:LYS:HD2	1.85	0.57
2:D:264:THR:OG1	2:D:313:VAL:HG11	2.04	0.57
2:C:156:GLU:OE1	2:C:156:GLU:N	2.25	0.57
2:C:140:LEU:HD12	2:C:141:SER:N	2.19	0.57
2:C:175:ILE:HD12	2:C:176:LEU:HD12	1.86	0.57
2:D:121:LEU:CD2	2:D:344:LYS:O	2.53	0.57
1:B:221:LEU:HD11	1:B:315:LYS:CG	2.22	0.57
2:D:186:GLU:CG	2:D:190:LYS:HE3	2.33	0.56
1:B:32:PRO:HD2	1:B:56:ASP:OD1	2.06	0.56
1:B:64:ILE:HB	1:B:65:LEU:HD22	1.87	0.56
2:C:352:LEU:HD23	2:C:355:GLN:NE2	2.21	0.56
2:C:182:ASN:CB	3:F:42:ARG:NH2	2.69	0.56
2:C:215:GLY:O	2:C:217:MET:HE2	2.06	0.56
1:A:142:LEU:HD13	1:A:152:VAL:HG23	1.88	0.56
1:A:188:TYR:HD1	1:A:267:LEU:HD23	1.71	0.56
1:B:241:GLU:HG2	1:B:247:VAL:HG22	1.87	0.56
2:D:185:VAL:HG12	2:D:269:VAL:HG11	1.84	0.56
1:A:259:GLU:C	1:A:261:LEU:H	2.13	0.55
2:C:229:VAL:HG22	2:C:230:PRO:CD	2.25	0.55
2:C:355:GLN:HA	2:C:358:MET:HG2	1.88	0.55
2:D:229:VAL:HG23	2:D:230:PRO:HD3	1.86	0.55
3:F:13:ILE:HD12	3:F:33:LYS:HD3	1.87	0.55
2:D:24:ILE:O	2:D:24:ILE:HG22	2.07	0.55
1:A:188:TYR:CD1	1:A:267:LEU:CD2	2.90	0.55
2:D:264:THR:O	2:D:268:MET:HG2	2.07	0.55
2:D:343:ARG:O	2:D:344:LYS:HB2	2.06	0.55
2:C:182:ASN:HD22	3:F:42:ARG:HH21	1.55	0.55
2:C:312:ASP:HA	2:C:315:THR:OG1	2.07	0.55
1:B:221:LEU:HD21	1:B:315:LYS:NZ	2.21	0.55
2:C:149:SER:O	2:C:153:VAL:HB	2.07	0.55
2:C:278:HIS:HB2	2:C:284:ILE:CD1	2.37	0.55
2:D:88:LYS:HA	2:D:91:GLU:HG3	1.88	0.55
2:D:182:ASN:OD1	2:D:186:GLU:OE2	2.24	0.55
2:C:257:VAL:HG23	2:C:304:TYR:O	2.06	0.54
2:D:117:GLU:HA	2:D:120:ARG:HB2	1.89	0.54
1:A:35:VAL:HA	1:A:54:VAL:HG22	1.88	0.54
1:A:156:GLY:O	1:A:181:ALA:HB1	2.07	0.54
2:C:77:LYS:HA	2:C:80:ILE:HG22	1.89	0.54
2:D:191:ALA:O	2:D:192:GLN:CG	2.55	0.54
2:C:222:PRO:HG2	2:C:352:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:264:THR:HB	2:C:314:LEU:HD11	1.88	0.54
2:C:229:VAL:CG2	2:C:230:PRO:HD2	2.27	0.54
2:D:142:VAL:HB	2:D:287:LYS:HB3	1.88	0.54
2:D:201:ARG:CZ	2:D:258:ALA:HB1	2.37	0.54
2:D:142:VAL:HG22	2:D:291:ILE:HD11	1.90	0.54
2:C:197:PRO:HB3	3:F:76:GLY:OXT	2.07	0.54
2:D:87:CYS:O	2:D:91:GLU:HG2	2.06	0.53
1:A:332:PRO:HD2	1:A:335:ARG:HG2	1.91	0.53
1:B:305:MET:HG2	1:B:335:ARG:HG3	1.91	0.53
2:C:47:VAL:HG23	2:C:346:GLN:NE2	2.23	0.53
2:D:229:VAL:CG1	2:D:232:ARG:NH1	2.71	0.53
2:D:322:ILE:HA	2:D:325:LYS:HG2	1.89	0.53
1:B:73:HIS:HB3	1:B:177:ARG:NH2	2.24	0.53
1:A:119:MET:CE	1:A:134:VAL:HG21	2.39	0.53
1:A:151:ILE:HD13	1:A:282:ILE:HG13	1.90	0.53
2:D:140:LEU:HD22	2:D:143:PHE:HD2	1.73	0.53
1:A:62:ARG:HG3	1:A:67:LEU:HD11	1.90	0.53
1:A:331:ALA:HB1	1:A:335:ARG:HD3	1.90	0.53
2:D:159:VAL:C	2:D:160:THR:HG22	2.33	0.53
2:D:140:LEU:CD2	2:D:143:PHE:CE2	2.91	0.53
1:B:189:LEU:HA	1:B:192:ILE:HG12	1.90	0.53
3:F:8:LEU:HD11	3:F:70:VAL:HG13	1.91	0.53
1:B:11:ASP:HA	1:B:106:THR:OG1	2.10	0.52
2:C:29:SER:HA	2:C:32:LEU:HD12	1.92	0.52
2:C:144:ASN:HA	2:C:147:ARG:HD3	1.92	0.52
2:D:159:VAL:O	2:D:160:THR:CG2	2.53	0.52
1:B:87:HIS:O	1:B:91:TYR:HB2	2.09	0.52
2:C:135:LYS:CG	2:C:168:LEU:HD22	2.40	0.52
2:D:32:LEU:O	2:D:101:ARG:NH2	2.42	0.52
2:D:201:ARG:NH1	2:D:258:ALA:HB1	2.24	0.52
2:C:265:TYR:O	2:C:269:VAL:HG23	2.10	0.52
2:D:99:VAL:O	2:D:103:ALA:HB3	2.10	0.52
2:D:117:GLU:OE1	2:D:117:GLU:N	2.42	0.52
2:D:198:LYS:HB3	2:D:246:GLY:HA2	1.92	0.52
2:D:229:VAL:CG1	2:D:232:ARG:HH12	2.22	0.52
1:A:10:ILE:HD12	1:A:89:THR:HG21	1.91	0.52
2:D:261:SER:HA	2:D:305:HIS:NE2	2.25	0.52
2:D:25:GLU:HB3	2:D:49:TYR:HE1	1.75	0.52
2:D:142:VAL:HG21	2:D:287:LYS:O	2.10	0.51
2:D:160:THR:CG2	2:D:162:GLU:H	2.10	0.51
1:B:189:LEU:HD11	1:B:250:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:LYS:HG3	2:D:75:ASN:HB2	1.92	0.51
2:D:146:LEU:HD22	2:D:291:ILE:HD12	1.90	0.51
2:D:256:PHE:HE1	2:D:259:SER:HB2	1.74	0.51
1:A:162:THR:HG21	1:A:278:THR:HA	1.92	0.51
1:A:8:LEU:HD12	1:A:103:VAL:HG22	1.92	0.51
