



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:44 PM EDT

PDB ID : 1DJZ / pdb_00001djz
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM
RAT COMPLEXED WITH INOSITOL-4,5-BISPHOSPHATE
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.
Deposited on : 1996-08-24
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

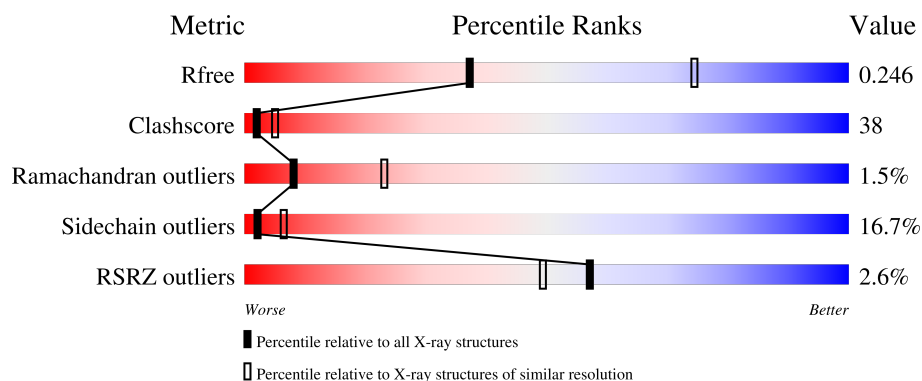
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	624	 2% 34% 36% 11% • 18%
1	B	624	 2% 36% 42% 10% • 10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8840 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 PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	82	0	0
			4057	2565	709	761	22			
1	B	561	Total	C	N	O	S	109	0	0
			4465	2818	776	847	24			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

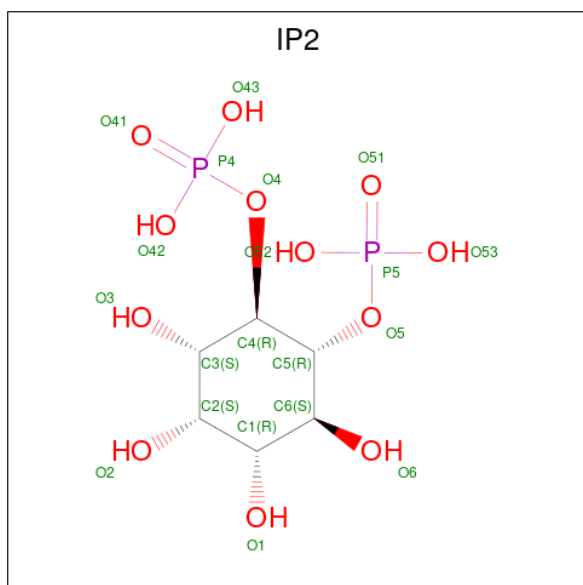
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is D-MYO-INOSITOL-4,5-BISPHOSPHATE (CCD ID: IP2) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		

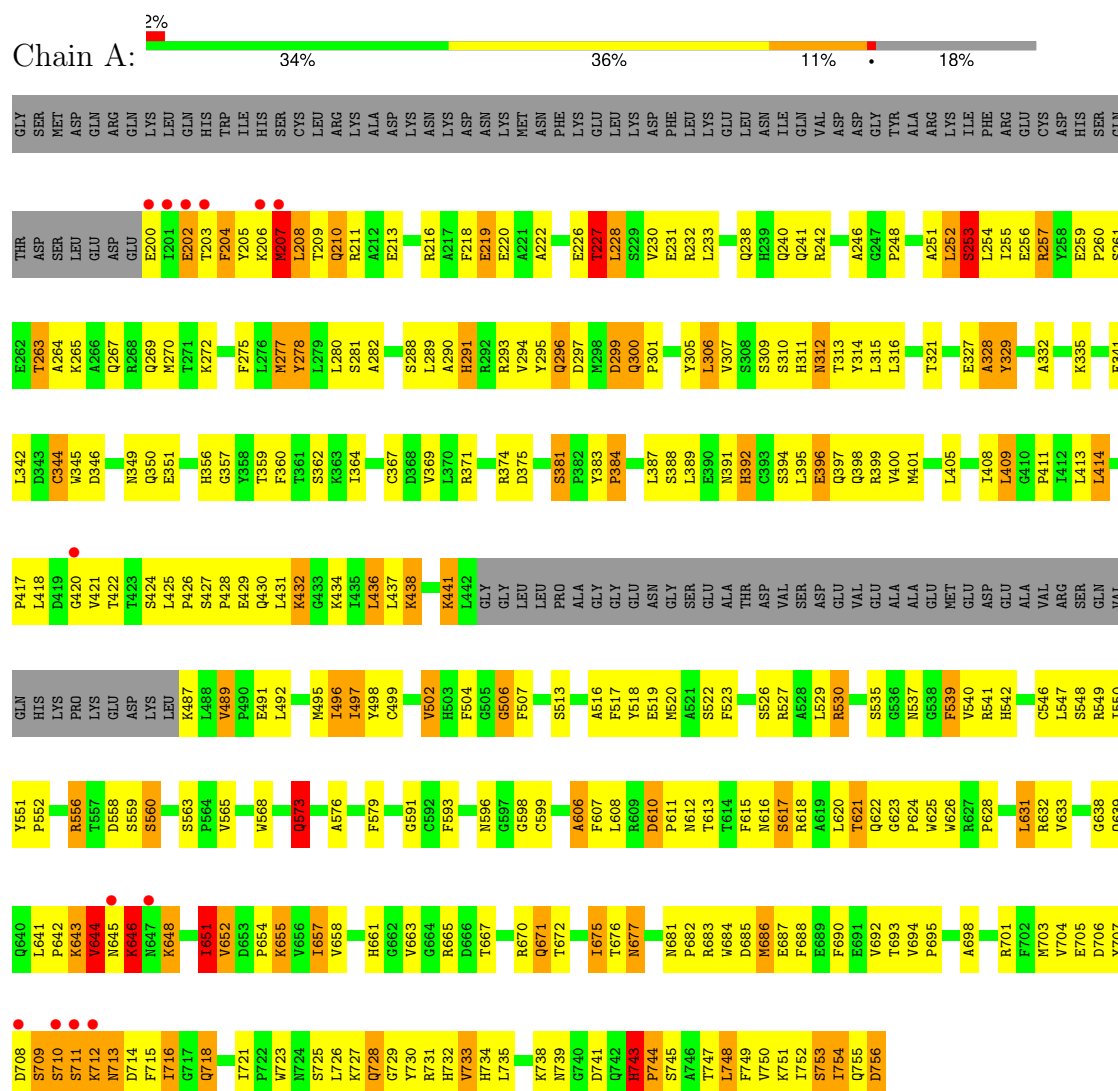
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		
5	B	141	Total	O	0	0
			141	141		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1



D706	G638	L547	GLU	L418	C344	T263	T193	GLY
Y707	Q639	S548	D484	L421	W345	A264	D194	SER
D708	Q640	R549	K485	T422	D346	K265	S195	MET
S709	P642	I550	L486	T423		A266	L196	ASP
S710		P552	K487	T424	Q350	Q267	E197	GLN
	K645	R556	L488	S424	E351	K268	L198	ARG
I715	K646		W489	L425	P362	Q269	E199	GLN
I716	K647		P490	P426	I353	K270	E200	LYS
G717	E491	S560	E491	S427		T271	T201	LEU
Q718	K648	S561	L492		H356	K272	E202	GLN
S719	N649	S562	S493	L431	Q357		T203	HIS
T720	S650	Y562	D494	K432	Y358	F275	F204	TRP
I721	I651	S563	M495	G433	T359	L276	Y205	ILE
P722	V652	P564	I496	K434		K277	K296	HIS
W723	D653	E566	L497	K435	S362		M207	SER
N724	P654	E567	Y498	L436	K363	L280		CYS
S725	K655	Q573	K500	L437	I364	S281	Q210	LEU
L726	V656		K509	L438	A282	A282	R211	ARG
K727	I657		S501	K438	D283	D283	A212	LYS
Q728	V658	A576	H502	G439	G284	G284	E213	ALA
F629	E659	L577	H503	K440			E214	ASP
I660	I660	N578	F504	K441	L370		D215	LYS
Y730	H661	F579	G505	L445	R371	F287		ASN
H731		Q580	G506		R374		F218	LYS
H732	R665	T581	F507	LEU	D375	A290		ASP
V733			S508	PRO	Y376	H291	A221	H158
H734		D887	S509	ALA	A377	R292		K159
L735	R670	V588	P510	GLY	F378	R293	E226	M160
L736	Q671		G511	GLU	K379	V294	T227	H161
S737	T672	Y889	G512	ASN		Y295	L228	F162
K738	A673	L590	T512	GLY	Y383	Q296	S229	K163
N739	V674	G591	S513	SER	P384	D297	V230	E164
G740	I675	C592	G514	GLU	V385	H298		L165
D741	T676	F593	Q515	GLU		D299		K166
Q742	M677	Q594	A516	ALA	S388	Q300	V234	D167
H743	N678	D595	F517	THR	L389	F301	T235	F168
P744		N596	Y518	ASP	E390		F236	L169
	N681	G597	E519	VAL	N391	Y305	L237	K170
T747	P682	G598	M520	SER	H392	L306		E171
L748	R683	C599		ASP	C393		Q238	L172
F749	W684		F523	GLU	S394	S309	H239	M173
V750	D685	F607	S524	VAL	L395	S310	Q240	I174
K751	M686	D610	E525	GLU	E396	H311	Q241	G175
I752	E687	P611	S526	ALA	Q397	N312	R242	G176
S753	P688	M612	R527	ALA	Q398	T313	E243	D177
I754	E689	T613	A528	GLU	R399	Y314	E244	D178
D755		T614	L529	MET	V400	L315	E245	G179
