Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 12:23 AM EDT

PDB ID	:	2P1N
Title	:	Mechanism of Auxin Perception by the TIR1 Ubiqutin Ligase
Authors	:	Tan, X.; Calderon-Villalobos, L.I.A.; Sharon, M.; Robinson, C.V.; Estelle, M.; Zheng, C.; Zheng, N.
Deposited on	:	2007-03-06
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

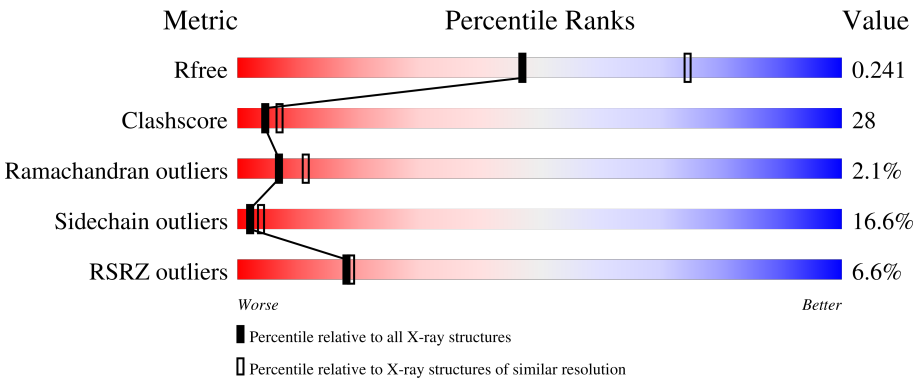
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	160	28% 36% 31% 10% • 21%
1	D	160	24% 35% 29% 12% • 21%
2	B	594	% 55% 31% 8% • •
2	E	594	% 53% 32% 9% • •
3	C	13	8% 15% 38% 38% 8%

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Mol	Chain	Length	Quality of chain
3	F	13	46% 31% 15% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11872 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 SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	126	1009	638	165	201	5	0	0	0
1	D	127	1023	649	167	202	5	0	0	0

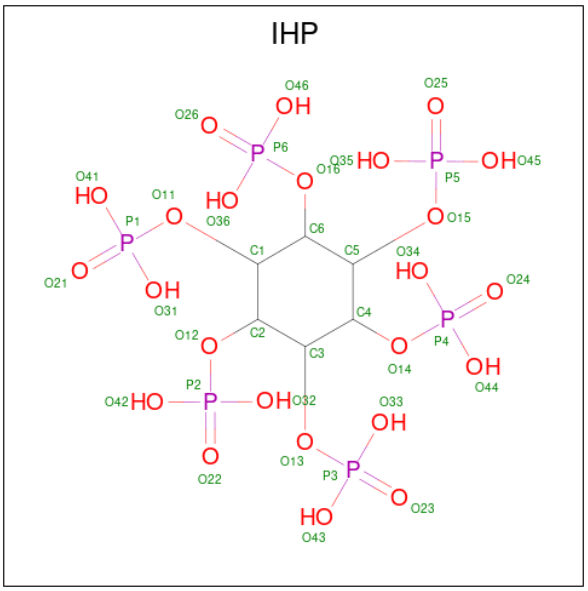
- Molecule 2 is a protein called TRANSPORT INHIBITOR RESPONSE 1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	571	4495	2871	759	828	37	0	0	0
2	E	571	4495	2871	759	828	37	0	0	0

- Molecule 3 is a protein called Auxin-responsive protein IAA7.

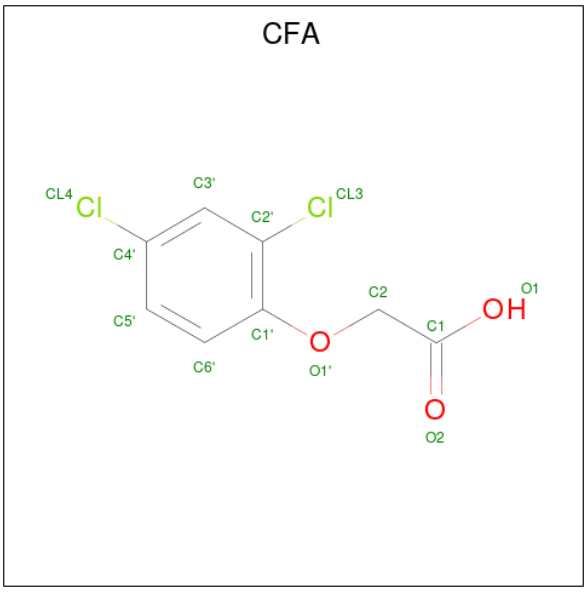
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	13	114	74	23	17	0	0	0
3	F	13	114	74	23	17	0	0	0

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	B	1	36	6	24	6	0	0
			Total	C	O	P		
4	E	1	36	6	24	6	0	0

- Molecule 5 is (2,4-DICHLOROPHENOXY)ACETIC ACID (three-letter code: CFA) (formula: $C_8H_6Cl_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	O		
5	B	1	13	8	2	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	O		
5	E	1	13	8	2	3	0	0

- Molecule 6 is water.

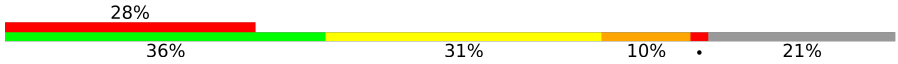
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	25	25	25	0	0
6	B	217	217	217	0	0
6	C	6	6	6	0	0
6	D	32	32	32	0	0
6	E	240	240	240	0	0
6	F	4	4	4	0	0

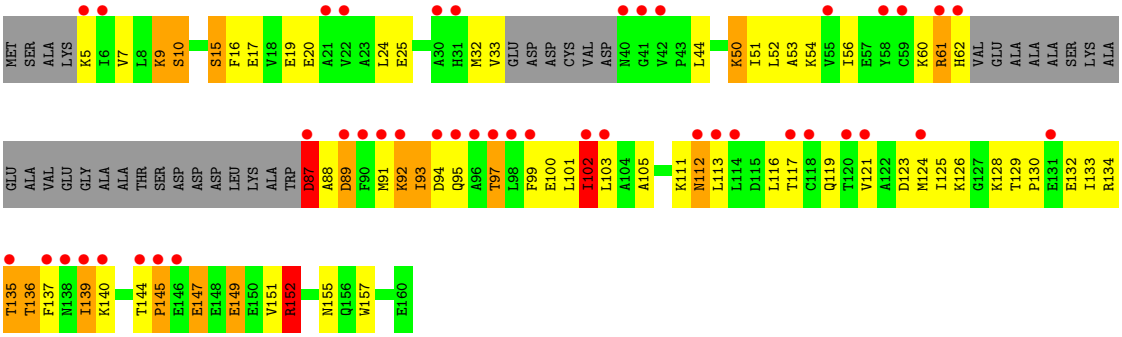
3 Residue-property plots (i)

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: SKP1-like protein 1A

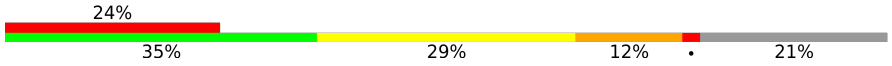
Chain A:

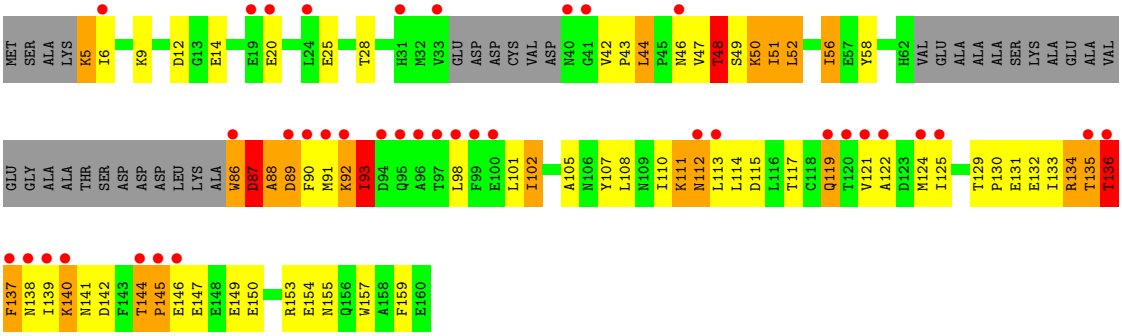




• Molecule 1: SKP1-like protein 1A

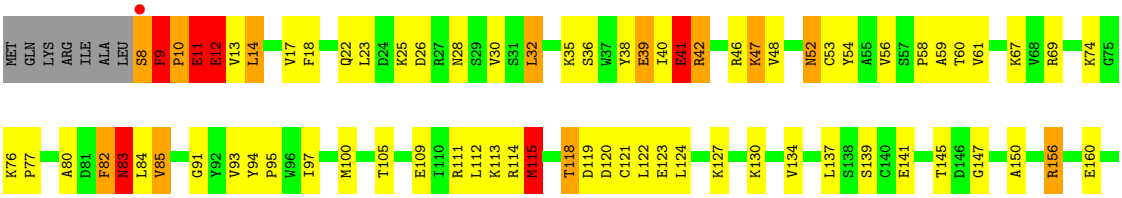
Chain D:

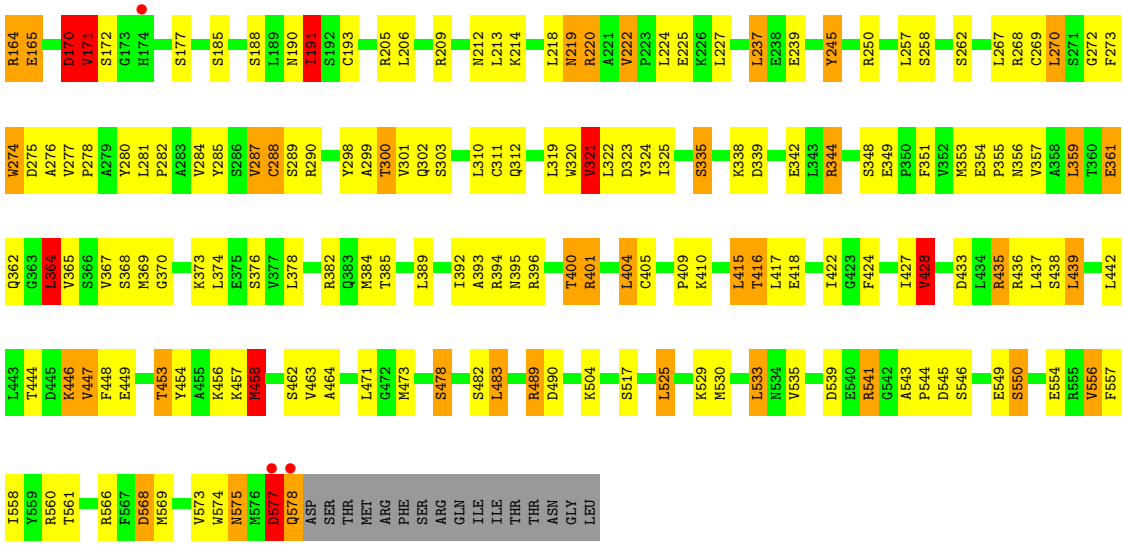




• Molecule 2: TRANSPORT INHIBITOR RESPONSE 1 protein

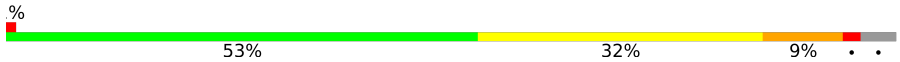
Chain B:

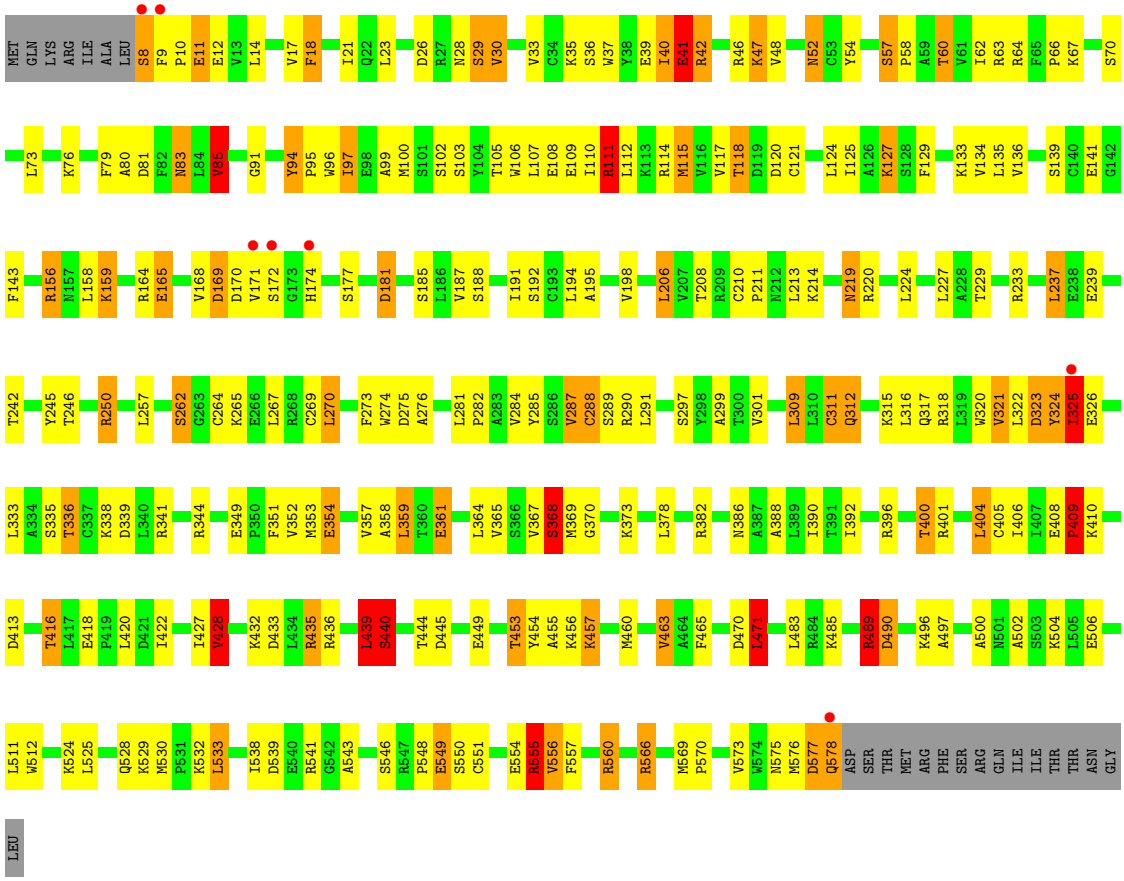




- Molecule 2: TRANSPORT INHIBITOR RESPONSE 1 protein

Chain E:

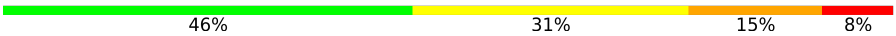


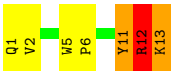


- Molecule 3: Auxin-responsive protein IAA7

Chain C:

• Molecule 3: Auxin-responsive protein IAA7

Chain F: 



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.67Å 82.75Å 125.79Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-2.50) 90.5 (49.55-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.274 0.235 , 0.241	Depositor DCC
R_{free} test set	3305 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11872	wwPDB-VP
Average B, all atoms (Å^2)	7.0	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 52.31 % 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 4.9529e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, CFA

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	1.01	2/1022 (0.2%)	1.03	5/1377 (0.4%)
1	D	0.92	2/1038 (0.2%)	1.14	5/1400 (0.4%)
2	B	1.31	11/4593 (0.2%)	1.36	53/6226 (0.9%)
2	E	1.29	13/4593 (0.3%)	1.34	39/6226 (0.6%)
3	C	4.02	1/118 (0.8%)	0.90	0/159
3	F	1.12	0/118	1.06	0/159
All	All	1.30	29/11482 (0.3%)	1.30	102/15547 (0.7%)

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	A	3	3
1	D	0	4
2	B	2	14
2	E	3	7
3	F	0	3
All	All	8	31

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	13	LYS	C-OXT	-41.90	0.43	1.23
2	E	440	SER	CB-OG	-8.13	1.31	1.42
1	A	20	GLU	CB-CG	7.43	1.66	1.52
1	A	20	GLU	CG-CD	7.25	1.62	1.51
2	E	408	GLU	CB-CG	7.25	1.66	1.52
2	B	428	VAL	CB-CG2	-7.25	1.37	1.52
2	B	225	GLU	CD-OE2	6.93	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	30	VAL	CB-CG2	-6.82	1.38	1.52
2	B	39	GLU	CG-CD	6.28	1.61	1.51
2	B	448	PHE	CE2-CZ	5.97	1.48	1.37
2	E	512	TRP	CE3-CZ3	5.78	1.48	1.38
2	E	557	PHE	CD1-CE1	5.77	1.50	1.39
2	E	555	ARG	CG-CD	-5.73	1.37	1.51
2	E	79	PHE	CG-CD1	5.63	1.47	1.38
2	B	56	VAL	CA-CB	5.50	1.66	1.54
2	B	193	CYS	CB-SG	5.50	1.91	1.82
2	B	245	TYR	CE2-CZ	5.39	1.45	1.38
1	D	14	GLU	CG-CD	-5.35	1.44	1.51
2	B	225	GLU	CB-CG	-5.30	1.42	1.52
2	B	405	CYS	CB-SG	5.28	1.91	1.82
1	D	14	GLU	CB-CG	-5.26	1.42	1.52
2	E	85	VAL	CB-CG2	-5.20	1.42	1.52
2	E	405	CYS	CB-SG	5.19	1.91	1.82
2	E	428	VAL	CB-CG1	-5.13	1.42	1.52
2	E	336	THR	CB-CG2	5.13	1.69	1.52
2	B	550	SER	C-N	-5.11	1.22	1.34
2	E	195	ALA	CA-CB	5.10	1.63	1.52
2	B	274	TRP	CB-CG	5.09	1.59	1.50
2	E	502	ALA	C-O	5.04	1.32	1.23

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	144	THR	C-N-CD	-19.80	77.03	120.60
2	B	220	ARG	N-CA-CB	-16.51	80.88	110.60
2	E	435	ARG	NE-CZ-NH2	-12.82	113.89	120.30
2	E	555	ARG	NE-CZ-NH1	12.14	126.37	120.30
2	B	339	ASP	CB-CG-OD1	10.63	127.86	118.30
2	E	560	ARG	NE-CZ-NH2	-9.63	115.48	120.30
2	B	205	ARG	NE-CZ-NH2	-9.24	115.68	120.30
2	E	359	LEU	CB-CG-CD2	8.81	125.97	111.00
2	B	401	ARG	NE-CZ-NH1	-8.65	115.97	120.30
2	B	321	VAL	CB-CA-C	-8.21	95.80	111.40
2	E	339	ASP	CB-CG-OD1	8.16	125.65	118.30
2	B	115	MET	CG-SD-CE	8.15	113.25	100.20
2	B	267	LEU	CB-CG-CD2	-8.12	97.20	111.00
2	E	270	LEU	CB-CG-CD2	-8.09	97.24	111.00
2	B	401	ARG	NE-CZ-NH2	8.01	124.31	120.30
2	E	339	ASP	CB-CG-OD2	-7.95	111.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	321	VAL	CB-CA-C	-7.87	96.46	111.40
2	E	555	ARG	NE-CZ-NH2	-7.78	116.41	120.30
2	B	311	CYS	CA-CB-SG	-7.76	100.03	114.00
2	B	550	SER	CB-CA-C	-7.72	95.43	110.10
2	E	97	ILE	CG1-CB-CG2	-7.69	94.48	111.40
2	E	471	LEU	CB-CG-CD2	-7.61	98.06	111.00
2	E	323	ASP	CB-CG-OD1	7.36	124.93	118.30
2	B	321	VAL	CG1-CB-CG2	7.22	122.45	110.90
2	B	409	PRO	C-N-CA	-7.15	103.83	121.70
2	B	541	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	B	359	LEU	CB-CG-CD2	6.96	122.84	111.00
2	B	433	ASP	CB-CG-OD2	6.92	124.52	118.30
2	E	433	ASP	CB-CG-OD2	6.91	124.51	118.30
2	E	409	PRO	N-CA-C	6.87	129.96	112.10
2	E	511	LEU	CB-CG-CD2	6.87	122.67	111.00
2	B	458	MET	CG-SD-CE	6.79	111.06	100.20
2	E	111	ARG	NE-CZ-NH2	-6.76	116.92	120.30
2	B	541	ARG	NE-CZ-NH2	-6.71	116.94	120.30
2	E	566	ARG	NE-CZ-NH2	-6.66	116.97	120.30
2	B	478	SER	N-CA-C	6.63	128.90	111.00
1	A	87	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	44	LEU	CB-CG-CD1	6.58	122.19	111.00
2	B	435	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	B	556	VAL	CG1-CB-CG2	6.34	121.05	110.90
2	B	191	ILE	CA-CB-CG2	6.32	123.54	110.90
2	B	344	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	E	321	VAL	CG1-CB-CG2	6.25	120.90	110.90
2	E	94	TYR	C-N-CD	6.24	141.50	128.40
2	B	205	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	E	556	VAL	CG1-CB-CG2	6.16	120.76	110.90
2	B	409	PRO	N-CA-C	6.16	128.11	112.10
2	B	560	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	E	311	CYS	CA-CB-SG	-6.03	103.14	114.00
2	E	490	ASP	CB-CG-OD2	6.01	123.71	118.30
2	E	556	VAL	CB-CA-C	-6.00	100.00	111.40
2	B	191	ILE	CA-CB-CG1	-5.97	99.66	111.00
1	D	44	LEU	CB-CG-CD1	5.97	121.14	111.00
2	E	435	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	B	389	LEU	CA-CB-CG	-5.95	101.61	115.30
2	E	489	ARG	NE-CZ-NH2	-5.89	117.36	120.30
2	B	436	ARG	NE-CZ-NH2	5.80	123.20	120.30
2	E	560	ARG	NE-CZ-NH1	5.78	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	316	LEU	CB-CG-CD1	-5.77	101.19	111.00
2	B	353	MET	CG-SD-CE	5.77	109.43	100.20
2	E	135	LEU	CB-CG-CD1	-5.75	101.23	111.00
2	B	323	ASP	CB-CG-OD1	5.68	123.42	118.30
2	B	191	ILE	CB-CG1-CD1	-5.65	98.08	113.90
2	B	222	VAL	CB-CA-C	-5.62	100.72	111.40
2	E	107	LEU	CB-CG-CD2	-5.60	101.48	111.00
2	B	382	ARG	NE-CZ-NH1	-5.53	117.54	120.30
2	B	213	LEU	CB-CG-CD2	-5.49	101.67	111.00
2	B	225	GLU	OE1-CD-OE2	5.49	129.89	123.30
1	D	93	ILE	N-CA-C	-5.49	96.18	111.00
2	B	473	MET	CA-CB-CG	-5.48	103.99	113.30
2	E	309	LEU	CB-CG-CD2	5.45	120.26	111.00
2	B	568	ASP	CB-CG-OD1	5.45	123.20	118.30
2	E	81	ASP	CB-CG-OD1	5.38	123.15	118.30
2	B	556	VAL	CA-CB-CG1	5.38	118.97	110.90
2	B	14	LEU	CB-CG-CD1	-5.33	101.94	111.00
2	B	100	MET	CG-SD-CE	5.31	108.69	100.20
2	B	122	LEU	CB-CG-CD2	-5.30	101.99	111.00
2	B	170	ASP	CB-CG-OD2	5.29	123.06	118.30
2	B	267	LEU	CA-CB-CG	-5.28	103.16	115.30
2	B	364	LEU	CB-CG-CD2	5.27	119.96	111.00
1	D	87	ASP	CB-CG-OD2	5.27	123.04	118.30
2	E	102	SER	N-CA-C	5.26	125.20	111.00
2	B	556	VAL	CB-CA-C	-5.25	101.42	111.40
2	E	368	SER	CB-CA-C	-5.25	100.13	110.10
1	A	94	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	89	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	112	ASN	N-CA-C	5.22	125.09	111.00
2	B	111	ARG	CG-CD-NE	-5.22	100.84	111.80
1	A	89	ASP	CB-CG-OD2	5.21	122.99	118.30
2	B	447	VAL	CB-CA-C	-5.19	101.55	111.40
2	E	81	ASP	CB-CG-OD2	-5.17	113.65	118.30
2	B	525	LEU	CB-CG-CD2	5.16	119.77	111.00
2	E	198	VAL	CG1-CB-CG2	5.12	119.08	110.90
2	B	32	LEU	CA-CB-CG	5.11	127.06	115.30
2	B	483	LEU	CB-CG-CD2	5.11	119.69	111.00
2	E	318	ARG	NE-CZ-NH2	-5.11	117.75	120.30
2	E	576	MET	N-CA-C	5.07	124.68	111.00
2	B	437	LEU	CB-CG-CD1	5.06	119.61	111.00
2	E	490	ASP	CB-CG-OD1	-5.06	113.75	118.30
2	B	550	SER	O-C-N	-5.06	114.61	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	378	LEU	CB-CG-CD1	5.06	119.60	111.00
2	B	409	PRO	O-C-N	-5.03	114.66	122.70

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	99	PHE	CA
1	A	112	ASN	CA
1	A	153	ARG	CA
2	B	60	THR	CA
2	B	478	SER	CA
2	E	41	GLU	CA
2	E	60	THR	CA
2	E	390	ILE	CB

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Peptide
1	A	87	ASP	Peptide
1	A	97	THR	Peptide
2	B	10	PRO	Peptide
2	B	11	GLU	Peptide
2	B	170	ASP	Peptide
2	B	171	VAL	Peptide
2	B	191	ILE	Peptide
2	B	218	LEU	Peptide
2	B	262	SER	Peptide
2	B	287	VAL	Peptide
2	B	41	GLU	Peptide
2	B	415	LEU	Peptide
2	B	549	GLU	Peptide
2	B	577	ASP	Peptide
2	B	82	PHE	Peptide
2	B	9	PHE	Peptide
1	D	136	THR	Peptide
1	D	86	TRP	Peptide
1	D	87	ASP	Peptide
1	D	88	ALA	Peptide
2	E	169	ASP	Peptide
2	E	17	VAL	Peptide
2	E	262	SER	Peptide

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Mol	Chain	Res	Type	Group
2	E	324	TYR	Peptide
2	E	40	ILE	Peptide
2	E	439	LEU	Peptide
2	E	533	LEU	Peptide
3	F	1	GLN	Peptide
3	F	11	TYR	Peptide
3	F	12	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1009	0	1003	71	3
1	D	1023	0	1013	114	0
2	B	4495	0	4529	219	0
2	E	4495	0	4529	220	0
3	C	114	0	118	24	3
3	F	114	0	118	17	0
4	B	36	0	6	1	0
4	E	36	0	6	2	0
5	B	13	0	5	1	0
5	E	13	0	5	0	0
6	A	25	0	0	3	0
6	B	217	0	0	21	0
6	C	6	0	0	1	0
6	D	32	0	0	6	0
6	E	240	0	0	22	0
6	F	4	0	0	1	0
All	All	11872	0	11332	642	3

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 28.