1:A:190:MET:HG3	1:A:209:VAL:HG21	1.93	0.51
1:A:340:TRP:C	1:A:342:GLY:H	2.19	0.51
1:A:360:GLN:O	1:A:364:GLU:HG2	2.11	0.51
1:B:211:ASP:O	1:B:215:LYS:HB2	2.10	0.51
1:A:107:GLU:HB3	1:A:134:VAL:HG11	1.92	0.51
1:A:188:TYR:CD1	1:A:267:LEU:HD23	2.45	0.51
2:D:195:ARG:NH1	2:D:198:LYS:NZ	2.59	0.51
2:C:218:LYS:O	2:C:221:SER:HB2	2.10	0.51
2:D:77:LYS:O	2:D:81:GLU:HG2	2.10	0.51
1:B:369:ILE:HG13	1:B:372:ARG:HH21	1.76	0.51
2:D:140:LEU:HD22	2:D:143:PHE:CE2	2.45	0.51
2:D:256:PHE:CE1	2:D:259:SER:HB2	2.46	0.51
2:D:153:VAL:CG2	2:D:273:ASP:OD2	2.57	0.50
1:A:153:MET:HE3	1:A:304:THR:HG22	1.92	0.50
2:C:203:ARG:HD3	3:F:74:ARG:NH1	2.26	0.50
2:D:121:LEU:HD21	2:D:344:LYS:O	2.12	0.50
2:D:263:THR:HG22	2:D:295:TRP:CH2	2.46	0.50
1:A:345:ILE:O	1:A:349:LEU:HG	2.11	0.50
2:C:217:MET:CE	2:C:234:VAL:HG21	2.42	0.50
1:A:120:THR:OG1	1:A:370:VAL:HG11	2.12	0.50
1:A:18:LYS:HG2	1:A:30:VAL:HG13	1.93	0.50
1:B:32:PRO:CD	1:B:56:ASP:OD1	2.60	0.50
1:B:189:LEU:O	1:B:193:LEU:HB2	2.12	0.49
1:A:119:MET:HE3	1:A:134:VAL:HG21	1.95	0.49
2:D:257:VAL:HG13	2:D:258:ALA:N	2.26	0.49
2:C:153:VAL:HG12	2:C:154:LYS:HG2	1.93	0.49
2:D:326:ALA:HB3	2:D:328:ILE:HG12	1.94	0.49
2:C:47:VAL:O	2:C:51:GLU:HB2	2.13	0.49
1:A:136:ILE:HG22	1:A:138:ALA:H	1.77	0.49
2:D:147:ARG:NE	2:D:160:THR:OG1	2.46	0.49
2:C:278:HIS:O	2:C:284:ILE:HD12	2.12	0.49
2:D:196:TYR:N	2:D:197:PRO:CD	2.76	0.49
3:F:26:VAL:O	3:F:30:ILE:HG13	2.12	0.49
1:B:156:GLY:O	1:B:181:ALA:HB1	2.12	0.49
2:C:278:HIS:O	2:C:284:ILE:HD13	2.13	0.49
2:D:32:LEU:C	2:D:101:ARG:HH21	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:LEU:C	2:D:148:ASP:H	2.20	0.49
2:C:156:GLU:CG	2:C:157:TYR:N	2.73	0.49
2:C:43:ILE:O	2:C:47:VAL:HG22	2.13	0.48
3:E:42:ARG:HB2	3:E:70:VAL:O	2.13	0.48
1:A:76:VAL:HG21	1:A:79:TRP:CZ2	2.48	0.48
1:B:132:MET:HE2	1:B:132:MET:HB3	1.79	0.48
3:F:33:LYS:HG3	3:F:34:GLU:HG2	1.95	0.48
2:C:316:GLU:HG3	2:C:317:PRO:HD2	1.95	0.48
2:D:74:GLN:HG2	2:D:119:ARG:HH12	1.78	0.48
3:F:30:ILE:HG22	3:F:36:ILE:HD12	1.95	0.48
1:B:93:GLU:O	1:B:94:LEU:C	2.54	0.48
2:C:79:ALA:O	2:C:83:ILE:HG12	2.12	0.48
2:C:133:VAL:HA	2:C:136:GLN:HG2	1.94	0.48
2:D:182:ASN:O	2:D:183:ASP:HB2	2.13	0.48
2:C:124:THR:HG23	2:C:215:GLY:HA3	1.95	0.48
1:A:208:ILE:HG21	1:A:242:LEU:HD22	1.96	0.48
2:C:47:VAL:HG21	2:C:342:PHE:CE2	2.48	0.48
2:D:140:LEU:CD2	2:D:143:PHE:HE2	2.27	0.48
1:A:79:TRP:HH2	1:A:119:MET:HG2	1.79	0.48
1:B:227:MET:SD	1:B:255:PHE:CE1	2.99	0.48
1:A:153:MET:HE2	1:A:299:LEU:HG	1.96	0.48
2:C:182:ASN:ND2	3:F:70:VAL:CG2	2.53	0.47
2:C:331:ASN:O	2:C:331:ASN:CG	2.56	0.47
1:A:79:TRP:CH2	1:A:119:MET:HG2	2.49	0.47
2:C:196:TYR:O	2:C:198:LYS:N	2.45	0.47
2:D:263:THR:HG22	2:D:295:TRP:HH2	1.78	0.47
1:B:116:ARG:HA	1:B:119:MET:HE2	1.95	0.47
1:A:152:VAL:HG22	1:A:298:VAL:HB	1.97	0.47
1:A:252:ASN:OD1	1:A:252:ASN:C	2.56	0.47
1:A:188:TYR:CD1	1:A:267:LEU:HD21	2.50	0.47
2:D:337:ASP:O	2:D:337:ASP:OD1	2.33	0.47
3:E:6:LYS:HB2	3:E:6:LYS:HE2	1.58	0.47
1:B:283:MET:C	1:B:285:CYS:H	2.22	0.47
1:A:219:VAL:HG22	1:A:258:PRO:CB	2.44	0.47
1:B:194:THR:HA	1:B:199:SER:HA	1.96	0.47
2:D:249:LYS:HD2	2:D:249:LYS:HA	1.69	0.47
1:B:189:LEU:HB2	1:B:257:CYS:SG	2.54	0.47
2:D:142:VAL:HA	2:D:145:GLU:HG2	1.95	0.47
1:B:62:ARG:HE	1:B:67:LEU:HD11	1.80	0.46
1:B:223:PHE:O	1:B:227:MET:HG2	2.14	0.46
2:C:268:MET:O	2:C:272:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:ILE:HG12	2:D:300:ILE:CG2	2.45	0.46
1:B:42:GLY:HA2	1:B:45:VAL:HB	1.95	0.46
1:B:305:MET:HE3	1:B:305:MET:HB3	1.80	0.46
2:C:225:THR:HG22	2:C:225:THR:O	2.15	0.46
1:A:73:HIS:HB3	1:A:177:ARG:NH2	2.30	0.46
1:A:103:VAL:HG12	1:A:104:LEU:N	2.29	0.46
1:B:229:THR:O	1:B:229:THR:CG2	2.63	0.46
2:C:47:VAL:HG21	2:C:342:PHE:HE2	1.81	0.46
1:B:215:LYS:HE3	1:B:215:LYS:HB3	1.81	0.46
2:D:182:ASN:HA	2:D:186:GLU:OE1	2.16	0.46