	V692	F615	R530	GLU	N401	L316	A246	Y180
	T693	N616	L531	ASP				A181
V694	V694	F616	L532	GLU	L405	E327	A251	R182
P695	S617	S617	Q533	ALA	A328	A328	L252	K183
D696	R618	R618	E534	VAL	T408	T329	S253	I184
A698			S535	ARG	L409	I330	L254	F185
L699	T621	Q622	G536	SER	G410	R331	T255	R186
V700	G623	G623	N537	GLN	P411	A332	E256	E187
R701	P624	W625		VAL	I412	L333	R257	C188
F702	W626		R541	GLN	I413		Y258	D189
M703			H542	HIS	L414	L340	E259	H190
V704			H545	LYS	D415	E341	P260	S191
E705		R632	C546	PRO	Q416	L342	S261	Q192

4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	396.49Å 396.49Å 396.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.95 10.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.95) 91.8 (10.00-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.89Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.212 , 0.270 0.194 , 0.246	Depositor DCC
R_{free} test set	2048 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 106.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8840	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IP2, CA, ACT

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	1.32	23/4152 (0.6%)	1.36	39/5624 (0.7%)
1	B	1.31	15/4565 (0.3%)	1.35	41/6174 (0.7%)
All	All	1.31	38/8717 (0.4%)	1.35	80/11798 (0.7%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	692	VAL	CA-CB	-8.46	1.43	1.53
1	B	565	VAL	CA-CB	-8.34	1.44	1.54
1	B	520	MET	SD-CE	-8.04	1.59	1.79
1	B	330	ILE	CA-CB	-7.94	1.44	1.54
1	A	277	MET	SD-CE	7.92	1.99	1.79
1	A	658	VAL	CA-C	-7.13	1.44	1.52
1	B	588	VAL	CA-CB	-6.99	1.45	1.54
1	A	540	VAL	CA-CB	-6.86	1.46	1.54
1	A	686	MET	SD-CE	6.33	1.95	1.79
1	A	328	ALA	CA-CB	-6.30	1.43	1.53
1	B	733	VAL	CA-CB	-6.23	1.46	1.54
1	B	632	ARG	CA-C	-6.21	1.45	1.52
1	B	673	ALA	CA-CB	-6.15	1.44	1.53
1	A	606	ALA	CA-CB	-6.12	1.43	1.53
1	A	703	MET	SD-CE	-6.04	1.64	1.79
1	B	670	ARG	CA-C	-6.04	1.45	1.52
1	A	663	VAL	CA-CB	-6.02	1.48	1.54
1	A	307	VAL	CA-CB	-5.94	1.47	1.54
1	A	329	TYR	CG-CD1	-5.94	1.26	1.39
1	B	314	TYR	CE2-CZ	-5.91	1.24	1.38
1	A	332	ALA	CA-C	-5.87	1.45	1.52
1	A	733	VAL	CA-CB	-5.80	1.47	1.54
1	A	565	VAL	CA-CB	-5.57	1.48	1.54
1	A	408	ILE	CA-CB	-5.55	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	734	HIS	CA-CB	-5.46	1.46	1.53
1	B	435	ILE	CA-CB	-5.43	1.47	1.54
1	A	329	TYR	CG-CD2	-5.42	1.27	1.39
1	A	291	HIS	CA-C	-5.38	1.45	1.52
1	B	314	TYR	CG-CD2	-5.33	1.28	1.39
1	A	294	VAL	CA-CB	-5.32	1.45	1.53
1	B	234	VAL	CA-CB	-5.29	1.47	1.54
1	A	329	TYR	CE2-CZ	-5.27	1.25	1.38
1	A	387	LEU	CA-C	-5.25	1.46	1.52
1	A	631	LEU	CA-C	-5.21	1.46	1.52
1	A	313	THR	CA-CB	-5.19	1.44	1.53
1	B	290	ALA	CA-CB	-5.16	1.45	1.53
1	A	290	ALA	CA-CB	-5.09	1.45	1.53
1	B	502	VAL	CA-CB	-5.03	1.47	1.55

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	LEU	N-CA-C	-11.30	97.79	111.69
1	B	508	SER	N-CA-C	10.31	123.90	112.97
1	B	226	GLU	N-CA-C	-9.48	99.38	113.61
1	A	202	GLU	N-CA-C	-8.96	99.69	111.24
1	A	226	GLU	N-CA-C	-8.95	102.06	113.16
1	B	654	PRO	N-CA-C	8.82	125.41	111.38
1	B	743	HIS	C-N-CD	-8.65	89.52	125.00
1	A	743	HIS	C-N-CD	-8.65	89.54	125.00
1	B	509	SER	N-CA-C	-8.24	101.46	113.16
1	A	675	ILE	N-CA-C	-7.73	97.35	108.17