All (642) 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)
2:B:351:PHE:CD2	3:C:13:LYS:HD2	1.56	1.40
1:D:144:THR:CB	1:D:145:PRO:CD	2.02	1.35
1:A:129:THR:HG23	1:A:132:GLU:OE1	1.14	1.31
1:D:144:THR:CB	1:D:145:PRO:HD2	1.40	1.26
2:B:11:GLU:N	2:B:12:GLU:HG3	1.55	1.21
2:B:145:THR:OG1	2:B:171:VAL:O	1.59	1.20
1:D:93:ILE:HD11	1:D:98:LEU:HB2	1.23	1.20
2:B:453:THR:HG21	6:B:815:HOH:O	1.39	1.20
3:F:13:LYS:HB2	6:F:292:HOH:O	1.40	1.20
1:D:144:THR:HB	1:D:145:PRO:CD	1.63	1.19
2:B:373:LYS:HE3	6:B:810:HOH:O	1.44	1.15
1:D:86:TRP:CZ2	6:D:189:HOH:O	1.98	1.13
1:A:62:HIS:HE1	1:A:87:ASP:OD1	1.32	1.12
1:A:62:HIS:CE1	1:A:87:ASP:OD1	2.02	1.12
1:D:91:MET:HA	1:D:91:MET:HE3	1.29	1.11
1:D:86:TRP:CE2	6:D:189:HOH:O	1.99	1.11
2:B:530:MET:HB3	2:B:533:LEU:HD22	1.34	1.07
2:E:569:MET:HE2	2:E:573:VAL:CG1	1.83	1.07
1:A:89:ASP:HA	1:A:92:LYS:CG	1.86	1.06
2:E:569:MET:CE	2:E:573:VAL:HG12	1.85	1.05
1:A:32:MET:O	1:A:33:VAL:HG23	1.58	1.04
2:E:352:VAL:O	2:E:382:ARG:NH2	1.90	1.04
2:B:400:THR:HG22	2:B:401:ARG:HE	1.19	1.03
1:A:129:THR:CG2	1:A:132:GLU:OE1	2.06	1.03
2:E:569:MET:HE2	2:E:573:VAL:HG12	1.04	1.02
2:B:156:ARG:HG2	2:B:156:ARG:HH11	1.24	1.01
2:E:156:ARG:HG2	2:E:156:ARG:HH11	0.88	1.01
2:E:549:GLU:HB3	6:E:838:HOH:O	1.58	1.01
2:B:11:GLU:H	2:B:12:GLU:HG3	1.06	1.00
1:D:140:LYS:HZ2	1:D:140:LYS:HB2	1.23	1.00
1:A:89:ASP:HA	1:A:92:LYS:HG2	1.41	1.00
1:D:48:THR:HG21	1:D:50:LYS:HB3	1.42	1.00
2:B:369:MET:HG2	2:B:395:ASN:ND2	1.75	1.00
2:B:400:THR:CG2	2:B:401:ARG:HE	1.74	0.99
2:B:11:GLU:C	2:B:12:GLU:CG	2.30	0.98
2:B:13:VAL:O	2:B:17:VAL:HG23	1.64	0.98
3:F:12:ARG:O	3:F:12:ARG:HD3	1.61	0.98
2:E:156:ARG:HH11	2:E:156:ARG:CG	1.76	0.98
2:B:11:GLU:C	2:B:12:GLU:HG2	1.85	0.96
1:D:134:ARG:HD3	1:D:141:ASN:HB2	1.43	0.96
1:A:91:MET:HE1	1:A:117:THR:HG22	1.45	0.95
2:B:351:PHE:HD2	3:C:13:LYS:HD2	1.21	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:GLU:N	2:B:354:GLU:OE2	2.00	0.94
2:B:351:PHE:CD2	3:C:13:LYS:CD	2.50	0.94
1:D:144:THR:HB	1:D:145:PRO:HD3	1.45	0.94
2:B:11:GLU:O	2:B:12:GLU:HG2	1.68	0.94
2:E:181:ASP:OD1	2:E:181:ASP:N	1.97	0.93
3:F:13:LYS:O	3:F:13:LYS:HD3	1.70	0.92
1:A:89:ASP:HB2	1:A:92:LYS:HG3	1.49	0.92
2:E:353:MET:HB3	2:E:354:GLU:OE2	1.69	0.92
2:E:436:ARG:CD	2:E:460:MET:HE3	2.00	0.92
1:A:128:LYS:NZ	1:A:136:THR:HG21	1.83	0.92
2:B:575:ASN:HD22	2:B:577:ASP:H	1.18	0.91
2:E:156:ARG:HG2	2:E:156:ARG:NH1	1.60	0.91
1:A:149:GLU:HB2	6:A:183:HOH:O	1.69	0.91
1:D:140:LYS:HB2	1:D:140:LYS:NZ	1.86	0.90
1:D:58:TYR:OH	1:D:112:ASN:HB2	1.72	0.90
2:E:529:LYS:HG2	2:E:530:MET:CE	2.01	0.90
1:A:89:ASP:CB	1:A:92:LYS:HG3	2.01	0.89
2:E:354:GLU:CD	2:E:354:GLU:H	1.75	0.89
2:B:569:MET:HE1	2:B:575:ASN:N	1.86	0.89
1:D:91:MET:HE1	1:D:93:ILE:HD12	1.53	0.89
1:A:89:ASP:CA	1:A:92:LYS:HG3	2.03	0.89
1:D:48:THR:HG22	1:D:51:ILE:H	1.35	0.89
2:E:326:GLU:HB3	2:E:358:ALA:O	1.71	0.89
1:D:144:THR:OG1	1:D:145:PRO:HD2	1.72	0.88
2:B:118:THR:HG22	2:B:121:CYS:H	1.39	0.88
1:A:129:THR:OG1	1:A:132:GLU:HG3	1.74	0.88
2:E:299:ALA:O	2:E:322:LEU:HD12	1.74	0.87
2:B:285:TYR:O	2:B:288:CYS:HB2	1.73	0.87
2:E:410:LYS:N	6:E:809:HOH:O	1.79	0.87
2:E:436:ARG:NE	2:E:460:MET:HE3	1.88	0.87
2:E:436:ARG:HD2	2:E:460:MET:HE3	1.55	0.87
2:B:11:GLU:H	2:B:12:GLU:CG	1.87	0.87
1:D:153:ARG:HD3	6:D:177:HOH:O	1.74	0.86
1:D:86:TRP:N	1:D:89:ASP:H	1.72	0.86
1:D:129:THR:N	1:D:132:GLU:OE2	2.06	0.86
1:A:91:MET:CE	1:A:117:THR:HG22	2.05	0.86
1:D:91:MET:CE	1:D:93:ILE:HD12	2.05	0.86
1:D:91:MET:HA	1:D:91:MET:CE	2.05	0.85
2:B:569:MET:HE2	2:B:573:VAL:HG12	1.58	0.85
1:A:105:ALA:HB2	1:A:113:LEU:HD23	1.57	0.84
2:B:530:MET:CB	2:B:533:LEU:HD22	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LYS:NZ	1:D:140:LYS:CB	2.37	0.83
2:B:541:ARG:HD2	2:B:554:GLU:OE1	1.78	0.83
2:E:529:LYS:HG2	2:E:530:MET:HE2	1.57	0.83
2:E:354:GLU:CD	2:E:354:GLU:N	2.30	0.83
2:B:156:ARG:HH11	2:B:156:ARG:CG	1.92	0.82
6:B:818:HOH:O	3:C:2:VAL:HG11	1.80	0.82
2:B:156:ARG:HG2	2:B:156:ARG:NH1	1.87	0.81
1:D:91:MET:HE3	1:D:91:MET:CA	2.11	0.81
2:E:83:ASN:HA	6:E:693:HOH:O	1.79	0.81
1:A:89:ASP:HA	1:A:92:LYS:HG3	1.59	0.81
1:D:48:THR:CG2	1:D:50:LYS:N	2.44	0.81
1:A:128:LYS:HZ3	1:A:136:THR:HG21	1.45	0.80
2:E:353:MET:CB	2:E:354:GLU:OE2	2.30	0.80
3:F:13:LYS:O	3:F:13:LYS:CG	2.30	0.80
1:A:89:ASP:O	1:A:92:LYS:HB2	1.81	0.79
3:C:13:LYS:CG	3:C:13:LYS:O	2.30	0.79
3:F:13:LYS:O	3:F:13:LYS:CD	2.30	0.78
2:B:320:TRP:CE2	2:B:344:ARG:HD2	2.18	0.78
1:D:48:THR:HG22	1:D:50:LYS:N	1.99	0.78
2:B:76:LYS:NZ	2:B:141:GLU:OE2	2.12	0.77
2:E:325:ILE:CG2	2:E:325:ILE:O	2.31	0.77
2:E:416:THR:HG21	6:E:737:HOH:O	1.83	0.77
1:D:48:THR:HG21	1:D:50:LYS:CB	2.14	0.76
3:F:12:ARG:O	3:F:12:ARG:CD	2.32	0.76
1:D:93:ILE:CD1	1:D:98:LEU:HB2	2.12	0.76
3:C:8:VAL:HG13	3:C:10:ASN:OD1	1.85	0.75
2:E:413:ASP:HB3	2:E:416:THR:HG22	1.66	0.75
3:F:11:TYR:O	3:F:12:ARG:HG3	1.86	0.75
1:A:103:LEU:HD21	2:B:9:PHE:CB	2.17	0.75
2:B:529:LYS:HG2	2:B:530:MET:HE2	1.68	0.75
1:D:137:PHE:H	1:D:137:PHE:HD2	1.33	0.74
2:E:575:ASN:HD22	2:E:577:ASP:H	1.35	0.74
2:B:351:PHE:HD2	3:C:13:LYS:CD	1.94	0.74
2:B:575:ASN:ND2	2:B:577:ASP:H	1.85	0.74
3:C:12:ARG:O	3:C:13:LYS:HB3	1.84	0.74
2:E:432:LYS:HG2	6:E:842:HOH:O	1.88	0.74
2:E:118:THR:HG23	6:E:675:HOH:O	1.85	0.74
2:E:489:ARG:HD3	2:E:490:ASP:OD2	1.88	0.74
2:B:489:ARG:HD3	2:B:490:ASP:OD2	1.88	0.73
2:B:287:VAL:O	2:B:290:ARG:HG2	1.88	0.73
2:E:436:ARG:CZ	2:E:460:MET:HE3	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:529:LYS:HG2	2:B:530:MET:CE	2.18	0.73
2:E:416:THR:CG2	2:E:418:GLU:H	2.01	0.73
2:E:118:THR:CG2	2:E:120:ASP:HB2	2.18	0.72
2:B:77:PRO:HG3	2:B:557:PHE:CZ	2.25	0.72
1:D:121:VAL:O	1:D:124:MET:HB2	1.89	0.72
1:D:93:ILE:HD11	1:D:98:LEU:CB	2.13	0.72
1:A:89:ASP:CA	1:A:92:LYS:CG	2.60	0.72
2:B:41:GLU:OE1	6:B:733:HOH:O	2.08	0.72
1:D:133:ILE:C	1:D:135:THR:H	1.93	0.72
2:B:578:GLN:HA	6:B:795:HOH:O	1.88	0.71
1:D:131:GLU:O	1:D:135:THR:HB	1.90	0.71
2:E:18:PHE:H	2:E:18:PHE:HD2	1.38	0.71
2:E:428:VAL:HG13	2:E:454:TYR:HB2	1.72	0.71
1:D:5:LYS:O	1:D:6:ILE:HD13	1.90	0.71
1:D:91:MET:HE1	1:D:93:ILE:CD1	2.21	0.71
2:B:11:GLU:N	2:B:12:GLU:CG	2.46	0.70
2:B:400:THR:CG2	2:B:401:ARG:NE	2.53	0.70
1:D:132:GLU:O	1:D:136:THR:OG1	2.08	0.70
3:C:13:LYS:CD	3:C:13:LYS:O	2.39	0.70
2:B:35:LYS:HE3	6:B:808:HOH:O	1.91	0.70
2:E:282:PRO:HA	2:E:285:TYR:CE1	2.26	0.69
2:B:404:LEU:HD23	2:B:424:PHE:HZ	1.57	0.69
1:D:144:THR:HB	1:D:145:PRO:HD2	1.35	0.69
2:E:416:THR:HG22	2:E:418:GLU:H	1.57	0.69
2:E:435:ARG:HD2	6:E:679:HOH:O	1.90	0.69
2:E:118:THR:HG22	2:E:121:CYS:H	1.58	0.69
1:A:105:ALA:HB2	1:A:113:LEU:CD2	2.21	0.69
3:C:5:TRP:CG	3:C:6:PRO:HA	2.27	0.69
2:E:524:LYS:HE2	2:E:549:GLU:OE1	1.93	0.69
2:E:233:ARG:HD3	6:E:714:HOH:O	1.92	0.68
1:A:103:LEU:HD21	2:B:9:PHE:HB3	1.74	0.68
1:D:155:ASN:HD22	2:E:28:ASN:HB3	1.58	0.68
2:B:9:PHE:HD1	2:B:9:PHE:O	1.75	0.68
2:B:9:PHE:CD1	2:B:9:PHE:N	2.52	0.68
2:E:325:ILE:O	2:E:325:ILE:HG22	1.92	0.68
3:C:13:LYS:O	3:C:13:LYS:HG2	1.91	0.68
2:B:529:LYS:CG	2:B:530:MET:HE2	2.23	0.68
1:A:155:ASN:HB3	2:B:28:ASN:ND2	2.08	0.67
2:E:210:CYS:HB3	6:E:661:HOH:O	1.93	0.67
3:F:13:LYS:O	3:F:13:LYS:HG2	1.93	0.67
2:B:11:GLU:CA	2:B:12:GLU:HG3	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:351:PHE:CD2	3:F:13:LYS:HD2	2.30	0.67
2:E:400:THR:HG22	2:E:401:ARG:HG3	1.75	0.67
2:B:25:LYS:HG2	6:B:647:HOH:O	1.94	0.67
2:E:171:VAL:O	2:E:172:SER:HB3	1.92	0.67
1:A:32:MET:O	1:A:33:VAL:CG2	2.41	0.67
2:E:320:TRP:CE2	2:E:344:ARG:HD2	2.30	0.67
2:B:191:ILE:HD12	2:B:191:ILE:C	1.97	0.67
1:D:129:THR:HB	1:D:130:PRO:HD2	1.77	0.67
2:B:164:ARG:C	2:B:165:GLU:HG2	2.15	0.66
2:B:369:MET:HB3	6:B:686:HOH:O	1.95	0.66
1:D:131:GLU:HG3	1:D:134:ARG:HH21	1.60	0.66
2:E:529:LYS:HG2	2:E:530:MET:HE3	1.78	0.66
3:C:13:LYS:O	3:C:13:LYS:HD3	1.95	0.66
2:E:422:ILE:O	6:E:717:HOH:O	2.13	0.66
1:D:48:THR:CG2	1:D:50:LYS:HB3	2.20	0.66
2:E:409:PRO:CA	6:E:809:HOH:O	2.44	0.66
1:A:105:ALA:CB	1:A:113:LEU:HD23	2.25	0.66
1:D:48:THR:CG2	1:D:50:LYS:CB	2.73	0.66
2:E:118:THR:HG21	2:E:120:ASP:HB2	1.77	0.65
2:E:245:TYR:HB3	2:E:276:ALA:HA	1.79	0.65
1:D:154:GLU:HG2	1:D:159:PHE:HE1	1.60	0.65
2:E:264:CYS:HB2	2:E:267:LEU:HD12	1.79	0.65
2:E:354:GLU:OE2	2:E:354:GLU:N	2.29	0.65
2:E:76:LYS:NZ	2:E:141:GLU:OE2	2.30	0.65
2:E:281:LEU:N	2:E:282:PRO:CD	2.59	0.65
2:E:575:ASN:ND2	2:E:577:ASP:H	1.93	0.65
2:B:160:GLU:HG2	2:B:188:SER:HB3	1.76	0.65
2:B:139:SER:HA	2:B:165:GLU:O	1.97	0.64
1:D:155:ASN:ND2	2:E:28:ASN:HB3	2.12	0.64
2:B:300:THR:HG22	2:B:324:TYR:CE1	2.32	0.64
2:E:436:ARG:HD2	2:E:460:MET:CE	2.25	0.64
2:B:145:THR:HG1	2:B:171:VAL:C	1.86	0.64
2:B:220:ARG:NH2	2:B:275:ASP:OD2	2.31	0.64
1:D:91:MET:CE	1:D:91:MET:CA	2.71	0.64
2:E:250:ARG:HG2	2:E:250:ARG:HH11	1.63	0.64
2:B:578:GLN:O	6:B:623:HOH:O	2.14	0.64
3:C:12:ARG:O	3:C:13:LYS:CB	2.45	0.64
1:D:119:GLN:HB3	6:D:170:HOH:O	1.97	0.64
2:B:109:GLU:HG2	2:B:134:VAL:HB	1.80	0.64
2:E:288:CYS:O	2:E:312:GLN:O	2.16	0.64
2:B:344:ARG:HG2	2:B:378:LEU:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:ARG:NH1	2:B:490:ASP:OD2	2.25	0.63
2:B:83:ASN:HA	6:B:672:HOH:O	1.98	0.63
2:B:351:PHE:CE2	3:C:13:LYS:HD2	2.27	0.63
2:E:164:ARG:C	2:E:165:GLU:HG2	2.17	0.63
1:D:140:LYS:CB	1:D:140:LYS:HZ3	2.11	0.63
2:E:400:THR:HG22	2:E:401:ARG:HE	1.62	0.63
2:E:42:ARG:HB3	2:E:64:ARG:O	1.98	0.63
1:D:155:ASN:HB3	2:E:28:ASN:ND2	2.13	0.62