2:D:355:GLN:HG3	2:D:359:HIS:CE1	2.51	0.46
3:F:61:ILE:CG2	3:F:67:LEU:HD21	2.46	0.46
1:A:10:ILE:HG23	1:A:105:LEU:HD23	1.98	0.46
2:C:223:ASN:HD21	2:C:227:ASN:HB3	1.80	0.46
2:C:316:GLU:HG2	2:C:318:PHE:CD1	2.51	0.46
3:E:23:ILE:HG12	3:E:54:ARG:O	2.16	0.46
1:A:142:LEU:HD22	1:A:165:ILE:HD13	1.98	0.45
1:A:160:THR:HB	1:A:178:LEU:HB3	1.98	0.45
1:A:241:GLU:HG2	1:A:247:VAL:HG22	1.98	0.45
1:A:353:GLN:C	1:A:356:TRP:CD1	2.89	0.45
1:A:357:ILE:HG23	1:A:369:ILE:HD13	1.97	0.45
2:D:175:ILE:HG23	2:D:295:TRP:CE3	2.51	0.45
3:E:26:VAL:HG21	3:E:56:LEU:HD21	1.98	0.45
1:B:31:PHE:HB2	1:B:56:ASP:OD1	2.16	0.45
2:C:28:ILE:HG22	2:C:28:ILE:O	2.17	0.45
3:E:33:LYS:HG3	3:E:34:GLU:HG2	1.96	0.45
1:B:78:ASN:HB3	1:B:81:ASP:HB2	1.97	0.45
1:B:213:LYS:O	1:B:217:CYS:HB2	2.16	0.45
2:C:44:LEU:HB3	2:C:346:GLN:HG2	1.97	0.45
2:C:72:PHE:CE2	2:C:334:VAL:HA	2.51	0.45
1:A:159:VAL:HG22	1:A:160:THR:N	2.30	0.45
2:D:37:LEU:HD21	2:D:42:PHE:HD1	1.81	0.45
2:C:289:ASN:OD1	2:C:331:ASN:OD1	2.35	0.45
2:D:126:TYR:O	2:D:130:LEU:HD13	2.17	0.45
1:B:133:TYR:HE2	1:B:135:ALA:HB2	1.81	0.45
1:B:68:LYS:HD2	1:B:81:ASP:OD2	2.16	0.45
1:B:97:ALA:HA	1:B:98:PRO:HD3	1.82	0.45
1:B:164:PRO:O	1:B:170:ALA:HA	2.16	0.45
2:D:300:ILE:H	2:D:300:ILE:HG13	1.59	0.45
1:A:237:GLU:HG2	1:A:251:GLY:HA3	1.99	0.45
2:C:355:GLN:O	2:C:356:SER:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:13:ILE:HD13	3:F:30:ILE:HG23	1.99	0.44
1:A:96:VAL:HG22	1:A:97:ALA:N	2.32	0.44
1:B:209:VAL:O	1:B:209:VAL:HG12	2.17	0.44
3:E:40:GLN:HG3	3:E:72:ARG:O	2.18	0.44
1:A:9:VAL:HG12	1:A:104:LEU:HB3	1.98	0.44
1:B:153:MET:HE3	1:B:299:LEU:HD22	1.99	0.44
2:D:106:ALA:HA	2:D:109:LEU:HG	1.99	0.44
1:A:226:GLU:C	1:A:228:ALA:N	2.68	0.44
2:C:119:ARG:HE	2:C:123:GLU:HG3	1.82	0.44
1:A:229:THR:HG22	1:A:236:LEU:HD11	1.99	0.44
1:A:250:ILE:HG22	1:A:254:ARG:CG	2.36	0.44
1:A:252:ASN:OD1	1:A:253:GLU:N	2.50	0.44
1:B:208:ILE:HD13	1:B:243:PRO:HD2	1.99	0.44
2:D:175:ILE:HG22	2:D:176:LEU:HD23	2.00	0.44
2:D:254:THR:HA	2:D:255:PRO:HD3	1.79	0.44
2:D:337:ASP:HB2	2:D:339:HIS:CE1	2.53	0.44
2:D:358:MET:HE3	2:D:358:MET:HB2	1.90	0.44
1:A:161:HIS:CD2	1:A:177:ARG:HB2	2.53	0.44
3:E:15:LEU:HD22	3:E:26:VAL:HG13	2.00	0.44
1:B:13:GLY:O	1:B:14:SER:C	2.59	0.44
1:B:27:PRO:HG3	1:B:340:TRP:CG	2.52	0.44
1:B:54:VAL:HG21	1:B:84:LYS:HB3	2.00	0.44
2:D:352:LEU:O	2:D:355:GLN:HB3	2.16	0.44
1:A:130:PRO:HA	1:A:359:LYS:HE2	2.00	0.44
1:A:190:MET:O	1:A:194:THR:HG23	2.18	0.44
1:A:353:GLN:CA	1:A:356:TRP:CD1	3.00	0.44
2:C:278:HIS:HB3	2:C:284:ILE:HD12	1.99	0.44
1:A:304:THR:HA	1:A:309:ILE:HD13	2.00	0.43
2:C:358:MET:HB2	2:C:358:MET:HE3	1.76	0.43
2:D:358:MET:O	2:D:362:LEU:HB2	2.18	0.43
1:A:103:VAL:CG1	1:A:104:LEU:N	2.81	0.43
1:A:160:THR:N	1:A:178:LEU:O	2.35	0.43
1:A:163:VAL:HG13	1:A:175:ILE:HG12	2.00	0.43
2:D:153:VAL:CG1	2:D:269:VAL:CG1	2.77	0.43
2:C:260:LEU:HD12	2:C:260:LEU:HA	1.84	0.43
1:A:196:ARG:NH2	1:A:252:ASN:HD21	2.16	0.43
1:A:340:TRP:C	1:A:342:GLY:N	2.76	0.43
1:B:113:LYS:H	1:B:113:LYS:HG3	1.39	0.43
2:C:181:LEU:HD21	2:C:185:VAL:HB	1.99	0.43
1:A:239:SER:HB3	1:A:247:VAL:HG12	2.00	0.43
1:A:204:ALA:O	1:A:207:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:140:LEU:HD11	2:C:141:SER:OG	2.15	0.43
2:C:203:ARG:HG3	3:F:74:ARG:HD2	2.01	0.43
2:C:356:SER:O	2:C:359:HIS:HB2	2.19	0.43
2:D:103:ALA:C	2:D:105:VAL:H	2.26	0.43
3:E:1:MET:HE2	3:E:1:MET:HB3	1.79	0.43
1:A:193:LEU:HD22	1:A:198:TYR:HD2	1.83	0.43
1:A:370:VAL:HG23	1:A:371:HIS:N	2.33	0.43
1:B:87:HIS:C	1:B:89:THR:H	2.26	0.43
1:A:35:VAL:HG21	1:A:81:ASP:HB3	2.01	0.42
1:A:259:GLU:C	1:A:261:LEU:N	2.75	0.42
1:B:155:SER:OG	1:B:304:THR:HG23	2.19	0.42
2:C:63:PHE:O	2:C:67:ILE:HG12	2.18	0.42
1:A:343:GLY:C	1:A:345:ILE:N	2.76	0.42
1:B:137:GLN:HA	1:B:339:VAL:HG13	2.01	0.42
2:C:116:ASN:O	2:C:120:ARG:HG3	2.18	0.42