1	B	646	LYS	N-CA-C	-7.71	104.34	113.21
1	B	645	ASN	N-CA-C	7.37	126.49	110.80
1	B	675	ILE	N-CA-C	-7.24	97.42	107.99
1	A	654	PRO	N-CA-C	7.09	122.65	111.38
1	B	715	PHE	N-CA-C	-7.01	99.13	110.20
1	A	644	VAL	CB-CA-C	6.95	122.68	111.29
1	A	408	ILE	N-CA-C	6.90	117.51	110.82
1	B	566	GLU	N-CA-C	6.85	119.59	111.71
1	A	709	SER	N-CA-C	-6.85	103.74	111.07
1	B	748	LEU	N-CA-C	-6.83	98.79	109.72
1	B	591	GLY	N-CA-C	-6.83	104.23	112.49
1	B	573	GLN	N-CA-C	6.74	121.64	113.41
1	A	591	GLY	N-CA-C	-6.71	104.38	112.49
1	A	278	TYR	N-CA-C	-6.59	103.78	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	677	ASN	N-CA-C	6.41	120.26	111.54
1	A	573	GLN	N-CA-C	6.37	121.18	113.41
1	A	207	MET	N-CA-C	6.35	121.03	113.28
1	B	560	SER	N-CA-C	-6.35	102.15	110.53
1	A	299	ASP	N-CA-C	6.30	121.25	113.50
1	B	613	THR	CB-CA-C	-6.26	98.41	109.62
1	A	230	VAL	CB-CA-C	-6.21	103.90	112.04
1	B	202	GLU	N-CA-C	-6.19	103.47	111.02
1	B	400	VAL	CB-CA-C	-6.13	104.01	112.04
1	A	748	LEU	N-CA-C	-6.11	99.95	109.72
1	A	306	LEU	N-CA-C	-6.09	99.34	109.46
1	A	565	VAL	CB-CA-C	-6.00	104.20	111.88
1	B	306	LEU	N-CA-C	-6.00	99.89	109.96
1	B	172	LEU	N-CA-C	-5.99	100.98	109.96
1	A	716	ILE	CB-CA-C	-5.94	105.59	111.30
1	B	754	ILE	CB-CA-C	-5.94	101.83	110.63
1	A	428	PRO	N-CA-C	-5.91	105.32	113.53
1	A	205	TYR	N-CA-C	-5.83	104.93	111.28
1	B	265	LYS	N-CA-C	-5.80	103.94	111.02
1	B	565	VAL	CB-CA-C	-5.68	104.60	112.04
1	A	253	SER	N-CA-C	-5.66	105.19	111.36
1	B	229	SER	N-CA-C	-5.62	102.20	110.52
1	A	752	ILE	CB-CA-C	-5.61	103.22	110.84
1	A	384	PRO	N-CA-C	5.56	119.94	111.15
1	B	408	ILE	N-CA-C	5.54	116.20	110.82
1	B	176	VAL	N-CA-C	5.54	116.46	108.48
1	A	750	VAL	N-CA-C	5.53	116.67	108.65
1	B	174	ILE	N-CA-C	5.52	116.52	107.24
1	B	385	VAL	CB-CA-C	-5.52	102.61	110.83
1	B	594	GLN	N-CA-C	-5.51	105.43	111.82
1	A	667	THR	CB-CA-C	5.46	118.62	109.89
1	A	754	ILE	CB-CA-C	-5.45	103.06	110.42
1	B	427	SER	N-CA-C	-5.45	103.27	110.40
1	A	312	ASN	N-CA-C	-5.42	103.90	111.39
1	A	496	ILE	CB-CA-C	-5.42	106.06	111.80
1	A	282	ALA	N-CA-C	-5.41	106.52	113.01
1	B	716	ILE	CB-CA-C	-5.38	106.33	111.44
1	B	581	THR	N-CA-C	5.34	120.07	109.01
1	B	700	VAL	CA-C-N	-5.33	115.48	122.99
1	B	700	VAL	C-N-CA	-5.33	115.48	122.99
1	B	230	VAL	CB-CA-C	-5.25	105.17	112.04
1	A	718	GLN	N-CA-CB	-5.22	103.42	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	614	THR	N-CA-C	-5.20	106.62	113.17
1	A	227	THR	N-CA-C	5.17	117.05	109.24
1	A	568	TRP	N-CA-C	-5.13	105.68	111.28
1	B	723	TRP	N-CA-C	5.12	119.82	111.37
1	A	735	LEU	N-CA-C	5.12	117.71	110.50
1	B	282	ALA	N-CA-C	-5.11	106.31	112.54
1	A	560	SER	N-CA-C	-5.09	103.76	110.43
1	A	392	HIS	N-CA-C	-5.09	104.89	111.71
1	A	651	ILE	CB-CA-C	-5.09	103.91	111.19
1	B	412	ILE	CB-CA-C	-5.09	104.27	112.16
1	A	288	SER	N-CA-C	5.09	121.64	110.80
1	B	258	TYR	N-CA-C	5.05	121.15	114.12
1	A	506	GLY	N-CA-C	-5.00	103.44	110.75
1	B	394	SER	N-CA-C	-5.00	103.87	110.43

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	4057	0	3972	305	0
1	B	4465	0	4375	332	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	20	0	9	3	0
4	B	20	0	9	4	0
5	A	125	0	0	4	0
5	B	141	0	0	19	0
All	All	8840	0	8371	629	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 38.