2:E:428:VAL:HG22	2:E:455:ALA:HB2	1.80	0.62
3:C:1:GLN:HB3	3:C:13:LYS:HE2	1.81	0.62
1:A:125:ILE:O	1:A:128:LYS:HB2	2.00	0.62
1:D:46:ASN:HB2	1:D:107:TYR:CE2	2.35	0.62
3:F:5:TRP:CG	3:F:6:PRO:HA	2.35	0.62
1:A:103:LEU:HD21	2:B:9:PHE:HB2	1.80	0.62
1:A:135:THR:O	1:A:137:PHE:N	2.33	0.62
2:B:282:PRO:HA	2:B:285:TYR:CE1	2.35	0.62
2:B:209:ARG:HD3	6:B:804:HOH:O	1.98	0.61
1:D:130:PRO:O	1:D:134:ARG:HB2	2.00	0.61
1:D:142:ASP:OD1	1:D:142:ASP:N	2.27	0.61
2:B:277:VAL:HG21	2:B:280:TYR:HD1	1.64	0.61
1:D:129:THR:OG1	1:D:132:GLU:HG3	2.01	0.61
2:E:80:ALA:HA	2:E:85:VAL:HG13	1.80	0.61
2:E:21:ILE:O	2:E:21:ILE:HG22	2.00	0.61
2:E:439:LEU:HD12	2:E:439:LEU:H	1.65	0.61
2:B:145:THR:CB	2:B:171:VAL:O	2.49	0.60
2:B:349:GLU:HG3	2:B:356:ASN:ND2	2.15	0.60
2:B:364:LEU:HD13	2:B:392:ILE:HD13	1.83	0.60
2:E:18:PHE:HD2	2:E:18:PHE:N	1.99	0.60
2:B:9:PHE:HD1	2:B:9:PHE:H	1.49	0.60
1:A:56:ILE:HG22	1:A:60:LYS:HE3	1.82	0.60
1:D:48:THR:HG22	1:D:51:ILE:N	2.12	0.60
2:E:416:THR:HG23	2:E:418:GLU:HB2	1.84	0.60
1:D:144:THR:CB	1:D:145:PRO:HD3	1.90	0.60
2:B:385:THR:HG21	2:B:415:LEU:HD12	1.82	0.60
1:D:42:VAL:HG12	1:D:42:VAL:O	2.02	0.60
2:E:281:LEU:N	2:E:282:PRO:HD3	2.17	0.60
2:E:129:PHE:HB3	6:E:701:HOH:O	2.02	0.59
2:B:449:GLU:O	2:B:453:THR:HG23	2.02	0.59
1:A:102:ILE:HD11	1:A:121:VAL:HG21	1.84	0.59
2:E:109:GLU:HG2	2:E:134:VAL:HB	1.84	0.59
1:D:133:ILE:O	1:D:135:THR:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ASN:CA	6:B:672:HOH:O	2.50	0.59
2:E:577:ASP:O	2:E:578:GLN:OE1	2.20	0.59
2:B:118:THR:HG23	2:B:120:ASP:H	1.67	0.59
2:B:335:SER:HA	2:B:338:LYS:HZ1	1.68	0.59
2:B:52:ASN:HD22	2:B:52:ASN:C	2.06	0.59
1:D:86:TRP:HB3	1:D:88:ALA:HB3	1.83	0.59
1:D:134:ARG:HD3	1:D:141:ASN:CB	2.25	0.59
2:E:220:ARG:HH21	2:E:275:ASP:CG	2.05	0.59
2:B:569:MET:CE	2:B:575:ASN:HB2	2.33	0.59
2:E:529:LYS:CD	2:E:530:MET:HE3	2.33	0.59
1:D:86:TRP:N	1:D:89:ASP:HB3	2.18	0.59
2:B:299:ALA:O	2:B:322:LEU:HD12	2.03	0.58
1:A:125:ILE:N	1:A:125:ILE:HD13	2.18	0.58
2:B:22:GLN:HE22	2:B:46:ARG:HD2	1.69	0.58
2:B:300:THR:HG22	2:B:324:TYR:HE1	1.66	0.58
2:B:361:GLU:N	2:B:361:GLU:OE2	2.35	0.58
2:E:127:LYS:CG	2:E:127:LYS:O	2.50	0.58
1:A:102:ILE:HG21	2:B:13:VAL:HG11	1.85	0.58
2:E:436:ARG:CZ	2:E:460:MET:CE	2.81	0.58
1:D:86:TRP:C	1:D:88:ALA:N	2.57	0.58
1:D:48:THR:HG23	1:D:50:LYS:H	1.69	0.58
2:B:14:LEU:HD12	2:B:40:ILE:HG13	1.86	0.58
2:B:428:VAL:HG13	2:B:454:TYR:HB2	1.86	0.57
2:B:464:ALA:HA	2:B:489:ARG:O	2.03	0.57
2:B:569:MET:HE1	2:B:575:ASN:HB2	1.85	0.57
2:E:351:PHE:CD2	3:F:13:LYS:CD	2.87	0.57
2:E:156:ARG:CG	2:E:156:ARG:NH1	2.44	0.57
2:B:439:LEU:CD1	2:B:463:VAL:HG23	2.34	0.57
1:D:43:PRO:O	1:D:44:LEU:HD23	2.05	0.57
2:B:569:MET:HG2	2:B:573:VAL:CG1	2.33	0.57
2:E:96:TRP:O	2:E:100:MET:HG3	2.04	0.57
1:A:7:VAL:HG12	1:A:17:GLU:HG3	1.86	0.57
1:A:135:THR:C	1:A:137:PHE:H	2.07	0.57
1:A:134:ARG:HB2	1:A:139:ILE:HB	1.86	0.57
1:A:144:THR:OG1	1:A:147:GLU:HG3	2.04	0.57
1:D:135:THR:C	1:D:137:PHE:O	2.43	0.57
2:E:58:PRO:O	2:E:62:ILE:HD12	2.03	0.57
2:B:416:THR:O	2:B:417:LEU:HB2	2.05	0.57
1:A:91:MET:O	1:A:93:ILE:N	2.30	0.56
2:E:219:ASN:HD22	2:E:219:ASN:H	1.52	0.56
2:E:127:LYS:O	2:E:127:LYS:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ALA:HB2	2:B:427:ILE:HD13	1.87	0.56
1:D:102:ILE:HG12	1:D:117:THR:HB	1.86	0.56
2:E:485:LYS:NZ	4:E:601:IHP:O36	2.38	0.56
2:B:533:LEU:N	2:B:533:LEU:HD13	2.21	0.56
2:E:239:GLU:HA	2:E:269:CYS:HB2	1.86	0.56
1:A:50:LYS:O	1:A:53:ALA:HB3	2.05	0.56
2:B:569:MET:CE	2:B:573:VAL:HG12	2.34	0.56
2:E:541:ARG:HD2	2:E:554:GLU:OE1	2.06	0.56
2:E:106:TRP:HB2	6:E:726:HOH:O	2.06	0.56
2:E:400:THR:CG2	2:E:401:ARG:HE	2.18	0.56
2:B:281:LEU:N	2:B:282:PRO:HD3	2.20	0.56
3:C:5:TRP:CD2	3:C:6:PRO:HA	2.41	0.56
1:D:86:TRP:C	1:D:88:ALA:H	2.09	0.55
1:D:133:ILE:C	1:D:135:THR:N	2.58	0.55
1:D:134:ARG:CD	1:D:141:ASN:HB2	2.28	0.55
2:E:60:THR:HB	2:E:63:ARG:HH12	1.71	0.55
2:B:338:LYS:HE3	2:B:370:GLY:O	2.07	0.55
1:A:52:LEU:O	1:A:52:LEU:HD23	2.07	0.55
2:E:18:PHE:N	2:E:18:PHE:CD2	2.68	0.55
2:B:11:GLU:CA	2:B:12:GLU:CG	2.82	0.55
1:D:137:PHE:N	1:D:137:PHE:CD2	2.67	0.55
2:E:219:ASN:HD22	2:E:219:ASN:N	2.05	0.55
2:B:416:THR:HG22	2:B:418:GLU:H	1.73	0.54
1:D:86:TRP:N	1:D:89:ASP:N	2.48	0.54
2:B:543:ALA:O	2:B:546:SER:HB2	2.06	0.54
1:D:135:THR:O	1:D:137:PHE:O	2.26	0.54
2:E:91:GLY:O	2:E:115:MET:HE3	2.07	0.54
1:A:151:VAL:HG12	2:B:32:LEU:HD21	1.88	0.54
1:D:91:MET:CE	1:D:93:ILE:CD1	2.81	0.54
2:E:529:LYS:CG	2:E:530:MET:HE3	2.37	0.54
1:D:48:THR:HG23	1:D:50:LYS:N	2.21	0.54
2:B:52:ASN:ND2	2:B:54:TYR:H	2.06	0.54
2:B:416:THR:HG23	2:B:418:GLU:HG3	1.90	0.54
1:D:86:TRP:N	1:D:89:ASP:CB	2.71	0.54
2:B:277:VAL:CG2	2:B:280:TYR:HD1	2.21	0.54
1:D:52:LEU:HD22	1:D:56:ILE:HD11	1.90	0.54
2:B:539:ASP:OD2	2:B:541:ARG:HD3	2.07	0.54
2:E:117:VAL:O	2:E:143:PHE:HB3	2.08	0.54
2:B:26:ASP:O	2:B:30:VAL:HG13	2.08	0.53
2:B:118:THR:HG21	6:B:718:HOH:O	2.07	0.53
2:E:365:VAL:O	2:E:368:SER:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:TYR:HH	1:D:112:ASN:HB2	1.70	0.53
2:E:63:ARG:NH2	6:E:667:HOH:O	2.33	0.53
2:E:8:SER:O	2:E:9:PHE:CD2	2.62	0.53
2:E:439:LEU:CD1	2:E:463:VAL:HG23	2.39	0.53
2:B:281:LEU:N	2:B:282:PRO:CD	2.72	0.53
2:E:80:ALA:CA	2:E:85:VAL:HG13	2.39	0.53
2:E:416:THR:CG2	2:E:418:GLU:HB2	2.39	0.53
1:D:91:MET:HE3	1:D:93:ILE:HD12	1.90	0.53
1:A:151:VAL:HG12	2:B:32:LEU:CD2	2.40	0.52
2:B:320:TRP:NE1	2:B:344:ARG:HD2	2.24	0.52
2:E:529:LYS:HE3	2:E:530:MET:CE	2.39	0.52
1:D:134:ARG:NH1	1:D:141:ASN:HB2	2.25	0.52
3:C:1:GLN:CB	3:C:13:LYS:HE2	2.38	0.52
1:A:89:ASP:O	1:A:92:LYS:CB	2.54	0.52
1:D:52:LEU:O	1:D:56:ILE:HG12	2.09	0.52
1:D:131:GLU:HG3	6:D:168:HOH:O	2.09	0.52
2:E:351:PHE:HD2	3:F:13:LYS:HD2	1.73	0.52
2:B:9:PHE:O	2:B:9:PHE:CD1	2.62	0.52
3:C:1:GLN:OE1	3:C:13:LYS:HG3	2.10	0.51
1:A:133:ILE:O	1:A:137:PHE:HB2	2.10	0.51
2:B:410:LYS:O	2:B:442:LEU:HB2	2.10	0.51
1:D:88:ALA:N	1:D:90:PHE:H	2.08	0.51
2:E:449:GLU:O	2:E:453:THR:HG23	2.10	0.51
1:D:115:ASP:O	1:D:119:GLN:HG3	2.10	0.51
1:D:134:ARG:HH11	1:D:141:ASN:HB2	1.74	0.51
2:B:58:PRO:O	2:B:59:ALA:C	2.48	0.51
2:B:119:ASP:O	2:B:123:GLU:HG3	2.09	0.51
2:B:160:GLU:CG	2:B:188:SER:HB3	2.41	0.51
1:D:122:ALA:O	1:D:125:ILE:N	2.33	0.51
2:E:539:ASP:OD2	2:E:541:ARG:HD3	2.11	0.51
2:B:404:LEU:HD23	2:B:424:PHE:CZ	2.44	0.51
2:E:158:LEU:C	2:E:159:LYS:HG2	2.31	0.51
2:B:214:LYS:HG3	6:B:799:HOH:O	2.11	0.51
2:E:538:ILE:O	2:E:555:ARG:HG2	2.11	0.51
2:B:400:THR:HG22	2:B:401:ARG:NE	2.05	0.50
1:A:87:ASP:O	1:A:87:ASP:OD2	2.30	0.50
2:B:147:GLY:O	2:B:150:ALA:HB3	2.11	0.50
2:B:578:GLN:C	2:B:578:GLN:OE1	2.49	0.50
2:B:439:LEU:HD13	2:B:463:VAL:HG23	1.92	0.50
2:B:442:LEU:HA	6:B:689:HOH:O	2.10	0.50
1:D:28:THR:HB	1:D:108:LEU:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ASN:O	1:D:138:ASN:OD1	2.30	0.50
1:D:154:GLU:HG2	1:D:159:PHE:CE1	2.44	0.50
2:E:73:LEU:HB2	2:E:112:LEU:CD2	2.41	0.50
2:E:416:THR:HG23	2:E:418:GLU:H	1.74	0.50
2:E:338:LYS:NZ	2:E:370:GLY:O	2.45	0.50
2:E:324:TYR:O	2:E:326:GLU:HG3	2.12	0.50
2:E:364:LEU:HG	2:E:392:ILE:HD13	1.94	0.49
4:B:601:IHP:O44	4:B:601:IHP:O33	2.31	0.49
2:E:413:ASP:CG	2:E:416:THR:HB	2.32	0.49
2:B:310:LEU:O	2:B:312:GLN:N	2.46	0.49
1:A:152:ARG:O	1:A:155:ASN:HB2	2.12	0.49
1:D:122:ALA:C	1:D:124:MET:N	2.66	0.49
2:E:229:THR:HA	6:E:819:HOH:O	2.13	0.49
1:D:48:THR:CG2	1:D:50:LYS:CA	2.91	0.49
1:D:48:THR:CG2	1:D:51:ILE:H	2.15	0.49
1:D:86:TRP:CG	1:D:87:ASP:N	2.80	0.49
1:A:56:ILE:CG2	1:A:60:LYS:HE3	2.43	0.49
2:B:9:PHE:HB2	2:B:10:PRO:HD2	1.94	0.49
2:E:118:THR:HG22	2:E:120:ASP:N	2.28	0.49
2:E:164:ARG:O	2:E:165:GLU:HG2	2.12	0.49
2:B:11:GLU:C	2:B:12:GLU:HG3	2.14	0.49
2:B:190:ASN:OD1	2:B:190:ASN:C	2.51	0.48
1:D:49:SER:O	1:D:50:LYS:C	2.51	0.48
2:B:8:SER:HB3	6:B:813:HOH:O	2.12	0.48
2:B:438:SER:CB	2:B:462:SER:HB2	2.43	0.48
2:E:97:ILE:HG22	2:E:124:LEU:HD23	1.94	0.48
2:B:91:GLY:O	2:B:115:MET:HB3	2.14	0.48
2:B:118:THR:HB	2:B:121:CYS:SG	2.53	0.48
1:A:135:THR:C	1:A:137:PHE:N	2.67	0.48
1:A:135:THR:HG22	1:A:136:THR:N	2.28	0.48
1:A:103:LEU:CD2	2:B:9:PHE:HB2	2.43	0.48
1:A:157:TRP:N	1:A:157:TRP:CD1	2.80	0.48
2:E:404:LEU:O	2:E:440:SER:HB2	2.14	0.48
2:B:404:LEU:CD2	2:B:424:PHE:HZ	2.26	0.48
1:D:88:ALA:H	1:D:90:PHE:H	1.60	0.48
2:B:438:SER:HB3	2:B:462:SER:HB2	1.95	0.47
2:B:569:MET:HE1	2:B:575:ASN:CB	2.44	0.47
2:E:325:ILE:O	2:E:325:ILE:HG23	2.12	0.47
2:B:52:ASN:C	2:B:52:ASN:ND2	2.66	0.47
1:D:144:THR:HB	1:D:145:PRO:CG	2.39	0.47
2:E:52:ASN:C	2:E:52:ASN:HD22	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:118:THR:HG21	6:E:759:HOH:O	2.14	0.47
1:A:9:LYS:O	1:A:10:SER:O	2.33	0.47
2:B:220:ARG:HB2	6:B:755:HOH:O	2.14	0.47
2:B:529:LYS:CG	2:B:530:MET:CE	2.89	0.47
1:A:7:VAL:HA	1:A:16:PHE:O	2.15	0.47
2:B:118:THR:CG2	2:B:120:ASP:HB2	2.43	0.47
2:B:239:GLU:HG2	2:B:269:CYS:HB2	1.96	0.47
2:E:323:ASP:O	2:E:325:ILE:O	2.32	0.47
2:E:569:MET:CE	2:E:575:ASN:N	2.77	0.47
2:B:93:VAL:HG13	2:B:97:ILE:HD12	1.97	0.47
2:B:444:THR:C	2:B:446:LYS:N	2.65	0.47
2:E:37:TRP:CD1	2:E:37:TRP:N	2.79	0.47
2:E:439:LEU:HD13	2:E:463:VAL:HG23	1.95	0.47
2:B:47:LYS:HE3	6:B:698:HOH:O	2.15	0.47
2:E:64:ARG:O	2:E:66:PRO:HD3	2.15	0.47
2:E:52:ASN:C	2:E:52:ASN:ND2	2.68	0.47
2:E:191:ILE:O	2:E:219:ASN:HB3	2.15	0.47
2:E:94:TYR:O	2:E:95:PRO:C	2.51	0.47
2:B:118:THR:CG2	2:B:120:ASP:N	2.78	0.46
1:D:131:GLU:CG	1:D:134:ARG:HH21	2.28	0.46