2:C:358:MET:HG3	2:C:359:HIS:N	2.33	0.42
2:D:63:PHE:O	2:D:67:ILE:HG12	2.19	0.42
2:D:120:ARG:HB3	2:D:216:ILE:O	2.18	0.42
2:D:177:SER:C	2:D:179:VAL:H	2.26	0.42
2:D:265:TYR:HE1	2:D:318:PHE:HZ	1.67	0.42
1:B:287:VAL:HG23	1:B:288:ASP:OD1	2.19	0.42
2:D:299:TYR:CD2	2:D:305:HIS:HD2	2.37	0.42
3:E:26:VAL:O	3:E:30:ILE:HG13	2.18	0.42
3:E:40:GLN:HG2	3:E:71:LEU:HB3	2.00	0.42
2:D:161:HIS:C	2:D:163:THR:H	2.28	0.42
1:A:180:LEU:HD21	1:A:260:ALA:O	2.19	0.42
2:D:39:GLU:HG2	2:D:109:LEU:HB3	2.00	0.42
2:D:260:LEU:O	2:D:261:SER:C	2.60	0.42
1:A:341:ILE:HG21	1:A:341:ILE:HD13	1.72	0.42
1:B:333:PRO:HD2	1:B:334:GLU:OE1	2.20	0.42
2:C:300:ILE:HD13	2:C:300:ILE:HG21	1.69	0.42
2:D:88:LYS:HA	2:D:91:GLU:CG	2.49	0.42
2:D:195:ARG:HH11	2:D:198:LYS:NZ	2.18	0.42
1:A:286:ASP:C	1:A:288:ASP:N	2.77	0.42
1:B:118:LYS:HD2	1:B:118:LYS:HA	1.90	0.42
2:C:257:VAL:CG2	2:C:304:TYR:O	2.68	0.42
2:C:275:ILE:HD12	2:C:322:ILE:HG22	2.01	0.42
2:D:32:LEU:C	2:D:101:ARG:NH2	2.77	0.42
2:D:180:MET:HE3	2:D:180:MET:HB3	1.92	0.42
2:D:203:ARG:C	2:D:205:GLU:N	2.75	0.42
1:B:20:GLY:HA2	1:B:94:LEU:CD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:O	1:B:217:CYS:SG	2.74	0.42
1:B:261:LEU:HB3	1:B:274:ILE:HD13	2.02	0.42
2:D:276:GLU:HA	2:D:279:LYS:HD3	2.02	0.42
2:D:285:GLU:HA	2:D:288:VAL:HG12	2.02	0.42
3:E:74:ARG:C	3:E:76:GLY:H	2.27	0.42
1:A:354:GLN:H	1:A:354:GLN:HG2	1.53	0.42
3:F:61:ILE:HG23	3:F:67:LEU:HD21	2.02	0.42
1:A:337:TYR:O	1:A:341:ILE:HG13	2.20	0.41
1:B:40:HIS:O	1:B:41:GLN:C	2.62	0.41
1:B:90:PHE:CD2	1:B:98:PRO:HG3	2.54	0.41
2:C:271:LEU:HD21	2:C:291:ILE:HG21	2.02	0.41
2:D:103:ALA:C	2:D:105:VAL:N	2.75	0.41
2:D:261:SER:HB3	2:D:313:VAL:HG21	2.02	0.41
3:F:1:MET:HG3	3:F:17:VAL:HG23	2.02	0.41
1:A:208:ILE:O	1:A:212:ILE:HG13	2.20	0.41
2:D:70:LEU:O	2:D:73:LYS:HG2	2.20	0.41
2:D:160:THR:OG1	2:D:161:HIS:N	2.45	0.41
1:A:294:TYR:O	1:A:327:ILE:HA	2.21	0.41
2:C:26:LEU:C	2:C:26:LEU:CD1	2.82	0.41
2:D:175:ILE:HA	2:D:175:ILE:HD13	1.85	0.41
2:D:77:LYS:HG2	2:D:80:ILE:HD12	2.02	0.41
2:D:147:ARG:HA	2:D:174:PHE:CZ	2.55	0.41
1:A:44:MET:H	1:A:44:MET:HG3	1.57	0.41
2:C:240:ASN:C	2:C:241:GLU:HG2	2.46	0.41
2:C:257:VAL:HG21	2:C:305:HIS:CA	2.46	0.41
2:D:117:GLU:HA	2:D:120:ARG:HD2	2.03	0.41
2:D:229:VAL:HG11	2:D:232:ARG:NH1	2.35	0.41
1:B:142:LEU:HD22	1:B:165:ILE:HD13	2.01	0.41
2:C:191:ALA:C	2:C:193:SER:H	2.29	0.41
2:C:292:ILE:CD1	2:C:330:LEU:HD11	2.50	0.41
2:D:280:THR:O	2:D:281:ASP:C	2.61	0.41
2:D:337:ASP:OD1	2:D:337:ASP:C	2.63	0.41
1:B:269:MET:HB3	1:B:269:MET:HE2	1.78	0.41
2:C:175:ILE:HD12	2:C:176:LEU:CD1	2.49	0.41
2:D:187:LEU:N	2:D:188:PRO:HD2	2.35	0.41
1:B:12:ASN:HB3	1:B:82:MET:HE1	2.02	0.41
2:D:283:ASP:OD1	2:D:287:LYS:HE2	2.21	0.41
3:E:15:LEU:HD23	3:E:17:VAL:HG13	2.02	0.41
1:A:219:VAL:HG22	1:A:258:PRO:HB3	2.02	0.41
1:B:96:VAL:HB	1:B:101:HIS:CE1	2.56	0.41
2:D:25:GLU:HB3	2:D:49:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:GLU:HA	2:D:94:LEU:HB3	2.01	0.41
3:E:40:GLN:HG2	3:E:72:ARG:N	2.35	0.41
3:E:63:LYS:HE2	3:E:63:LYS:HB2	1.89	0.41
2:D:146:LEU:C	2:D:148:ASP:N	2.79	0.41
1:A:142:LEU:HG	1:A:147:ARG:HB3	2.03	0.40
1:A:219:VAL:HG22	1:A:258:PRO:HB2	2.02	0.40
1:A:247:VAL:H	1:A:247:VAL:HG23	1.60	0.40
1:B:359:LYS:HE3	1:B:359:LYS:HB2	1.85	0.40
2:C:119:ARG:HD2	2:C:119:ARG:HA	1.77	0.40
1:A:332:PRO:C	1:A:334:GLU:N	2.79	0.40
1:B:133:TYR:CE2	1:B:135:ALA:HB2	2.57	0.40
2:C:313:VAL:HG23	2:C:314:LEU:CD1	2.40	0.40
2:D:350:PHE:CE1	2:D:354:ILE:CD1	3.04	0.40
3:E:37:PRO:HA	3:E:38:PRO:HD3	1.97	0.40
1:A:210:ARG:HE	1:A:210:ARG:HB2	1.76	0.40
2:C:215:GLY:HA2	2:C:301:LYS:HA	2.02	0.40
2:D:106:ALA:N	2:D:107:PRO:HD2	2.36	0.40
2:D:313:VAL:O	2:D:319:LEU:HD12	2.21	0.40
2:C:334:VAL:O	2:C:334:VAL:HG13	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	362/375 (96%)	332 (92%)	30 (8%)	0	100	100