All (629) 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:196:LEU:HD22	1:B:200:GLU:HB3	1.28	1.14
1:A:401:MET:HE2	1:A:492:LEU:HD11	1.38	1.03
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.23	1.01
1:B:401:MET:HE2	1:B:492:LEU:HD11	1.41	1.00
1:B:728:GLN:NE2	1:B:754:ILE:H	1.59	1.00
1:A:548:SER:H	1:A:573:GLN:NE2	1.61	0.96
1:A:613:THR:HG22	1:A:615:PHE:H	1.28	0.95
1:A:207:MET:HE1	1:A:210:GLN:HB3	1.49	0.94
1:A:241:GLN:HE22	1:A:730:TYR:H	1.06	0.94
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.02	0.93
1:A:520:MET:HE3	1:A:549:ARG:HB2	1.51	0.92
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.54	0.90
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.55	0.89
1:B:548:SER:H	1:B:573:GLN:NE2	1.69	0.89
1:B:642:PRO:HG3	1:B:743:HIS:CD2	2.08	0.88
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.37	0.88
1:B:728:GLN:HE22	1:B:754:ILE:H	1.21	0.88
1:A:728:GLN:HE22	1:A:754:ILE:H	1.16	0.88
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.56	0.87
1:A:516:ALA:HB3	1:A:519:GLU:HG3	1.57	0.87
1:B:196:LEU:CD2	1:B:200:GLU:HB3	2.05	0.86
1:A:556:ARG:HH11	1:A:556:ARG:HG2	1.38	0.86
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.55	0.86
1:B:168:PHE:CE1	1:B:172:LEU:HD21	2.09	0.86
1:A:728:GLN:NE2	1:A:754:ILE:H	1.72	0.86
1:A:316:LEU:HD23	1:A:328:ALA:HB2	1.59	0.85
1:B:607:PHE:HE2	5:B:821:HOH:O	1.59	0.84
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.24	0.82
1:B:692:VAL:HG12	1:B:695:PRO:HD3	1.61	0.82
1:B:549:ARG:C	1:B:550:ILE:HD13	2.05	0.82
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.15	0.81
1:B:701:ARG:HE	1:B:718:GLN:HE21	1.28	0.81
1:B:642:PRO:HG3	1:B:743:HIS:HD2	1.44	0.80
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.63	0.80
1:A:651:ILE:HD13	1:A:677:ASN:HD21	1.46	0.80
1:A:692:VAL:HG12	1:A:695:PRO:HD3	1.61	0.80
1:B:632:ARG:HH21	1:B:755:GLN:NE2	1.80	0.80
1:B:701:ARG:HE	1:B:718:GLN:NE2	1.79	0.79
1:B:530:ARG:HG3	1:B:530:ARG:HH11	1.45	0.79
1:A:573:GLN:NE2	1:A:573:GLN:H	1.82	0.78
1:A:420:GLY:O	1:A:422:THR:HG23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:MET:HE2	1:B:277:MET:HA	1.67	0.77
1:B:728:GLN:HE21	1:B:753:SER:HA	1.49	0.77
1:A:238:GLN:HG2	1:A:246:ALA:CB	2.16	0.76
1:A:207:MET:HE3	1:A:207:MET:O	1.84	0.76
1:B:196:LEU:HB3	1:B:201:ILE:CD1	2.15	0.76
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.21	0.75
1:B:234:VAL:O	1:B:238:GLN:HG3	1.86	0.75
1:B:221:ALA:HB1	1:B:228:LEU:HD21	1.68	0.74
1:A:504:PHE:HB3	1:A:527:ARG:NH2	1.99	0.74
1:B:426:PRO:CG	1:B:431:LEU:HD11	2.15	0.74
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.03	0.74
1:B:174:ILE:HG22	1:B:176:VAL:HG23	1.68	0.74
1:B:436:LEU:N	1:B:436:LEU:HD23	2.01	0.73
1:B:241:GLN:HE22	1:B:730:TYR:H	1.35	0.73
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.18	0.73
1:B:573:GLN:NE2	1:B:573:GLN:H	1.87	0.73
1:A:438:LYS:HG3	1:A:499:CYS:HB3	1.70	0.73
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.69	0.72
1:B:316:LEU:HD23	1:B:328:ALA:HB2	1.71	0.72
1:B:203:THR:O	1:B:207:MET:HG3	1.89	0.72
1:A:394:SER:O	1:A:398:GLN:HG3	1.88	0.72
1:A:436:LEU:N	1:A:436:LEU:HD23	2.05	0.72
1:B:168:PHE:HE1	1:B:172:LEU:HD21	1.54	0.72
1:A:395:LEU:HD22	1:A:489:VAL:HG12	1.72	0.72
1:A:346:ASP:OD2	1:A:394:SER:HB3	1.90	0.71
1:B:259:GLU:OE2	1:B:260:PRO:HD2	1.90	0.71
1:A:520:MET:CE	1:A:549:ARG:HB2	2.21	0.71
1:A:350:GLN:OE1	1:A:396:GLU:HG3	1.90	0.71
1:B:551:TYR:HB2	1:B:552:PRO:HD2	1.73	0.71
1:A:311:HIS:NE2	4:A:1:IP2:H2	2.04	0.70
1:A:312:ASN:HB3	1:A:315:LEU:HD12	1.73	0.70
1:B:188:CYS:O	1:B:200:GLU:HG2	1.91	0.70
1:A:203:THR:O	1:A:207:MET:HB2	1.92	0.70
1:B:728:GLN:NE2	1:B:754:ILE:N	2.38	0.70
1:A:417:PRO:HD3	1:A:497:ILE:HG13	1.73	0.70
1:B:730:TYR:CE1	1:B:751:LYS:HD3	2.27	0.70
1:B:504:PHE:HB3	1:B:527:ARG:NH2	2.07	0.70