2:E:317:GLN:HB3	2:E:341:ARG:HG2	1.96	0.46
2:E:388:ALA:O	2:E:392:ILE:HG13	2.16	0.46
2:E:538:ILE:HB	2:E:555:ARG:HG3	1.96	0.46
1:A:95:GLN:C	1:A:97:THR:H	2.18	0.46
2:E:539:ASP:OD1	2:E:541:ARG:NH1	2.48	0.46
2:E:578:GLN:HB2	6:E:710:HOH:O	2.15	0.46
2:B:18:PHE:N	2:B:18:PHE:CD2	2.80	0.46
1:D:140:LYS:HZ3	1:D:140:LYS:HB3	1.80	0.46
1:D:145:PRO:HG2	1:D:146:GLU:OE1	2.15	0.46
2:E:159:LYS:HB3	2:E:187:VAL:HG23	1.98	0.46
2:B:348:SER:C	2:B:349:GLU:HG2	2.35	0.46
2:E:242:THR:HG1	2:E:273:PHE:H	1.57	0.46
2:E:108:GLU:O	2:E:133:LYS:N	2.49	0.46
2:E:118:THR:CG2	2:E:120:ASP:N	2.79	0.46
1:A:51:ILE:HG13	1:A:100:GLU:HB3	1.96	0.46
2:B:219:ASN:HB3	2:B:222:VAL:HG23	1.97	0.46
2:B:543:ALA:HA	2:B:544:PRO:HD3	1.61	0.46
2:E:213:LEU:O	2:E:214:LYS:HD3	2.16	0.46
1:D:141:ASN:OD1	1:D:141:ASN:C	2.54	0.46
2:E:80:ALA:CB	2:E:85:VAL:HG13	2.46	0.46
2:E:285:TYR:O	2:E:288:CYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:GLU:HG2	6:D:162:HOH:O	2.15	0.46
2:B:164:ARG:O	2:B:164:ARG:HG3	2.15	0.46
2:B:94:TYR:HB3	2:B:95:PRO:HD3	1.98	0.45
2:B:444:THR:C	2:B:446:LYS:H	2.19	0.45
1:D:105:ALA:HB2	1:D:113:LEU:HD23	1.98	0.45
2:E:57:SER:OG	2:E:60:THR:HG23	2.16	0.45
2:B:303:SER:HB2	2:B:324:TYR:O	2.16	0.45
2:B:361:GLU:HG3	2:B:384:MET:HA	1.98	0.45
2:B:365:VAL:O	2:B:368:SER:HB2	2.16	0.45
2:B:367:VAL:HG12	2:B:374:LEU:HD22	1.97	0.45
2:B:369:MET:HG2	2:B:395:ASN:HD21	1.70	0.45
2:E:118:THR:HG22	2:E:121:CYS:N	2.29	0.45
2:E:282:PRO:HA	2:E:285:TYR:CD1	2.51	0.45
2:B:38:TYR:CE1	2:B:42:ARG:HD2	2.52	0.45
2:B:112:LEU:HD12	2:B:137:LEU:CD2	2.46	0.45
2:B:212:ASN:HB2	6:B:627:HOH:O	2.15	0.45
2:E:73:LEU:HB2	2:E:112:LEU:HD23	1.97	0.45
2:B:145:THR:CG2	2:B:171:VAL:O	2.64	0.45
2:E:192:SER:HB2	2:E:274:TRP:HH2	1.82	0.45
2:E:10:PRO:O	2:E:11:GLU:C	2.54	0.45
2:B:38:TYR:O	2:B:42:ARG:HG3	2.16	0.45
2:B:288:CYS:C	2:B:290:ARG:H	2.20	0.45
1:D:140:LYS:O	1:D:140:LYS:HG3	2.11	0.45
2:B:529:LYS:HE2	2:E:500:ALA:O	2.17	0.45
2:B:9:PHE:CD1	2:B:9:PHE:C	2.90	0.45
1:D:115:ASP:O	1:D:119:GLN:CG	2.65	0.45
2:B:82:PHE:CZ	3:C:7:PRO:HB2	2.52	0.44
2:B:457:LYS:HA	2:B:457:LYS:HD3	1.80	0.44
2:E:47:LYS:HB2	2:E:70:SER:HB3	1.97	0.44
2:E:548:PRO:C	2:E:550:SER:H	2.20	0.44
2:B:118:THR:CG2	2:B:120:ASP:H	2.30	0.44
2:E:35:LYS:O	2:E:39:GLU:HG2	2.17	0.44
2:E:333:LEU:HD23	2:E:367:VAL:HG21	1.98	0.44
2:B:9:PHE:HB2	2:B:10:PRO:CD	2.47	0.44
2:B:39:GLU:O	2:B:42:ARG:HB2	2.16	0.44
2:B:368:SER:HB3	2:B:395:ASN:HD22	1.82	0.44
2:B:395:ASN:O	2:B:396:ARG:CZ	2.66	0.44
2:E:36:SER:O	2:E:40:ILE:HG13	2.18	0.44
2:E:42:ARG:H	2:E:42:ARG:HG3	1.50	0.44
2:E:67:LYS:HA	2:E:67:LYS:HD2	1.71	0.44
2:E:400:THR:HG22	2:E:401:ARG:NE	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:THR:CG2	2:B:418:GLU:HG3	2.48	0.44
2:E:111:ARG:HB3	2:E:136:VAL:HB	2.00	0.44
2:E:471:LEU:HA	2:E:471:LEU:HD23	1.22	0.44
2:E:548:PRO:C	2:E:550:SER:N	2.69	0.44
3:F:11:TYR:C	3:F:12:ARG:HG3	2.38	0.44
1:A:123:ASP:HA	1:A:126:LYS:HG3	2.00	0.44
1:A:124:MET:O	1:A:128:LYS:HE3	2.17	0.44
1:A:149:GLU:HA	6:A:183:HOH:O	2.18	0.44
3:C:4:GLY:HA2	6:C:509:HOH:O	2.17	0.44
1:D:46:ASN:HB2	1:D:107:TYR:CD2	2.52	0.44
2:E:114:ARG:HA	2:E:139:SER:O	2.18	0.44
1:D:147:GLU:C	1:D:149:GLU:N	2.71	0.44
2:B:38:TYR:CD1	2:B:38:TYR:C	2.91	0.44
2:E:80:ALA:HB2	2:E:85:VAL:HG13	2.00	0.44
2:E:112:LEU:HB3	2:E:115:MET:HG3	1.98	0.44
2:E:129:PHE:CA	6:E:701:HOH:O	2.66	0.44
2:E:400:THR:HG22	2:E:401:ARG:CG	2.43	0.44
1:A:102:ILE:CG2	2:B:13:VAL:HG11	2.46	0.44
2:B:245:TYR:O	2:B:276:ALA:HA	2.18	0.44
2:B:529:LYS:C	2:B:530:MET:HE2	2.38	0.44
2:B:535:VAL:HG13	2:B:558:ILE:HG12	1.99	0.44
2:B:569:MET:HG2	2:B:573:VAL:HG12	2.00	0.44
2:B:578:GLN:C	2:B:578:GLN:CD	2.76	0.44
2:E:206:LEU:C	2:E:206:LEU:CD2	2.86	0.44
2:E:353:MET:CA	2:E:354:GLU:OE2	2.66	0.44
2:E:386:ASN:OD1	2:E:420:LEU:HA	2.18	0.44
2:B:224:LEU:HA	2:B:224:LEU:HD12	1.66	0.43
2:B:416:THR:HG22	2:B:417:LEU:N	2.33	0.43
1:D:122:ALA:C	1:D:124:MET:H	2.20	0.43
2:B:310:LEU:C	2:B:312:GLN:N	2.68	0.43
2:E:428:VAL:CG2	2:E:455:ALA:HB2	2.45	0.43
2:B:82:PHE:O	2:B:84:LEU:HG	2.19	0.43
2:B:118:THR:HG22	2:B:121:CYS:N	2.19	0.43
2:B:191:ILE:HD12	2:B:191:ILE:O	2.17	0.43
2:B:282:PRO:HA	2:B:285:TYR:CD1	2.54	0.43
5:B:602:CFA:H6'	5:B:602:CFA:C1	2.48	0.43
2:E:465:PHE:HZ	3:F:2:VAL:HG11	1.83	0.43
1:A:91:MET:C	1:A:93:ILE:N	2.72	0.43
3:C:10:ASN:OD1	3:C:10:ASN:N	2.50	0.43
2:E:270:LEU:HD23	2:E:270:LEU:HA	1.30	0.43
1:A:116:LEU:O	1:A:116:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:VAL:CG1	3:C:10:ASN:H	2.32	0.43
2:B:47:LYS:CE	6:B:698:HOH:O	2.66	0.43
2:B:191:ILE:HA	2:B:191:ILE:HD13	0.99	0.43
2:B:416:THR:HG23	2:B:418:GLU:CG	2.48	0.43
2:E:26:ASP:O	2:E:29:SER:HB2	2.19	0.43
1:A:91:MET:HE3	1:A:117:THR:HG22	1.95	0.43
1:D:125:ILE:HG23	1:D:133:ILE:HD13	2.01	0.43
2:E:143:PHE:CZ	2:E:168:VAL:HG22	2.53	0.43
1:D:157:TRP:CD2	2:E:560:ARG:HD2	2.54	0.43
2:E:177:SER:HA	6:E:636:HOH:O	2.18	0.43
2:E:110:ILE:HD13	2:E:125:ILE:CD1	2.49	0.43
2:E:361:GLU:OE2	2:E:361:GLU:N	2.52	0.43
2:E:396:ARG:HA	2:E:396:ARG:NE	2.34	0.43
2:E:400:THR:CG2	2:E:401:ARG:NE	2.82	0.43
2:E:470:ASP:HB3	2:E:497:ALA:HB2	2.01	0.43
1:A:132:GLU:O	1:A:136:THR:OG1	2.33	0.42
2:B:58:PRO:O	2:B:61:VAL:N	2.52	0.42
1:D:86:TRP:CE3	1:D:87:ASP:HB2	2.54	0.42
2:E:274:TRP:O	2:E:275:ASP:HB2	2.20	0.42
1:A:95:GLN:HG3	1:A:99:PHE:CE2	2.54	0.42
1:A:128:LYS:HZ2	1:A:136:THR:HG21	1.76	0.42
1:D:48:THR:HG22	1:D:50:LYS:CA	2.48	0.42
2:E:30:VAL:CG2	2:E:41:GLU:HG2	2.49	0.42
2:E:250:ARG:HH11	2:E:250:ARG:CG	2.29	0.42
2:E:529:LYS:HE3	6:E:692:HOH:O	2.19	0.42
2:B:288:CYS:C	2:B:290:ARG:N	2.73	0.42
2:E:287:VAL:O	2:E:287:VAL:CG1	2.67	0.42
1:A:119:GLN:HB3	6:A:164:HOH:O	2.20	0.42
2:B:250:ARG:HG2	2:B:250:ARG:HH11	1.84	0.42
2:B:274:TRP:NE1	2:B:298:TYR:CD1	2.87	0.42
2:B:47:LYS:HZ2	2:B:47:LYS:HG2	1.77	0.42
2:B:220:ARG:HG3	2:B:274:TRP:CD2	2.55	0.42
1:D:155:ASN:HB3	2:E:28:ASN:HD22	1.83	0.42
2:E:270:LEU:HD13	2:E:273:PHE:HZ	1.84	0.42
2:B:272:GLY:O	2:B:273:PHE:HB2	2.20	0.42
1:D:111:LYS:HZ2	1:D:111:LYS:HG2	1.34	0.42
2:E:529:LYS:HE3	2:E:530:MET:HE1	2.01	0.42
1:A:61:ARG:HA	1:A:61:ARG:HD2	1.49	0.42
3:C:8:VAL:HG13	3:C:10:ASN:H	1.85	0.42
2:E:533:LEU:HD23	2:E:560:ARG:HA	2.01	0.42
2:B:529:LYS:CB	2:B:530:MET:HE2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ARG:HG3	1:D:157:TRP:CE2	2.55	0.42
2:E:444:THR:O	2:E:445:ASP:C	2.58	0.42
2:B:36:SER:O	2:B:40:ILE:HG12	2.20	0.42
2:B:569:MET:HE1	2:B:574:TRP:C	2.38	0.42
2:E:52:ASN:ND2	2:E:54:TYR:H	2.18	0.41
2:E:210:CYS:HA	2:E:211:PRO:HD2	1.89	0.41
2:B:435:ARG:HA	2:B:458:MET:HA	2.02	0.41
2:E:62:ILE:CD1	2:E:99:ALA:HB1	2.50	0.41
2:E:237:LEU:HA	2:E:237:LEU:HD12	1.70	0.41
2:B:80:ALA:HA	2:B:85:VAL:HG13	2.01	0.41
2:B:342:GLU:HA	2:B:376:SER:O	2.20	0.41
1:D:105:ALA:HB2	1:D:113:LEU:CD2	2.50	0.41
1:A:144:THR:O	1:A:145:PRO:C	2.59	0.41
1:D:52:LEU:O	1:D:56:ILE:CG1	2.67	0.41
2:E:191:ILE:HB	2:E:194:LEU:HD12	2.01	0.41
2:E:471:LEU:C	2:E:471:LEU:HD22	2.41	0.41
2:B:41:GLU:O	2:B:42:ARG:C	2.58	0.41
1:D:5:LYS:HB3	1:D:5:LYS:HE2	1.53	0.41
1:D:145:PRO:CG	1:D:146:GLU:H	2.34	0.41
2:E:250:ARG:HG2	2:E:250:ARG:NH1	2.34	0.41
2:B:577:ASP:CG	2:B:578:GLN:N	2.73	0.41
2:E:351:PHE:CD2	3:F:13:LYS:HD3	2.56	0.41
2:E:439:LEU:HD12	2:E:439:LEU:N	2.32	0.41
2:E:570:PRO:HD2	2:E:573:VAL:CG2	2.50	0.41
4:E:601:IHP:O44	4:E:601:IHP:O33	2.39	0.41
2:B:74:LYS:HG2	2:B:113:LYS:HB3	2.03	0.41
2:E:9:PHE:HA	2:E:10:PRO:HD2	1.82	0.41
2:E:62:ILE:HD13	2:E:99:ALA:HB1	2.01	0.41
2:E:206:LEU:C	2:E:206:LEU:HD22	2.41	0.41
1:A:129:THR:HB	1:A:130:PRO:HD2	2.03	0.41
2:B:268:ARG:HA	2:B:268:ARG:HD3	1.78	0.41
2:B:300:THR:CG2	2:B:324:TYR:HE1	2.32	0.41
2:B:566:ARG:NH1	2:B:568:ASP:OD1	2.52	0.41
6:B:818:HOH:O	3:C:2:VAL:CG1	2.51	0.41
2:E:264:CYS:CB	2:E:267:LEU:HD12	2.50	0.41
2:B:39:GLU:OE2	2:B:42:ARG:HD3	2.21	0.41
2:B:319:LEU:HG	2:B:321:VAL:HG22	2.03	0.41
2:B:354:GLU:HA	2:B:355:PRO:HD3	1.76	0.41
2:E:282:PRO:HA	2:E:285:TYR:CZ	2.55	0.41
2:E:291:LEU:HD23	2:E:291:LEU:HA	1.93	0.41
2:E:322:LEU:HD23	2:E:322:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:ILE:HD11	2:E:420:LEU:HD11	2.03	0.41
2:E:413:ASP:OD1	2:E:416:THR:HB	2.21	0.41
2:E:543:ALA:O	2:E:546:SER:HB2	2.21	0.41
1:A:52:LEU:HD21	1:A:56:ILE:HD11	2.02	0.40
2:B:76:LYS:HA	2:B:77:PRO:HD3	1.90	0.40
1:A:95:GLN:C	1:A:97:THR:N	2.73	0.40
2:B:94:TYR:O	2:B:95:PRO:C	2.59	0.40
2:B:395:ASN:C	2:B:396:ARG:HG2	2.41	0.40
2:B:439:LEU:CD1	2:B:463:VAL:CG2	2.99	0.40
2:E:325:ILE:O	2:E:359:LEU:HD13	2.21	0.40
2:E:457:LYS:HD2	2:E:457:LYS:HA	1.94	0.40
3:F:5:TRP:CD2	3:F:6:PRO:HA	2.55	0.40
2:B:543:ALA:O	2:B:546:SER:CB	2.69	0.40
2:E:174:HIS:HD2	6:E:742:HOH:O	2.02	0.40
2:E:224:LEU:HD12	2:E:224:LEU:HA	1.52	0.40
2:B:114:ARG:HA	2:B:139:SER:O	2.20	0.40
2:E:416:THR:HG22	2:E:418:GLU:N	2.32	0.40
2:E:496:LYS:HB2	2:E:496:LYS:HE2	1.92	0.40
2:E:569:MET:HE3	2:E:575:ASN:N	2.36	0.40
2:B:237:LEU:HD12	2:B:237:LEU:HA	1.89	0.40
2:B:270:LEU:HD11	2:B:284:VAL:HG22	2.03	0.40
2:B:278:PRO:HD3	2:B:301:VAL:HG12	2.04	0.40
2:E:413:ASP:CB	2:E:416:THR:HG22	2.45	0.40
2:E:566:ARG:HG2	6:E:657:HOH:O	2.21	0.40
2:E:569:MET:HE1	2:E:575:ASN:N	2.36	0.40
3:F:5:TRP:CD1	3:F:6:PRO:HA	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:SER:O	3:C:11:TYR:O[1_545]	0.76	1.44
1:A:15:SER:O	3:C:11:TYR:C[1_545]	1.98	0.22
1:A:15:SER:C	3:C:11:TYR:O[1_545]	1.98	0.22