1	B	369/375 (98%)	340 (92%)	28 (8%)	1 (0%)	36	68
2	C	323/352 (92%)	302 (94%)	20 (6%)	1 (0%)	36	68
2	D	341/352 (97%)	310 (91%)	31 (9%)	0	100	100
3	E	76/78 (97%)	68 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
All	All	1546/1610 (96%)	1423 (92%)	121 (8%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	181	ALA
2	C	155	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	310/318 (98%)	277 (89%)	33 (11%)	6	27
1	B	313/318 (98%)	282 (90%)	31 (10%)	7	31
2	C	306/326 (94%)	276 (90%)	30 (10%)	7	31
2	D	319/326 (98%)	294 (92%)	25 (8%)	11	41
3	E	69/69 (100%)	49 (71%)	20 (29%)	0	1
3	F	69/69 (100%)	53 (77%)	16 (23%)	1	5
All	All	1386/1426 (97%)	1231 (89%)	155 (11%)	6	25

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	14	SER
1	A	24	ASP
1	A	40	HIS
1	A	44	MET
1	A	67	LEU
1	A	68	LYS
1	A	72	GLU
1	A	104	LEU

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Mol	Chain	Res	Type
1	A	120	THR
1	A	141	SER
1	A	147	ARG
1	A	151	ILE
1	A	161	HIS
1	A	190	MET
1	A	201	THR
1	A	211	ASP
1	A	222	ASP
1	A	232	SER
1	A	241	GLU
1	A	246	GLN
1	A	247	VAL
1	A	253	GLU
1	A	259	GLU
1	A	263	GLN
1	A	272	CYS
1	A	322	PRO
1	A	327	ILE
1	A	346	LEU
1	A	354	GLN
1	A	359	LYS
1	A	365	SER
1	A	368	SER
1	B	5	ILE
1	B	32	PRO
1	B	39	ARG
1	B	64	ILE
1	B	67	LEU
1	B	78	ASN
1	B	90	PHE
1	B	96	VAL
1	B	111	ASN
1	B	113	LYS
1	B	126	THR
1	B	134	VAL
1	B	140	LEU
1	B	141	SER
1	B	153	MET
1	B	162	THR
1	B	179	ASP
1	B	214	GLU

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Mol	Chain	Res	Type
1	B	235	SER
1	B	284	LYS
1	B	288	ASP
1	B	309	ILE
1	B	317	ILE
1	B	327	ILE
1	B	338	SER
1	B	341	ILE
1	B	350	SER
1	B	358	SER
1	B	365	SER
1	B	368	SER
1	B	369	ILE
2	C	30	LEU
2	C	33	ASP
2	C	37	LEU
2	C	48	LYS
2	C	73	LYS
2	C	80	ILE
2	C	91	GLU
2	C	110	LYS
2	C	142	VAL
2	C	153	VAL
2	C	159	VAL
2	C	166	LYS
2	C	185	VAL
2	C	188	PRO
2	C	189	LEU
2	C	228	LEU
2	C	229	VAL
2	C	233	ASP
2	C	237	ILE
2	C	239	ILE
2	C	255	PRO
2	C	268	MET
2	C	280	THR
2	C	282	LYS
2	C	310	VAL
2	C	311	VAL
2	C	317	PRO
2	C	338	THR
2	C	341	GLU

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Mol	Chain	Res	Type
2	C	358	MET
2	D	28	ILE
2	D	37	LEU
2	D	45	LEU
2	D	75	ASN
2	D	95	SER
2	D	104	GLU
2	D	130	LEU
2	D	134	ILE
2	D	137	GLU
2	D	168	LEU
2	D	175	ILE
2	D	194	GLU
2	D	206	LEU
2	D	216	ILE
2	D	231	VAL
2	D	279	LYS
2	D	284	ILE
2	D	291	ILE
2	D	300	ILE
2	D	328	ILE
2	D	330	LEU
2	D	341	GLU
2	D	354	ILE
2	D	362	LEU
2	D	364	GLU
3	E	0	SER
3	E	1	MET
3	E	5	VAL
3	E	6	LYS
3	E	8	LEU
3	E	9	THR
3	E	13	ILE
3	E	15	LEU
3	E	17	VAL
3	E	20	SER
3	E	24	GLU
3	E	29	LYS
3	E	33	LYS
3	E	43	LEU
3	E	49	GLN
3	E	62	GLN

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Mol	Chain	Res	Type
3	E	63	LYS
3	E	65	SER
3	E	73	LEU
3	E	74	ARG
3	F	3	ILE
3	F	9	THR
3	F	12	THR
3	F	13	ILE
3	F	15	LEU
3	F	16	GLU
3	F	17	VAL
3	F	18	GLU
3	F	22	THR
3	F	43	LEU
3	F	44	ILE
3	F	55	THR
3	F	63	LYS
3	F	70	VAL
3	F	72	ARG
3	F	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	59	GLN
1	A	353	GLN
1	A	354	GLN
1	B	92	ASN
1	B	111	ASN
1	B	161	HIS
1	B	280	ASN
1	B	314	GLN
2	C	90	ASN
2	C	220	ASN
2	C	355	GLN
2	D	74	GLN
2	D	112	ASN
2	D	184	ASN
2	D	213	ASN
2	D	227	ASN
2	D	293	ASN

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Mol	Chain	Res	Type
2	D	339	HIS
3	E	25	ASN
3	E	40	GLN
3	E	62	GLN
3	E	68	HIS
3	F	68	HIS

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	AR6	D	401	-	14,14,39	1.05	0	19,21,60	1.28	2 (10%)
4	PO4	C	401	-	4,4,4	1.21	0	6,6,6	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AR6	D	401	-	-	2/6/22/54	0/1/1/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	401	AR6	O1B-PB-O2B	3.19	123.28	110.83
5	D	401	AR6	C1D-C2D-C3D	2.37	105.20	102.29

There are no chirality outliers.