1:B:701:ARG:NH2	1:B:718:GLN:HG3	2.05	0.70
1:B:184:ILE:HG22	1:B:204:PHE:CD1	2.27	0.69
1:A:651:ILE:HD13	1:A:677:ASN:ND2	2.07	0.69
1:B:520:MET:CE	1:B:549:ARG:HB2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:HD12	5:B:767:HOH:O	1.91	0.69
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.28	0.69
1:A:675:ILE:HD13	1:A:684:TRP:NE1	2.07	0.69
1:B:174:ILE:CG2	1:B:176:VAL:HG23	2.22	0.69
1:A:548:SER:H	1:A:573:GLN:HE22	1.40	0.69
1:A:551:TYR:HB2	1:A:552:PRO:HD2	1.75	0.69
1:A:241:GLN:HE22	1:A:730:TYR:N	1.87	0.68
1:A:651:ILE:N	1:A:651:ILE:HD12	2.08	0.68
1:B:548:SER:H	1:B:573:GLN:HE22	1.40	0.68
1:B:701:ARG:NE	1:B:718:GLN:HE21	1.90	0.68
1:A:730:TYR:CE1	1:A:751:LYS:HD3	2.28	0.68
1:A:495:MET:O	1:A:497:ILE:HD13	1.93	0.68
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.23	0.68
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.76	0.68
1:B:346:ASP:OD2	1:B:394:SER:HB3	1.94	0.68
1:B:364:ILE:HD12	1:B:369:VAL:HG23	1.73	0.67
1:A:395:LEU:HD22	1:A:489:VAL:CG1	2.25	0.67
1:A:670:ARG:HD3	5:A:836:HOH:O	1.93	0.67
1:B:651:ILE:CG2	1:B:677:ASN:HA	2.25	0.66
1:A:356:HIS:ND1	1:A:359:THR:HG21	2.10	0.66
1:B:201:ILE:HD13	1:B:201:ILE:N	2.11	0.66
1:B:377:ALA:N	5:B:887:HOH:O	2.28	0.66
1:A:200:GLU:O	1:A:204:PHE:N	2.29	0.66
1:A:707:TYR:HA	1:A:713:ASN:OD1	1.96	0.66
1:B:342:LEU:HD12	1:B:342:LEU:N	2.12	0.65
1:A:426:PRO:HD3	1:A:498:TYR:CD2	2.31	0.65
1:A:204:PHE:O	1:A:208:LEU:N	2.30	0.65
1:A:549:ARG:NH1	4:A:1:IP2:O42	2.29	0.65
1:A:556:ARG:HG2	1:A:560:SER:OG	1.96	0.65
1:B:259:GLU:CD	1:B:260:PRO:HD2	2.20	0.65
1:B:651:ILE:HG22	1:B:677:ASN:HA	1.78	0.65
1:A:272:LYS:O	1:A:275:PHE:HB3	1.96	0.65
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.26	0.65
1:A:549:ARG:NH2	4:A:1:IP2:O3	2.29	0.65
1:B:728:GLN:NE2	1:B:753:SER:HA	2.11	0.65
1:A:617:SER:HA	1:A:620:LEU:HD21	1.79	0.64
1:A:238:GLN:HG2	1:A:246:ALA:HB1	1.78	0.64
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.80	0.64
1:A:497:ILE:HG22	1:A:498:TYR:CD1	2.32	0.64
1:B:549:ARG:HH22	4:B:1:IP2:C3	2.11	0.64
1:B:657:ILE:HD13	1:B:671:GLN:CB	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ASP:HB3	5:B:845:HOH:O	1.96	0.64
1:B:491:GLU:OE1	1:B:491:GLU:N	2.29	0.63
1:B:516:ALA:HB3	1:B:519:GLU:HG3	1.79	0.63
1:A:335:LYS:HE2	5:A:841:HOH:O	1.98	0.63
1:B:550:ILE:HD13	1:B:550:ILE:N	2.10	0.63
1:B:696:ASP:HB2	5:B:821:HOH:O	1.97	0.63
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.33	0.63
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.34	0.63
1:B:645:ASN:ND2	1:B:647:ASN:O	2.31	0.63
1:B:516:ALA:HB1	1:B:518:TYR:CE2	2.34	0.63
1:A:316:LEU:CD2	1:A:328:ALA:HB2	2.29	0.62
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.28	0.62
1:B:721:ILE:HG21	1:B:726:LEU:HD13	1.80	0.62
1:B:341:GLU:C	1:B:342:LEU:HD12	2.24	0.62
1:B:379:LYS:HE2	5:B:833:HOH:O	1.99	0.62
1:A:216:ARG:NH2	1:A:683:ARG:HH22	1.96	0.62
1:A:384:PRO:HG3	1:A:431:LEU:CB	2.30	0.62
1:B:705:GLU:C	1:B:716:ILE:HD12	2.25	0.62
1:A:218:PHE:CE1	1:A:272:LYS:HA	2.35	0.62
1:B:701:ARG:HH21	1:B:718:GLN:HG3	1.64	0.62
1:B:353:ILE:HD12	1:B:363:LYS:HG2	1.81	0.62
1:A:701:ARG:NH2	1:A:718:GLN:HG3	2.15	0.62
1:A:222:ALA:HB2	1:A:228:LEU:HD23	1.82	0.62
1:B:509:SER:N	1:B:510:PRO:HD2	2.15	0.61
1:A:259:GLU:CD	1:A:260:PRO:HD2	2.25	0.61
1:A:520:MET:HE3	1:A:549:ARG:CB	2.26	0.61
1:A:701:ARG:HH21	1:A:718:GLN:HG3	1.65	0.61
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.30	0.61
1:A:341:GLU:C	1:A:342:LEU:HD12	2.25	0.61
1:B:267:GLN:O	1:B:269:GLN:HG3	2.01	0.61
1:A:728:GLN:NE2	1:A:754:ILE:N	2.47	0.61
1:B:196:LEU:HB3	1:B:201:ILE:HD11	1.80	0.61
1:A:672:THR:HG22	1:A:688:PHE:CZ	2.37	0.60
1:B:515:GLN:HE21	1:B:542:HIS:HE1	1.49	0.60
1:A:675:ILE:HD13	1:A:684:TRP:CD1	2.36	0.60
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.32	0.60