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	120/160 (75%)	98 (82%)	15 (12%)	7 (6%)	1 1
1	D	121/160 (76%)	98 (81%)	18 (15%)	5 (4%)	3 3
2	B	569/594 (96%)	520 (91%)	41 (7%)	8 (1%)	11 20
2	E	569/594 (96%)	510 (90%)	50 (9%)	9 (2%)	9 17
3	C	11/13 (85%)	10 (91%)	1 (9%)	0	100 100
3	F	11/13 (85%)	8 (73%)	2 (18%)	1 (9%)	1 0
All	All	1401/1534 (91%)	1244 (89%)	127 (9%)	30 (2%)	7 11

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	92	LYS
2	B	42	ARG
2	B	83	ASN
2	B	219	ASN
2	B	550	SER
1	D	48	THR
1	D	87	ASP
1	D	145	PRO
2	E	11	GLU
2	E	18	PHE
2	E	41	GLU
1	A	88	ALA
2	B	12	GLU
2	B	289	SER
1	D	92	LYS
1	D	134	ARG
2	E	297	SER
2	E	325	ILE
2	E	506	GLU

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Mol	Chain	Res	Type
1	A	25	GLU
1	A	145	PRO
1	A	152	ARG
2	B	53	CYS
2	B	172	SER
3	F	12	ARG
2	E	301	VAL
2	E	311	CYS
1	A	102	ILE
2	E	409	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	113/137 (82%)	94 (83%)	19 (17%)	2 4
1	D	114/137 (83%)	88 (77%)	26 (23%)	1 1
2	B	504/525 (96%)	432 (86%)	72 (14%)	3 6
2	E	504/525 (96%)	420 (83%)	84 (17%)	2 4
3	C	12/12 (100%)	6 (50%)	6 (50%)	0 0
3	F	12/12 (100%)	10 (83%)	2 (17%)	2 4
All	All	1259/1348 (93%)	1050 (83%)	209 (17%)	2 4

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	9	LYS
1	A	15	SER
1	A	19	GLU
1	A	24	LEU
1	A	50	LYS
1	A	54	LYS
1	A	61	ARG

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Mol	Chain	Res	Type
1	A	93	ILE
1	A	101	LEU
1	A	102	ILE
1	A	111	LYS
1	A	112	ASN
1	A	135	THR
1	A	136	THR
1	A	139	ILE
1	A	140	LYS
1	A	147	GLU
1	A	149	GLU
2	B	8	SER
2	B	9	PHE
2	B	11	GLU
2	B	12	GLU
2	B	23	LEU
2	B	41	GLU
2	B	47	LYS
2	B	48	VAL
2	B	52	ASN
2	B	60	THR
2	B	67	LYS
2	B	69	ARG
2	B	83	ASN
2	B	85	VAL
2	B	105	THR
2	B	115	MET
2	B	118	THR
2	B	124	LEU
2	B	127	LYS
2	B	130	LYS
2	B	156	ARG
2	B	164	ARG
2	B	165	GLU
2	B	170	ASP
2	B	171	VAL
2	B	177	SER
2	B	185	SER
2	B	191	ILE
2	B	206	LEU
2	B	227	LEU
2	B	237	LEU