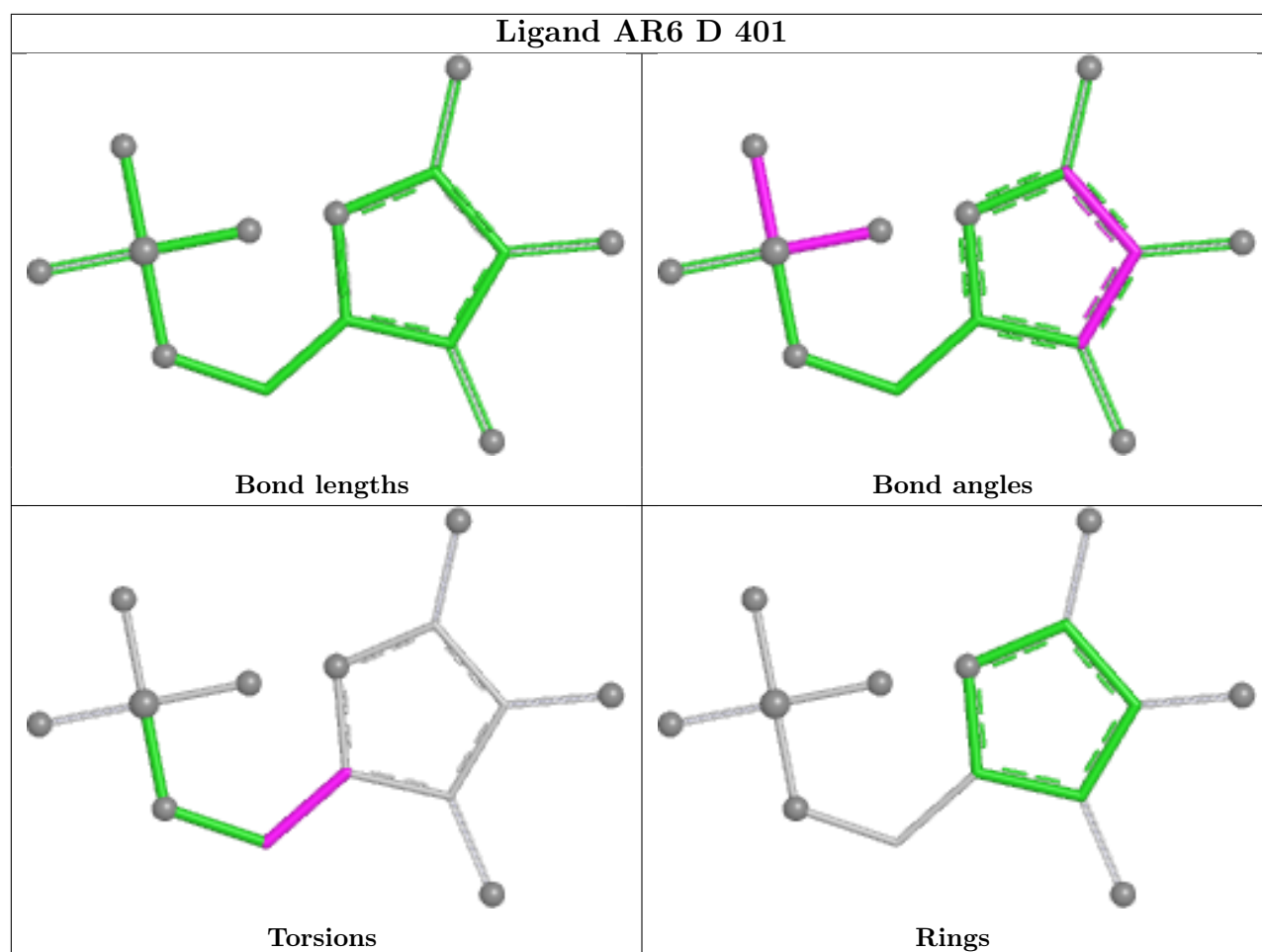
All (2) torsion outliers are listed below:

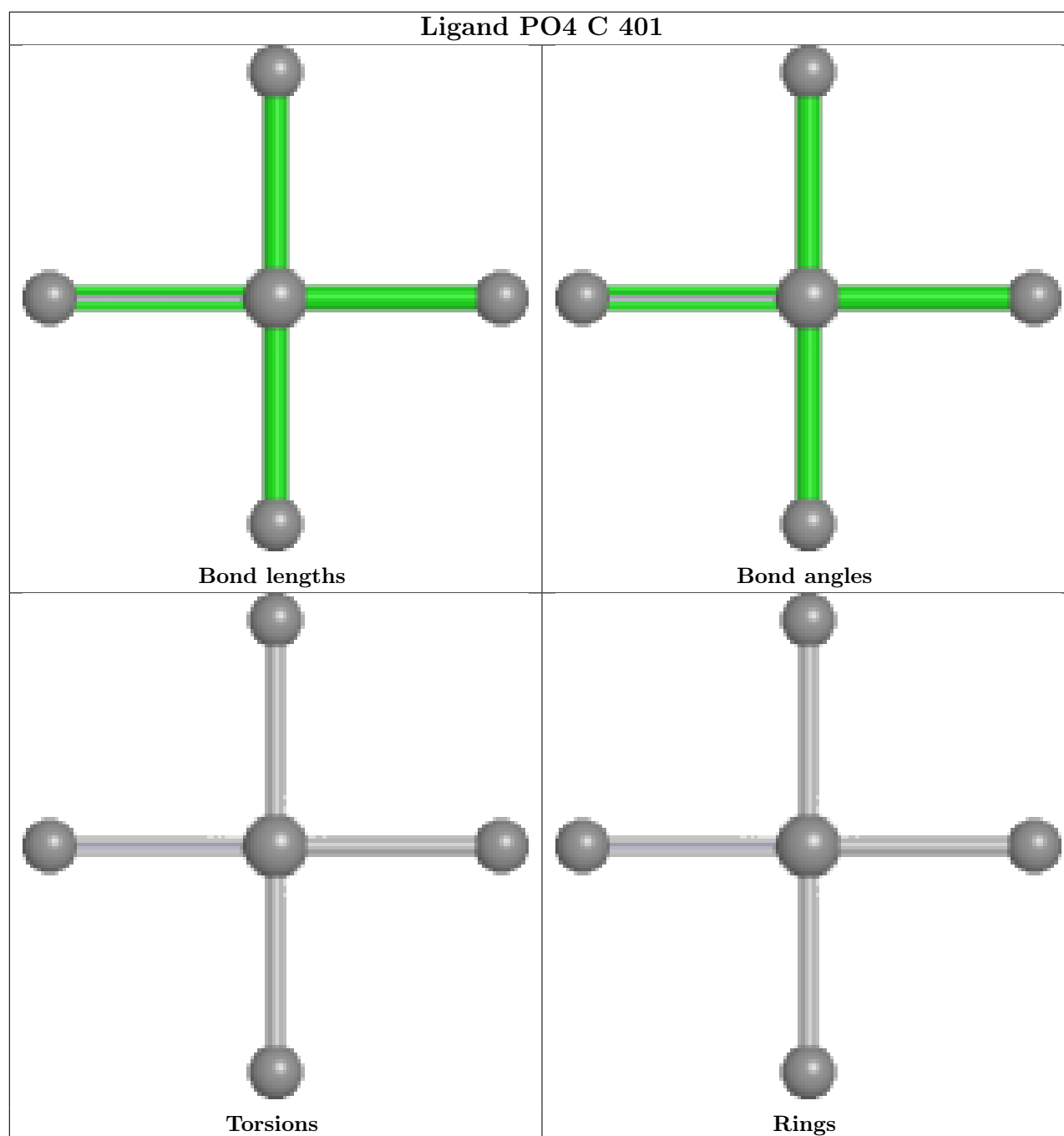
Mol	Chain	Res	Type	Atoms
5	D	401	AR6	O4D-C4D-C5D-O5D
5	D	401	AR6	C3D-C4D-C5D-O5D

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	366/375 (97%)	1.14	44 (12%)	9 6	5, 14, 37, 50	0
1	B	371/375 (98%)	1.17	58 (15%)	5 4	5, 17, 41, 77	0
2	C	331/352 (94%)	1.41	70 (21%)	2 2	8, 25, 50, 66	0
2	D	345/352 (98%)	1.51	90 (26%)	1 2	12, 31, 54, 67	0
3	E	78/78 (100%)	0.76	2 (2%)	57 37	11, 21, 35, 41	0
3	F	77/78 (98%)	0.91	4 (5%)	33 21	14, 25, 38, 50	0
All	All	1568/1610 (97%)	1.25	268 (17%)	4 3	5, 22, 48, 77	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	THR	7.9
1	B	15	GLY	5.4
1	A	250	ILE	5.2
1	B	39	ARG	5.0
2	D	227	ASN	4.9
2	D	247	TYR	4.9
2	C	217	MET	4.8
2	C	155	PRO	4.8
2	D	157	TYR	4.7
1	A	64	ILE	4.6
2	D	61	SER	4.5
2	D	200	ASP	4.3
2	D	161	HIS	4.2
2	C	216	ILE	3.9
1	B	217	CYS	3.9
1	B	51	ASP	3.9
2	C	200	ASP	3.8
2	C	140	LEU	3.8
2	C	182	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	105	VAL	3.8
2	D	216	ILE	3.8
3	E	76	GLY	3.7
1	A	365	SER	3.6
1	A	41	GLN	3.6
2	D	155	PRO	3.5
1	B	70	PRO	3.4
1	B	203	THR	3.4
2	C	191	ALA	3.4
2	D	213	ASN	3.3
2	D	45	LEU	3.3
1	A	226	GLU	3.3
1	A	31	PHE	3.3
1	B	71	ILE	3.3
2	D	351	GLY	3.3
1	B	201	THR	3.3
2	D	256	PHE	3.3
2	D	101	ARG	3.2
2	C	25	GLU	3.2
2	C	306	SER	3.2
1	A	257	CYS	3.2
2	D	283	ASP	3.2
1	A	44	MET	3.2
2	D	162	GLU	3.2
1	A	5	ILE	3.2
1	A	359	LYS	3.1
2	C	93	LEU	3.1
2	D	33	ASP	3.1
1	A	258	PRO	3.1
2	D	197	PRO	3.1
2	C	154	LYS	3.1
1	B	244	ASP	3.1
2	D	72	PHE	3.1
2	D	257	VAL	3.1
2	C	351	GLY	3.0
1	A	222	ASP	3.0
2	D	93	LEU	3.0
1	B	205	GLU	3.0
2	D	27	SER	3.0
2	D	28	ILE	3.0
2	D	39	GLU	3.0
2	C	343	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	45	VAL	3.0
2	D	94	LEU	2.9
2	D	244	ALA	2.9
2	C	103	ALA	2.9
2	C	123	GLU	2.9
1	B	62	ARG	2.9
3	F	75	GLY	2.9
2	D	102	LEU	2.9
2	D	163	THR	2.8
1	A	187	ASP	2.8