1:B:227:THR:HG21	1:B:269:GLN:CD	2.27	0.60
1:A:672:THR:HG22	1:A:688:PHE:HZ	1.66	0.60
1:A:227:THR:HG21	1:A:269:GLN:CD	2.26	0.60
1:A:711:SER:OG	1:A:712:LYS:N	2.33	0.60
1:B:376:TYR:N	5:B:887:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:ILE:HD13	1:B:671:GLN:HB3	1.84	0.59
1:B:327:GLU:OE2	1:B:331:ARG:HB2	2.02	0.59
1:A:364:ILE:HD12	1:A:369:VAL:HG23	1.82	0.59
1:A:259:GLU:OE1	1:A:270:MET:HA	2.02	0.59
1:A:616:ASN:OD1	1:A:618:ARG:HB2	2.02	0.59
1:A:395:LEU:O	1:A:399:ARG:HG3	2.03	0.59
1:A:730:TYR:CZ	1:A:751:LYS:HD3	2.38	0.59
1:B:515:GLN:NE2	1:B:542:HIS:HE1	2.01	0.59
1:A:573:GLN:H	1:A:573:GLN:HE21	1.51	0.59
1:A:739:ASN:HB2	1:A:741:ASP:OD2	2.02	0.59
1:B:183:LYS:HG2	1:B:184:ILE:HD13	1.84	0.59
1:B:184:ILE:HD13	1:B:184:ILE:N	2.16	0.58
1:B:364:ILE:HD12	1:B:369:VAL:CG2	2.33	0.58
1:A:263:THR:HG22	1:A:264:ALA:N	2.18	0.58
1:A:504:PHE:HD2	1:A:527:ARG:NH2	2.01	0.58
1:B:421:VAL:HG11	1:B:426:PRO:HD3	1.84	0.58
1:A:296:GLN:HG3	1:A:596:ASN:CG	2.29	0.58
1:A:621:THR:C	1:B:445:LEU:HD22	2.27	0.58
1:A:651:ILE:HG22	1:A:652:VAL:N	2.17	0.58
1:A:655:LYS:NZ	1:A:671:GLN:OE1	2.29	0.58
1:A:728:GLN:HE21	1:A:753:SER:HA	1.68	0.58
1:A:686:MET:HG3	1:A:687:GLU:N	2.17	0.58
1:A:623:GLY:HA3	1:A:625:TRP:CZ2	2.38	0.58
1:A:502:VAL:HG21	1:A:519:GLU:HB3	1.86	0.58
1:A:723:TRP:N	5:A:823:HOH:O	2.37	0.58
1:B:520:MET:HG3	1:B:547:LEU:O	2.04	0.58
1:A:401:MET:CE	1:A:492:LEU:HD11	2.24	0.57
1:B:300:GLN:O	1:B:427:SER:HA	2.05	0.57
1:A:216:ARG:HH21	1:A:683:ARG:NH2	1.99	0.57
1:A:251:ALA:O	1:A:255:ILE:HG13	2.04	0.57
1:A:617:SER:HB3	5:A:866:HOH:O	2.04	0.57
1:A:651:ILE:HG21	1:A:677:ASN:C	2.30	0.57
1:B:272:LYS:O	1:B:275:PHE:HB3	2.04	0.57
1:B:645:ASN:C	1:B:647:ASN:H	2.10	0.57
1:B:686:MET:HG3	1:B:687:GLU:N	2.19	0.57
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.68	0.57
1:A:549:ARG:C	1:A:550:ILE:HD13	2.29	0.57
1:B:729:GLY:O	1:B:751:LYS:HA	2.05	0.57
1:A:657:ILE:HD13	1:A:671:GLN:HB2	1.87	0.57
1:B:551:TYR:HB2	1:B:552:PRO:CD	2.34	0.57
1:A:359:THR:C	1:A:360:PHE:HD1	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ALA:HB1	1:A:518:TYR:CE2	2.41	0.56
1:A:657:ILE:HD13	1:A:671:GLN:CB	2.34	0.56
1:B:632:ARG:NH2	1:B:755:GLN:NE2	2.53	0.56
1:B:172:LEU:O	1:B:174:ILE:N	2.38	0.56
1:B:549:ARG:O	1:B:550:ILE:HD13	2.04	0.56
1:A:730:TYR:C	1:A:731:ARG:HG2	2.30	0.56
1:B:197:GLU:O	1:B:201:ILE:HG12	2.05	0.56
1:B:218:PHE:CE1	1:B:272:LYS:HA	2.41	0.56
1:B:549:ARG:NH1	1:B:549:ARG:HG2	2.20	0.56
1:A:289:LEU:HD12	1:A:289:LEU:O	2.05	0.56
1:A:327:GLU:HA	1:A:327:GLU:OE1	2.06	0.56
1:A:593:PHE:O	1:A:598:GLY:HA2	2.06	0.56
1:A:622:GLN:CB	1:B:445:LEU:HD13	2.33	0.56
1:A:398:GLN:O	1:A:401:MET:HB2	2.06	0.56
1:A:241:GLN:HB3	1:A:731:ARG:NH2	2.20	0.55
1:A:299:ASP:O	1:A:427:SER:HB3	2.06	0.55
1:B:730:TYR:CD1	1:B:751:LYS:HD3	2.41	0.55
1:A:253:SER:HB2	1:A:257:ARG:HH21	1.71	0.55
1:B:704:VAL:O	1:B:716:ILE:HB	2.06	0.55
1:A:207:MET:CE	1:A:210:GLN:HB3	2.30	0.55
1:A:686:MET:HE3	1:A:687:GLU:O	2.06	0.55
1:A:491:GLU:OE1	1:A:491:GLU:N	2.36	0.55
1:A:259:GLU:OE2	1:A:260:PRO:HD2	2.06	0.55
1:A:549:ARG:NH1	1:A:549:ARG:HG2	2.20	0.55
1:B:241:GLN:HE21	1:B:241:GLN:N	2.05	0.55
1:B:253:SER:HB2	1:B:257:ARG:HH21	1.72	0.55
1:A:693:THR:C	1:A:695:PRO:HD2	2.31	0.55
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.35	0.54
1:B:327:GLU:OE2	1:B:331:ARG:HD2	2.07	0.54
1:B:384:PRO:HG3	1:B:431:LEU:HB2	1.89	0.54
1:B:642:PRO:HD2	1:B:716:ILE:CG2	2.37	0.54
1:A:756:ASP:OD1	1:A:756:ASP:N	2.40	0.54
1:B:391:ASN:HD21	1:B:398:GLN:CD	2.15	0.54
1:B:393:CYS:N	5:B:871:HOH:O	2.41	0.54
1:B:409:LEU:HD13	1:B:409:LEU:N	2.23	0.54
1:B:184:ILE:HG22	1:B:204:PHE:CE1	2.43	0.54
1:B:213:GLU:HG2	1:B:214:ILE:N	2.22	0.54
1:B:418:LEU:HB2	1:B:421:VAL:HG21	1.90	0.54
1:B:296:GLN:HG3	1:B:596:ASN:ND2	2.23	0.54
1:A:523:PHE:O	1:A:550:ILE:HA	2.07	0.53