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Mol	Chain	Res	Type
2	B	257	LEU
2	B	258	SER
2	B	270	LEU
2	B	288	CYS
2	B	300	THR
2	B	302	GLN
2	B	321	VAL
2	B	325	ILE
2	B	335	SER
2	B	357	VAL
2	B	359	LEU
2	B	361	GLU
2	B	362	GLN
2	B	364	LEU
2	B	394	ARG
2	B	400	THR
2	B	404	LEU
2	B	416	THR
2	B	422	ILE
2	B	428	VAL
2	B	439	LEU
2	B	446	LYS
2	B	447	VAL
2	B	453	THR
2	B	456	LYS
2	B	458	MET
2	B	471	LEU
2	B	478	SER
2	B	482	SER
2	B	483	LEU
2	B	489	ARG
2	B	504	LYS
2	B	517	SER
2	B	525	LEU
2	B	533	LEU
2	B	545	ASP
2	B	556	VAL
2	B	561	THR
2	B	575	ASN
2	B	577	ASP
2	B	578	GLN
3	C	1	GLN

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Mol	Chain	Res	Type
3	C	8	VAL
3	C	10	ASN
3	C	11	TYR
3	C	12	ARG
3	C	13	LYS
1	D	5	LYS
1	D	9	LYS
1	D	12	ASP
1	D	20	GLU
1	D	25	GLU
1	D	47	VAL
1	D	48	THR
1	D	50	LYS
1	D	51	ILE
1	D	52	LEU
1	D	56	ILE
1	D	87	ASP
1	D	92	LYS
1	D	93	ILE
1	D	101	LEU
1	D	102	ILE
1	D	110	ILE
1	D	111	LYS
1	D	112	ASN
1	D	114	LEU
1	D	119	GLN
1	D	135	THR
1	D	136	THR
1	D	137	PHE
1	D	139	ILE
1	D	140	LYS
2	E	8	SER
2	E	12	GLU
2	E	14	LEU
2	E	23	LEU
2	E	29	SER
2	E	33	VAL
2	E	41	GLU
2	E	42	ARG
2	E	46	ARG
2	E	47	LYS
2	E	48	VAL

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Mol	Chain	Res	Type
2	E	52	ASN
2	E	57	SER
2	E	60	THR
2	E	83	ASN
2	E	85	VAL
2	E	103	SER
2	E	105	THR
2	E	111	ARG
2	E	115	MET
2	E	118	THR
2	E	127	LYS
2	E	156	ARG
2	E	159	LYS
2	E	165	GLU
2	E	169	ASP
2	E	170	ASP
2	E	181	ASP
2	E	185	SER
2	E	188	SER
2	E	206	LEU
2	E	208	THR
2	E	219	ASN
2	E	227	LEU
2	E	237	LEU
2	E	246	THR
2	E	250	ARG
2	E	257	LEU
2	E	262	SER
2	E	265	LYS
2	E	284	VAL
2	E	287	VAL
2	E	288	CYS
2	E	289	SER
2	E	290	ARG
2	E	309	LEU
2	E	312	GLN
2	E	315	LYS
2	E	321	VAL
2	E	325	ILE
2	E	335	SER
2	E	336	THR
2	E	349	GLU

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Mol	Chain	Res	Type
2	E	354	GLU
2	E	357	VAL
2	E	361	GLU
2	E	368	SER
2	E	369	MET
2	E	373	LYS
2	E	390	ILE
2	E	400	THR
2	E	404	LEU
2	E	416	THR
2	E	427	ILE
2	E	428	VAL
2	E	439	LEU
2	E	440	SER
2	E	453	THR
2	E	456	LYS
2	E	457	LYS
2	E	463	VAL
2	E	471	LEU
2	E	483	LEU
2	E	489	ARG
2	E	504	LYS
2	E	525	LEU
2	E	528	GLN
2	E	532	LYS
2	E	549	GLU
2	E	551	CYS
2	E	555	ARG
2	E	556	VAL
2	E	577	ASP
2	E	578	GLN
3	F	12	ARG
3	F	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	95	GLN
2	B	22	GLN
2	B	52	ASN
2	B	232	GLN

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Mol	Chain	Res	Type
2	B	302	GLN
2	B	383	GLN
2	B	395	ASN
2	B	501	ASN
2	B	575	ASN
1	D	31	HIS
2	E	52	ASN
2	E	83	ASN
2	E	131	ASN
2	E	174	HIS
2	E	219	ASN
2	E	312	GLN
2	E	383	GLN
2	E	501	ASN
2	E	575	ASN
2	E	578	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	CFA	B	602	-	13,13,13	1.43	3 (23%)	17,17,17	1.44	3 (17%)
5	CFA	E	602	-	13,13,13	1.79	3 (23%)	17,17,17	2.39	7 (41%)
4	IHP	E	601	-	36,36,36	3.03	14 (38%)	54,60,60	1.82	15 (27%)
4	IHP	B	601	-	36,36,36	2.67	10 (27%)	54,60,60	1.92	16 (29%)

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	CFA	B	602	-	-	0/5/5/5	0/1/1/1
5	CFA	E	602	-	-	0/5/5/5	0/1/1/1
4	IHP	E	601	-	-	3/30/54/54	0/1/1/1
4	IHP	B	601	-	-	5/30/54/54	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	601	IHP	P2-O42	7.67	1.84	1.54
4	B	601	IHP	P3-O13	7.37	1.73	1.59
4	E	601	IHP	P3-O43	6.67	1.80	1.54
4	B	601	IHP	P5-O15	6.65	1.71	1.59
4	B	601	IHP	P2-O32	6.12	1.78	1.54
4	E	601	IHP	P2-O12	6.10	1.70	1.59
4	E	601	IHP	P5-O15	5.56	1.69	1.59
4	E	601	IHP	P1-O11	5.22	1.69	1.59
4	B	601	IHP	P3-O43	5.20	1.74	1.54
4	E	601	IHP	P2-O32	5.11	1.74	1.54
4	E	601	IHP	P1-O41	4.60	1.72	1.54
4	E	601	IHP	P3-O13	4.44	1.67	1.59
4	B	601	IHP	P2-O12	4.09	1.67	1.59
4	E	601	IHP	P6-O16	3.97	1.66	1.59
4	B	601	IHP	P2-O42	3.76	1.69	1.54
4	B	601	IHP	P1-O41	3.68	1.69	1.54
4	B	601	IHP	P3-O33	3.46	1.68	1.54
4	E	601	IHP	P4-O14	3.45	1.65	1.59
5	E	602	CFA	O1'-C1'	-3.05	1.31	1.37
5	B	602	CFA	C2-C1	2.74	1.58	1.50
5	E	602	CFA	C4'-CL4	-2.67	1.68	1.74
4	E	601	IHP	C4-C3	2.53	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	IHP	O16-C6	-2.50	1.35	1.44
5	E	602	CFA	C2-C1	2.42	1.57	1.50
4	E	601	IHP	P1-O31	2.17	1.63	1.54
4	E	601	IHP	P4-O24	2.11	1.57	1.50
5	B	602	CFA	C4'-CL4	-2.10	1.69	1.74
4	E	601	IHP	P4-O44	2.03	1.62	1.54
4	B	601	IHP	C4-C3	2.02	1.56	1.52
5	B	602	CFA	C5'-C4'	2.01	1.41	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	IHP	O41-P1-O31	-5.37	87.11	107.64
4	E	601	IHP	O41-P1-O31	5.32	127.95	107.64
5	E	602	CFA	C1'-C2'-CL3	-5.16	113.36	119.43
5	E	602	CFA	C2'-C3'-C4'	-4.75	113.40	118.71
4	B	601	IHP	O12-C2-C3	-4.23	98.72	108.69
4	B	601	IHP	O14-C4-C5	-3.59	100.22	108.69
4	B	601	IHP	O32-P2-O22	3.43	124.10	110.68
4	E	601	IHP	C5-C6-C1	3.33	117.71	110.41
4	E	601	IHP	C6-C5-C4	3.33	117.70	110.41
5	B	602	CFA	C3'-C4'-CL4	-3.26	115.07	119.15
4	E	601	IHP	O12-P2-O22	-3.19	97.07	109.39
4	E	601	IHP	O14-C4-C5	-3.12	101.34	108.69
5	E	602	CFA	C3'-C2'-CL3	3.07	123.44	118.49
4	B	601	IHP	O12-C2-C1	-3.02	101.58	108.69
4	E	601	IHP	O45-P5-O15	-2.82	93.36	105.99
4	E	601	IHP	C6-C1-C2	2.82	116.58	110.41
4	B	601	IHP	O31-P1-O21	2.80	121.65	110.68
4	B	601	IHP	O45-P5-O15	-2.72	93.79	105.99
5	E	602	CFA	C6'-C1'-C2'	2.72	123.13	118.84
4	B	601	IHP	O36-P6-O26	2.72	121.33	110.68
5	E	602	CFA	C6'-C5'-C4'	2.71	122.10	119.24
5	E	602	CFA	C5'-C6'-C1'	-2.69	114.94	120.06
4	B	601	IHP	O13-P3-O23	-2.67	99.07	109.39
4	B	601	IHP	O11-C1-C6	-2.55	102.69	108.69
4	B	601	IHP	O15-C5-C6	2.54	114.68	108.69
4	E	601	IHP	O12-C2-C1	-2.48	102.84	108.69
4	E	601	IHP	O13-C3-C4	2.47	114.52	108.69
5	B	602	CFA	C5'-C6'-C1'	-2.45	115.38	120.06
4	B	601	IHP	O44-P4-O34	2.44	116.95	107.64
4	B	601	IHP	O45-P5-O35	2.36	116.66	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	IHP	O41-P1-O21	2.36	119.92	110.68
5	E	602	CFA	C5'-C4'-CL4	-2.30	115.76	119.35
5	B	602	CFA	C5'-C4'-CL4	2.20	122.79	119.35
4	E	601	IHP	O31-P1-O21	-2.13	102.36	110.68
4	E	601	IHP	O12-C2-C3	-2.12	103.68	108.69
4	E	601	IHP	O11-P1-O21	2.12	117.56	109.39
4	B	601	IHP	O15-P5-O25	2.11	117.52	109.39
4	E	601	IHP	O45-P5-O35	2.08	115.57	107.64
4	E	601	IHP	O14-P4-O24	2.06	117.35	109.39
4	E	601	IHP	O35-P5-O25	2.06	118.73	110.68
4	B	601	IHP	O36-P6-O16	-2.05	96.83	105.99

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	IHP	C1-O11-P1-O21
4	B	601	IHP	C2-O12-P2-O22
4	B	601	IHP	C3-O13-P3-O23
4	E	601	IHP	C2-O12-P2-O22
4	E	601	IHP	C4-O14-P4-O24
4	B	601	IHP	C4-O14-P4-O44
4	B	601	IHP	C5-O15-P5-O35
4	E	601	IHP	C3-O13-P3-O33

There are no ring outliers.

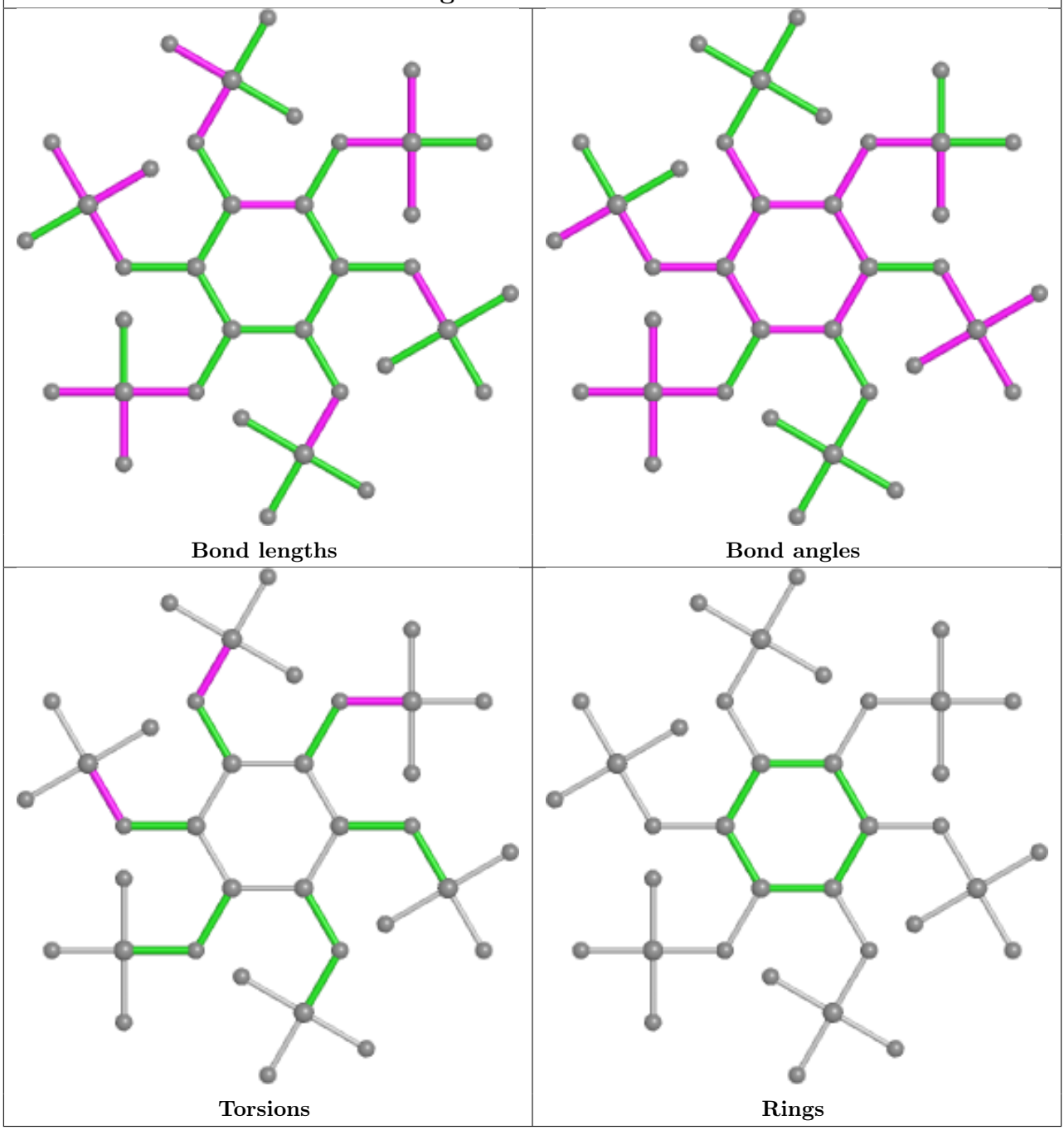
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	602	CFA	1	0
4	E	601	IHP	2	0
4	B	601	IHP	1	0