2	C	99	VAL	2.8
1	A	10	ILE	2.8
1	B	47	MET	2.7
1	B	41	GLN	2.7
2	D	179	VAL	2.7
2	D	30	LEU	2.7
2	D	115	ASP	2.7
2	D	150	TYR	2.7
1	B	204	ALA	2.7
2	C	141	SER	2.7
2	C	73	LYS	2.7
2	D	64	PHE	2.7
1	B	94	LEU	2.7
2	C	181	LEU	2.7
2	C	227	ASN	2.7
1	B	354	GLN	2.7
2	C	292	ILE	2.7
1	B	106	THR	2.7
2	D	41	ASP	2.7
1	A	83	GLU	2.6
2	D	276	GLU	2.6
3	F	76	GLY	2.6
2	D	338	THR	2.6
1	A	260	ALA	2.6
2	D	29	SER	2.6
1	B	34	ILE	2.6
2	C	139	ASP	2.6
2	D	260	LEU	2.6
2	C	184	ASN	2.6
2	C	62	GLY	2.6
1	B	297	THR	2.6
2	C	189	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	308	SER	2.6
2	D	259	SER	2.6
1	B	346	LEU	2.6
2	C	159	VAL	2.6
1	B	250	ILE	2.5
1	B	40	HIS	2.5
2	D	214	PRO	2.5
2	D	118	SER	2.5
2	D	177	SER	2.5
2	D	24	ILE	2.5
1	B	375	PHE	2.5
1	A	185	LEU	2.5
2	C	248	SER	2.5
1	B	225	GLN	2.5
2	D	140	LEU	2.5
1	B	24	ASP	2.5
2	D	139	ASP	2.5
2	D	156	GLU	2.5
1	A	249	THR	2.5
2	D	130	LEU	2.5
1	A	99	GLU	2.5
1	B	96	VAL	2.5
1	A	375	PHE	2.5
2	D	366	PHE	2.5
2	C	341	GLU	2.4
2	C	33	ASP	2.4
2	D	232	ARG	2.4
2	D	352	LEU	2.4
2	C	49	TYR	2.4
2	D	87	CYS	2.4
1	B	187	ASP	2.4
1	B	38	PRO	2.4
2	D	107	PRO	2.4
1	A	138	ALA	2.4
1	B	260	ALA	2.4
2	D	284	ILE	2.4
2	C	63	PHE	2.4
2	D	143	PHE	2.4
3	F	73	LEU	2.4
1	B	351	THR	2.4
2	D	254	THR	2.4
1	B	81	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	198	TYR	2.4
2	C	233	ASP	2.4
2	D	83	ILE	2.4
2	D	363	GLN	2.4
2	D	70	LEU	2.4
1	A	15	GLY	2.3
1	B	92	ASN	2.3
2	C	300	ILE	2.3
1	B	31	PHE	2.3
1	B	267	LEU	2.3
2	D	261	SER	2.3
2	D	52	LYS	2.3
2	D	246	GLY	2.3
1	A	231	ALA	2.3
2	C	258	ALA	2.3
2	D	291	ILE	2.3
1	A	244	ASP	2.3
1	B	262	PHE	2.3
2	D	367	LYS	2.3
2	D	108	ARG	2.3
1	B	342	GLY	2.3
2	C	259	SER	2.3
2	D	66	ASP	2.3
2	D	97	GLN	2.3
2	C	39	GLU	2.3
2	C	68	GLU	2.3
2	D	96	GLU	2.3
1	B	49	GLN	2.3
2	C	74	GLN	2.3
2	D	185	VAL	2.3
1	A	232	SER	2.3
1	B	218	TYR	2.3
2	C	76	TYR	2.3
2	D	279	LYS	2.3
1	A	45	VAL	2.3
2	C	41	ASP	2.3
2	C	283	ASP	2.3
2	D	32	LEU	2.2
1	B	14	SER	2.2
1	A	196	ARG	2.2
1	A	247	VAL	2.2