1:A:715:PHE:CE2	1:A:718:GLN:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:HB2	1:B:421:VAL:CG2	2.37	0.53
1:B:556:ARG:HG2	1:B:556:ARG:HH11	1.71	0.53
1:A:280:LEU:HD23	1:A:732:HIS:CE1	2.43	0.53
1:A:291:HIS:HD2	1:A:725:SER:OG	1.91	0.53
1:B:401:MET:CE	1:B:492:LEU:HD11	2.28	0.53
1:B:657:ILE:HD13	1:B:671:GLN:HB2	1.91	0.53
1:A:607:PHE:CE2	1:A:625:TRP:HB3	2.43	0.53
1:B:556:ARG:HG2	1:B:560:SER:OG	2.08	0.53
1:A:253:SER:HA	1:A:256:GLU:OE1	2.09	0.53
1:A:383:TYR:HB3	1:A:384:PRO:CD	2.38	0.53
1:B:311:HIS:CE1	1:B:312:ASN:HD22	2.26	0.53
1:B:356:HIS:ND1	1:B:359:THR:HG21	2.24	0.53
1:A:643:LYS:O	1:A:645:ASN:N	2.41	0.53
1:B:507:PHE:O	1:B:510:PRO:HG2	2.09	0.52
1:A:721:ILE:HG21	1:A:726:LEU:HD13	1.90	0.52
1:B:525:GLU:O	1:B:529:LEU:HG	2.08	0.52
1:B:607:PHE:CD2	1:B:625:TRP:HB3	2.45	0.52
1:A:252:LEU:O	1:A:256:GLU:HG3	2.10	0.52
1:A:556:ARG:HG2	1:A:556:ARG:NH1	2.14	0.52
1:B:395:LEU:O	1:B:399:ARG:HG3	2.08	0.52
1:A:607:PHE:CD2	1:A:625:TRP:HB3	2.44	0.52
1:A:622:GLN:HA	1:B:445:LEU:HD11	1.91	0.52
1:B:683:ARG:NH2	1:B:685:ASP:OD2	2.43	0.52
1:A:705:GLU:C	1:A:716:ILE:HD12	2.35	0.52
1:B:436:LEU:HD23	1:B:436:LEU:H	1.75	0.52
1:B:523:PHE:O	1:B:550:ILE:HA	2.10	0.52
1:A:729:GLY:O	1:A:751:LYS:HA	2.10	0.52
1:B:438:LYS:HG3	1:B:499:CYS:HB3	1.92	0.52
1:A:367:CYS:HB2	1:A:371:ARG:NH2	2.25	0.52
1:A:441:LYS:HG3	1:A:496:ILE:HB	1.92	0.52
1:B:346:ASP:OD1	1:B:393:CYS:HA	2.10	0.51
1:A:296:GLN:HG3	1:A:596:ASN:ND2	2.25	0.51
1:A:391:ASN:HD21	1:A:398:GLN:CD	2.18	0.51
1:A:401:MET:HE2	1:A:492:LEU:CD1	2.27	0.51
1:B:440:LYS:HA	5:B:770:HOH:O	2.09	0.51
1:B:607:PHE:CE2	5:B:821:HOH:O	2.47	0.51
1:A:300:GLN:O	1:A:427:SER:HA	2.11	0.51
1:A:360:PHE:CD1	1:A:360:PHE:N	2.79	0.51
1:B:593:PHE:O	1:B:598:GLY:HA2	2.10	0.51
1:B:707:TYR:O	1:B:708:ASP:OD1	2.29	0.51
1:A:227:THR:HG21	1:A:269:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:GLN:HB2	1:B:747:THR:OG1	2.10	0.51
1:A:342:LEU:HD12	1:A:342:LEU:N	2.25	0.51
1:A:708:ASP:N	1:A:713:ASN:OD1	2.37	0.51
1:B:234:VAL:HG23	1:B:251:ALA:HB2	1.93	0.51
1:B:632:ARG:NE	5:B:815:HOH:O	2.24	0.51
1:A:504:PHE:CE1	1:A:507:PHE:CE1	2.99	0.51
1:B:180:TYR:CE1	1:B:184:ILE:HG12	2.45	0.51
1:A:397:GLN:O	1:A:400:VAL:HB	2.11	0.50
1:A:706:ASP:HB3	1:A:714:ASP:HB2	1.93	0.50
1:B:169:LEU:O	1:B:172:LEU:O	2.29	0.50
1:B:183:LYS:O	1:B:187:GLU:HG3	2.11	0.50
1:B:350:GLN:HA	1:B:397:GLN:HE21	1.73	0.50
1:B:549:ARG:HG2	1:B:549:ARG:HH11	1.76	0.50
1:B:549:ARG:NH2	4:B:1:IP2:O3	2.44	0.50
1:B:647:ASN:CG	1:B:648:LYS:H	2.20	0.50
1:A:692:VAL:HG12	1:A:695:PRO:CD	2.35	0.50
1:B:240:GLN:HA	1:B:240:GLN:OE1	2.12	0.50
1:A:504:PHE:CZ	1:A:507:PHE:CE1	2.99	0.50
1:A:549:ARG:HG2	1:A:549:ARG:HH11	1.74	0.50
1:A:610:ASP:OD1	1:A:611:PRO:HD2	2.11	0.50
1:B:287:PHE:CE2	1:B:722:PRO:HD2	2.47	0.50
1:B:311:HIS:NE2	1:B:312:ASN:ND2	2.60	0.50
1:B:426:PRO:HB2	1:B:431:LEU:HD12	1.93	0.50
1:B:651:ILE:O	1:B:653:ASP:OD1	2.29	0.50
1:B:259:GLU:OE1	1:B:270:MET:HA	2.12	0.50
1:B:530:ARG:HH11	1:B:530:ARG:CG	2.19	0.50
1:B:398:GLN:O	1:B:401:MET:HB2	2.12	0.50
1:A:222:ALA:HB2	1:A:228:LEU:CD2	2.41	0.50
1:A:504:PHE:CD2	1:A:527:ARG:NH2	2.79	0.50
1:B:655:LYS:NZ	1:B:671:GLN:OE1	2.30	0.49
1:A:228:LEU:CD1	1:A:233:LEU:HA	2.42	0.49
1:A:405:LEU:HD23	1:A:409:LEU:CD2	2.42	0.49
1:A:520:MET:HG3	1:A:547:LEU:O	2.12	0.49
1:A:551:TYR:HB2	1:A:552:PRO:CD	2.40	0.49
1:B:189:ASP:OD1	1:B:191:SER:OG	2.30	0.49
1:B:375:ASP:C	5:B:887:HOH:O	2.54	0.49
1:A:409:LEU:HD13	1:A:409:LEU:N	2.27	0.49
1:A:497:ILE:CG2	1:A:498:TYR:CE1	2.96	0.49
1:B:263:THR:O	1:B:266:ALA:HB3	2.12	0.49
1:B:736:LEU:HD23	1:B:742:GLN:HA	1.92	0.49
1:A:537:ASN:ND2	1:A:613:THR:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:THR:HG21	1:B:269:GLN:OE1	2.12	0.49
1:B:411:PRO:O	1:B:434:LYS:NZ	2.45	0.49
1:B:573:GLN:H	1:B:573:GLN:HE21	1.61	0.49