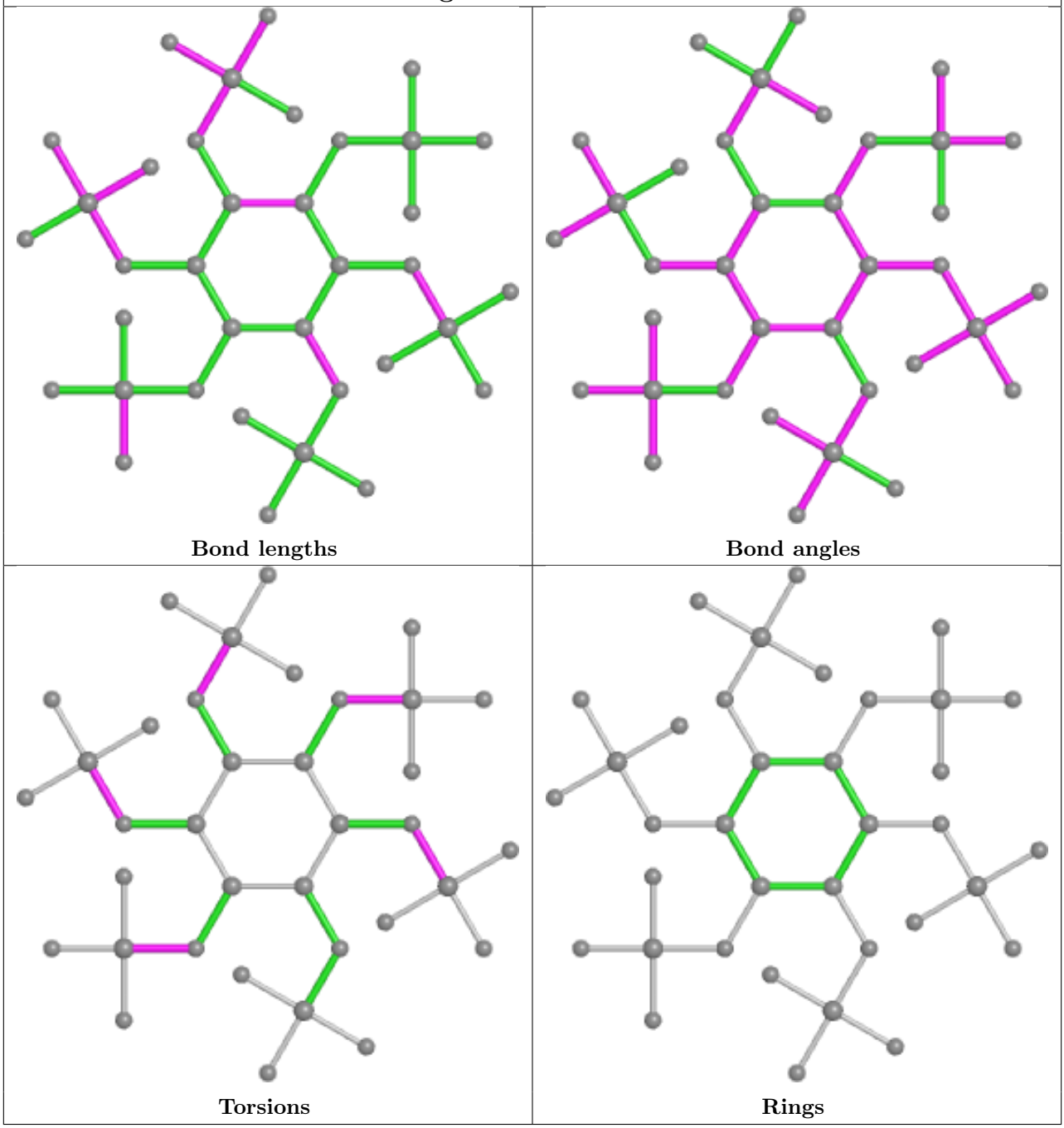
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand IHP E 601



Ligand IHP B 601



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 (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	126/160 (78%)	1.58	44 (34%)	0	0	2, 6, 13, 22	0
1	D	127/160 (79%)	1.37	38 (29%)	0	0	2, 6, 13, 22	0
2	B	571/594 (96%)	-0.07	4 (0%)	87	89	2, 6, 18, 41	0
2	E	571/594 (96%)	0.04	7 (1%)	79	80	2, 6, 16, 32	0
3	C	13/13 (100%)	0.56	1 (7%)	13	13	5, 8, 13, 16	0
3	F	13/13 (100%)	0.51	0	100	100	2, 7, 11, 12	0
All	All	1421/1534 (92%)	0.26	94 (6%)	18	19	2, 6, 16, 41	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ALA	5.5
1	D	137	PHE	5.2
1	A	90	PHE	4.4
1	A	99	PHE	4.4
1	A	40	ASN	4.3
1	A	97	THR	4.3
1	A	138	ASN	4.1
1	D	31	HIS	4.0
1	D	89	ASP	4.0
1	D	113	LEU	4.0
1	D	40	ASN	4.0
2	E	325	ILE	3.9
1	D	41	GLY	3.8
2	E	172	SER	3.8
1	A	124	MET	3.7
2	B	578	GLN	3.7
2	E	8	SER	3.7
1	A	58	TYR	3.6
1	A	41	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	124	MET	3.4
1	A	87	ASP	3.3
1	A	31	HIS	3.3
1	A	121	VAL	3.3
1	A	98	LEU	3.3
1	A	144	THR	3.3
1	D	146	GLU	3.2
1	A	22	VAL	3.2
1	A	21	ALA	3.2
1	A	145	PRO	3.1
1	D	96	ALA	3.1
1	D	144	THR	3.1
1	A	61	ARG	3.1
2	E	174	HIS	3.1
1	A	89	ASP	3.0
1	D	122	ALA	3.0
1	D	90	PHE	2.9
2	B	8	SER	2.9
1	D	97	THR	2.9
1	A	94	ASP	2.9
1	A	137	PHE	2.9
1	D	99	PHE	2.9
1	A	91	MET	2.8
1	D	91	MET	2.8
2	B	174	HIS	2.8
1	A	95	GLN	2.8
1	D	86	TRP	2.8
1	D	92	LYS	2.8
1	A	59	CYS	2.8
1	A	6	ILE	2.8
1	A	92	LYS	2.8
1	D	139	ILE	2.7
1	A	118	CYS	2.7
1	D	112	ASN	2.7
1	A	114	LEU	2.7
1	A	139	ILE	2.6
3	C	1	GLN	2.6
1	A	103	LEU	2.6
1	A	113	LEU	2.6
1	D	20	GLU	2.6
1	A	146	GLU	2.6
1	A	42	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	9	PHE	2.5
1	A	62	HIS	2.5
1	D	100	GLU	2.5
1	A	5	LYS	2.5
1	A	117	THR	2.5
1	A	30	ALA	2.5
1	D	138	ASN	2.4
1	D	119	GLN	2.4
2	E	171	VAL	2.4
1	A	120	THR	2.4
1	D	98	LEU	2.4
1	D	46	ASN	2.4
1	A	131	GLU	2.4
1	A	55	VAL	2.3
1	D	121	VAL	2.3
1	D	145	PRO	2.3
1	D	136	THR	2.3
1	A	112	ASN	2.2
2	E	578	GLN	2.2
1	A	140	LYS	2.2
1	D	135	THR	2.2
1	D	140	LYS	2.2
1	D	120	THR	2.2
1	D	6	ILE	2.1
1	D	125	ILE	2.1
1	D	33	VAL	2.1
1	D	24	LEU	2.1
1	D	95	GLN	2.1
2	B	577	ASP	2.1
1	A	135	THR	2.0
1	D	19	GLU	2.0
1	A	102	ILE	2.0
1	D	94	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

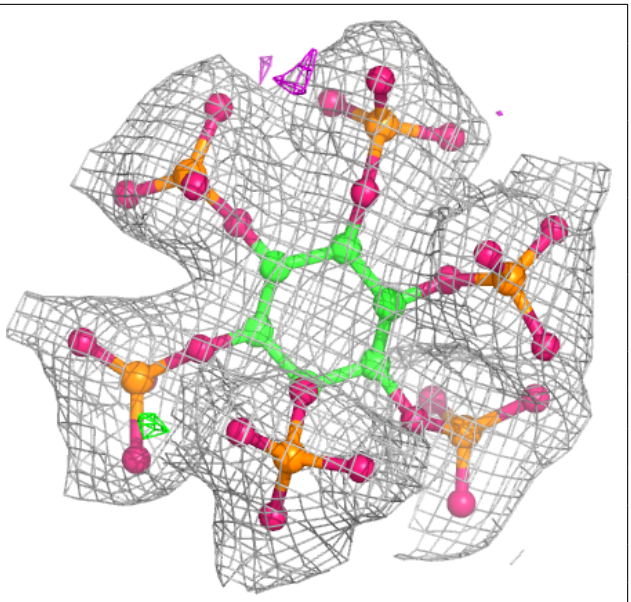
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

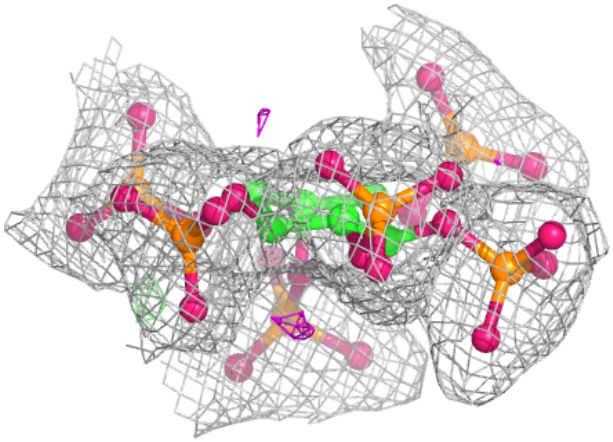
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IHP	B	601	36/36	0.96	0.16	2,6,30,44	0
4	IHP	E	601	36/36	0.97	0.17	2,7,25,32	0
5	CFA	B	602	13/13	0.97	0.16	2,2,9,10	0
5	CFA	E	602	13/13	0.97	0.15	2,2,10,16	0

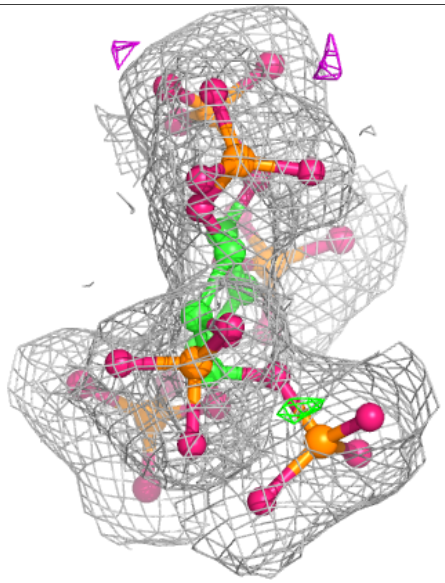
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IHP B 601:

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

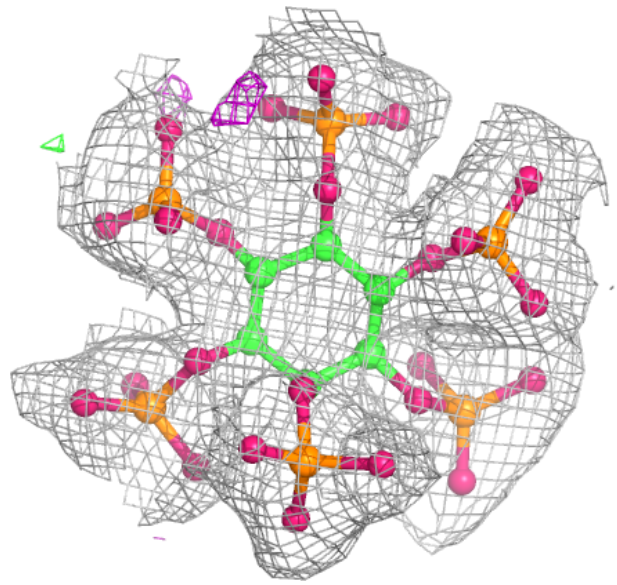


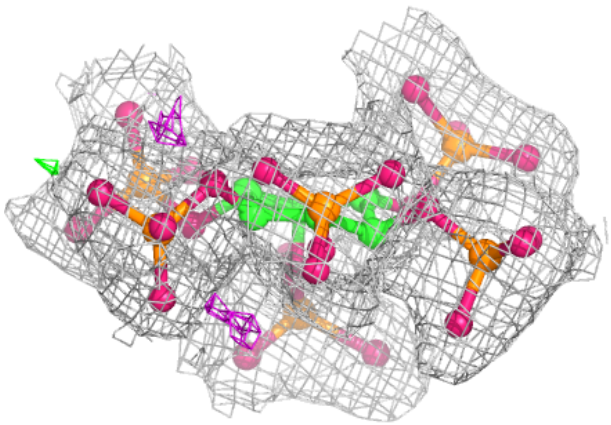


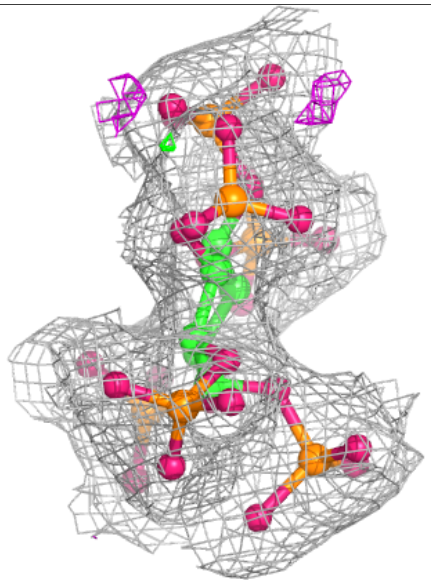


Electron density around IHP E 601:

$2mF_o$-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.