2	D	273	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	67	ILE	2.2
2	C	246	GLY	2.2
2	D	225	THR	2.2
2	C	85	ASP	2.2
2	D	109	LEU	2.2
1	B	340	TRP	2.2
1	A	246	GLN	2.2
1	B	64	ILE	2.2
1	A	92	ASN	2.2
2	C	75	ASN	2.2
2	D	131	GLU	2.2
1	B	272	CYS	2.2
2	D	357	ALA	2.2
1	B	166	TYR	2.2
2	C	363	GLN	2.2
2	C	26	LEU	2.2
2	D	135	LYS	2.2
2	D	184	ASN	2.2
2	D	194	GLU	2.2
1	B	13	GLY	2.2
1	A	62	ARG	2.2
1	A	272	CYS	2.2
2	C	115	ASP	2.2
2	D	43	ILE	2.1
2	C	34	SER	2.1
2	D	199	LYS	2.1
2	C	104	GLU	2.1
1	A	78	ASN	2.1
1	B	56	ASP	2.1
2	D	354	ILE	2.1
2	C	50	LEU	2.1
2	C	355	GLN	2.1
2	C	221	SER	2.1
3	E	64	GLU	2.1
1	A	252	ASN	2.1
1	A	24	ASP	2.1
2	C	38	ASP	2.1
2	C	312	ASP	2.1
1	A	309	ILE	2.1
1	B	10	ILE	2.1
2	D	250	THR	2.1
2	D	280	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	322	ILE	2.1
2	D	127	ALA	2.1
2	C	131	GLU	2.1
1	A	281	SER	2.1
1	B	35	VAL	2.1
1	B	222	ASP	2.1
2	C	148	ASP	2.1
2	C	314	LEU	2.1
2	D	192	GLN	2.1
2	D	245	GLY	2.1
1	A	364	GLU	2.1
2	C	156	GLU	2.1
2	C	118	SER	2.1
2	D	40	SER	2.1
2	D	266	SER	2.1
1	B	248	ILE	2.1
1	A	20	GLY	2.1
2	D	329	LYS	2.0
1	A	341	ILE	2.0
1	B	85	ILE	2.0
2	C	90	ASN	2.0
3	F	3	ILE	2.0
1	B	154	ASP	2.0
2	C	307	TYR	2.0
2	C	338	THR	2.0
1	A	262	PHE	2.0
1	B	90	PHE	2.0
1	A	30	VAL	2.0
2	C	121	LEU	2.0
1	A	233	SER	2.0
1	B	338	SER	2.0
2	C	239	ILE	2.0
2	C	127	ALA	2.0
1	B	91	TYR	2.0
1	B	240	TYR	2.0
1	A	17	CYS	2.0
2	C	162	GLU	2.0
2	D	319	LEU	2.0
2	C	296	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

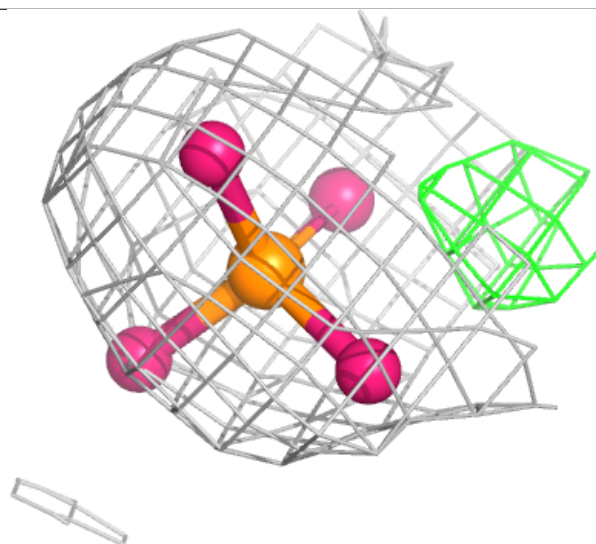
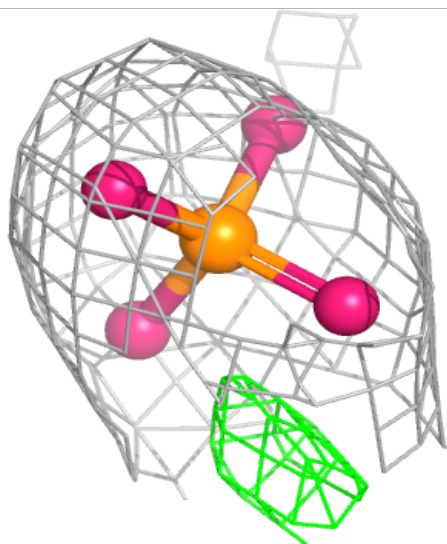
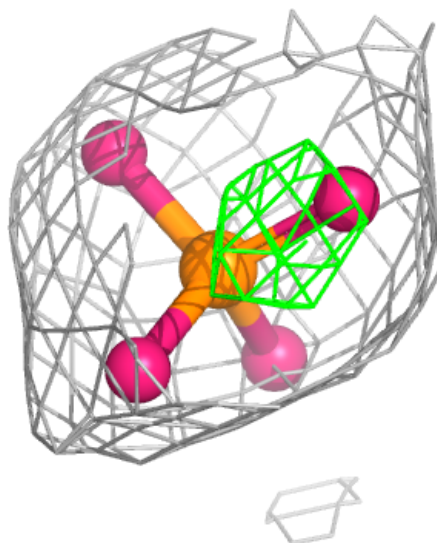
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

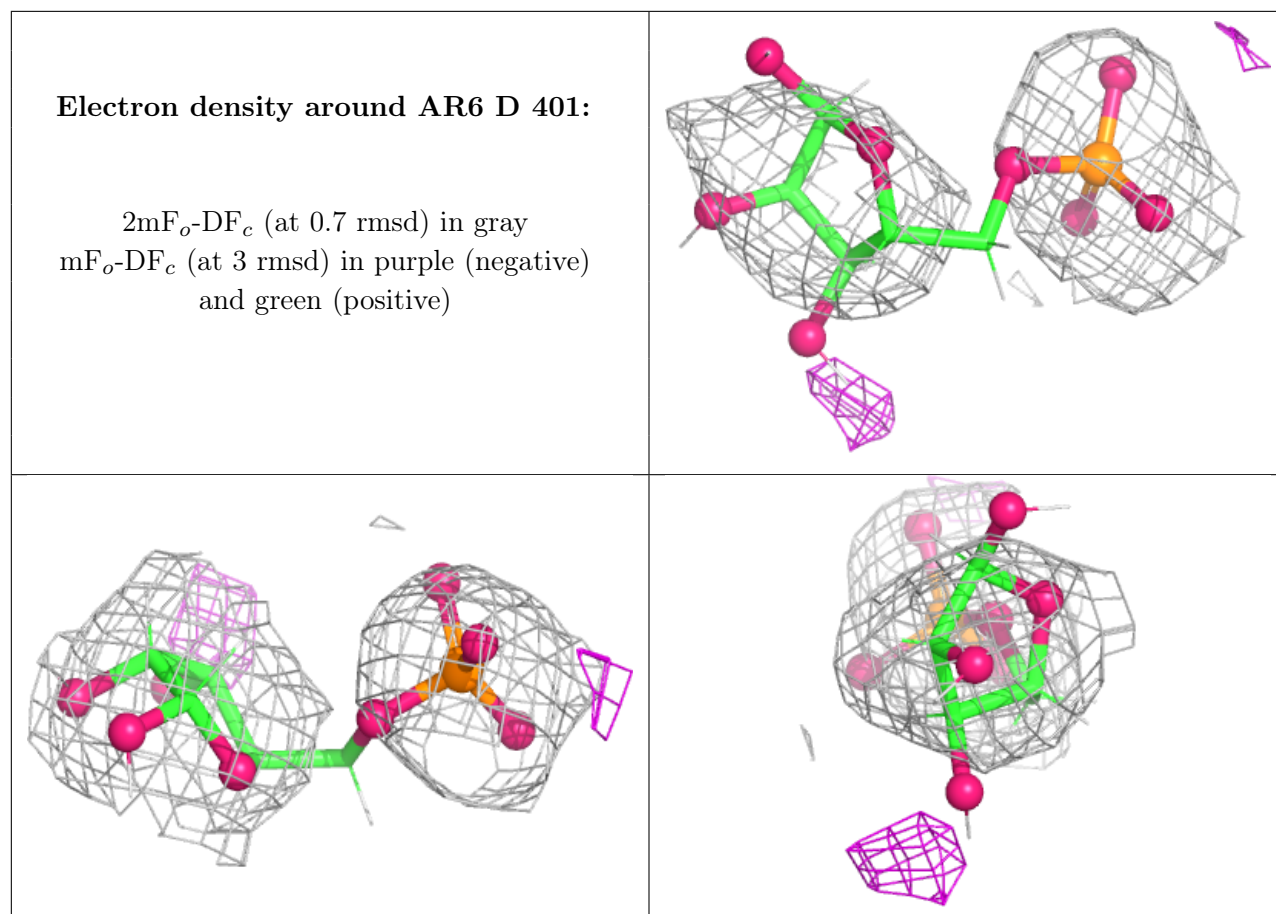
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	C	401	5/5	0.77	0.19	28,48,63,66	0
5	AR6	D	401	14/36	0.79	0.25	30,44,70,70	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PO4 C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.