1:B:702:PHE:CD2	1:B:733:VAL:HG21	2.48	0.49
1:A:426:PRO:HA	1:A:430:GLN:OE1	2.13	0.49
1:A:291:HIS:HA	1:A:295:TYR:CE2	2.48	0.49
1:A:218:PHE:CD1	1:A:272:LYS:HA	2.48	0.48
1:A:241:GLN:NE2	1:A:729:GLY:HA3	2.28	0.48
1:A:728:GLN:NE2	1:A:753:SER:HA	2.26	0.48
1:B:261:SER:O	1:B:265:LYS:HB2	2.13	0.48
1:B:434:LYS:HA	1:B:434:LYS:HD2	1.66	0.48
1:B:500:LYS:HE3	5:B:770:HOH:O	2.12	0.48
1:A:371:ARG:O	1:A:374:ARG:HB3	2.13	0.48
1:B:251:ALA:O	1:B:255:ILE:HG13	2.12	0.48
1:B:259:GLU:OE2	1:B:271:THR:HG23	2.13	0.48
1:A:356:HIS:HB3	1:A:359:THR:OG1	2.14	0.48
1:A:438:LYS:HA	1:A:499:CYS:HB2	1.94	0.48
1:A:622:GLN:HA	1:B:445:LEU:CD1	2.43	0.48
1:A:704:VAL:O	1:A:716:ILE:HB	2.13	0.48
1:A:755:GLN:HG2	1:A:756:ASP:N	2.22	0.48
1:B:395:LEU:HD22	1:B:489:VAL:CG1	2.43	0.48
1:B:509:SER:N	1:B:510:PRO:CD	2.76	0.48
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.48	0.48
1:A:507:PHE:CD1	1:A:542:HIS:ND1	2.81	0.48
1:B:221:ALA:CB	1:B:228:LEU:HD21	2.40	0.48
1:B:533:GLN:OE1	1:B:618:ARG:NH1	2.47	0.48
1:B:622:GLN:HG3	1:B:623:GLY:N	2.27	0.48
1:B:504:PHE:HD2	1:B:527:ARG:NH2	2.11	0.48
1:B:701:ARG:CZ	1:B:718:GLN:HG3	2.44	0.48
1:A:360:PHE:HD1	1:A:360:PHE:N	2.12	0.48
1:A:639:GLN:HB2	1:A:747:THR:OG1	2.13	0.48
1:B:244:GLU:C	1:B:246:ALA:H	2.20	0.48
1:B:418:LEU:HD12	1:B:426:PRO:HB3	1.95	0.48
1:B:284:GLY:O	1:B:731:ARG:HB3	2.14	0.48
1:B:395:LEU:HD22	1:B:489:VAL:HG12	1.96	0.48
1:B:241:GLN:CA	1:B:241:GLN:NE2	2.76	0.48
1:A:252:LEU:HD23	1:A:256:GLU:OE2	2.14	0.48
1:B:549:ARG:NH1	4:B:1:IP2:O43	2.46	0.48
1:A:280:LEU:HD23	1:A:732:HIS:ND1	2.29	0.47
1:B:168:PHE:O	1:B:171:GLU:HB2	2.14	0.47
1:B:426:PRO:HG2	1:B:431:LEU:CD1	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:PHE:CE2	1:B:625:TRP:HB3	2.49	0.47
1:B:721:ILE:CG2	1:B:726:LEU:HD13	2.44	0.47
1:A:202:GLU:O	1:A:206:LYS:N	2.29	0.47
1:A:522:SER:HA	1:A:549:ARG:O	2.13	0.47
1:B:169:LEU:HA	1:B:172:LEU:HD12	1.95	0.47
1:A:622:GLN:CA	1:B:445:LEU:HD13	2.44	0.47
1:B:291:HIS:HD2	1:B:725:SER:OG	1.96	0.47
1:B:371:ARG:O	1:B:374:ARG:HB3	2.13	0.47
1:A:743:HIS:HA	1:A:744:PRO:HD3	1.53	0.47
1:B:162:PHE:O	1:B:165:LEU:HB3	2.14	0.47
1:B:394:SER:O	1:B:398:GLN:HG3	2.14	0.47
1:B:542:HIS:C	1:B:542:HIS:CD2	2.92	0.47
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.73	0.47
1:B:162:PHE:CZ	1:B:182:ARG:HA	2.50	0.47
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.15	0.47
1:A:712:LYS:HB3	1:A:713:ASN:H	1.28	0.47
1:B:162:PHE:CZ	1:B:182:ARG:HB2	2.49	0.47
1:B:610:ASP:OD1	1:B:611:PRO:HD2	2.13	0.47
1:B:651:ILE:HG22	1:B:651:ILE:O	2.13	0.47
1:A:367:CYS:SG	1:A:371:ARG:NH2	2.88	0.47
1:B:587:ASP:HB3	1:B:718:GLN:NE2	2.30	0.47
1:A:530:ARG:CZ	1:A:530:ARG:HB2	2.30	0.47
1:A:623:GLY:HA3	1:A:625:TRP:CE2	2.50	0.47
1:A:670:ARG:HG3	1:A:690:PHE:CZ	2.50	0.47
1:B:610:ASP:O	1:B:612:ASN:N	2.48	0.47
1:A:200:GLU:O	1:A:203:THR:N	2.48	0.46
1:A:438:LYS:CG	1:A:499:CYS:HB3	2.43	0.46
1:A:651:ILE:N	1:A:651:ILE:CD1	2.78	0.46
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.14	0.46
1:B:733:VAL:HB	1:B:748:LEU:HB2	1.97	0.46
1:A:497:ILE:CD1	1:A:497:ILE:N	2.78	0.46
1:B:254:LEU:O	1:B:258:TYR:N	2.44	0.46
1:B:294:VAL:HA	1:B:596:ASN:OD1	2.15	0.46
1:B:311:HIS:CE1	1:B:312:ASN:ND2	2.82	0.46
1:B:623:GLY:HA3	1:B:625:TRP:CZ2	2.50	0.46
1:A:726:LEU:HD12	1:A:726:LEU:HA	1.46	0.46
1:B:280:LEU:HD23	1:B:732:HIS:ND1	2.31	0.46
1:B:509:SER:HB3	1:B:510:PRO:CD	2.46	0.46
1:B:549:ARG:HH22	4:B:1:IP2:H3	1.81	0.46
1:A:248:PRO:O	1:A:252:LEU:HB2	2.16	0.46
1:A:381:SER:HB2	1:A:599:CYS:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ILE:CG2	1:A:498:TYR:CD1	2.98	0.46
1:B:227:THR:CG2	1:B:269:GLN:HB3	2.46	0.46
1:B:384:PRO:HG3	1:B:431:LEU:CB	2.46	0.46
1:A:693:THR:OG1	1:A:694:VAL:HG23	2.16	0.46
1:B:207:MET:HE2	1:B:207:MET:HB3	1.87	0.46
1:B:316:LEU:CD2	1:B:328:ALA:HB2	2.43	0.46
1:A:213:GLU:HG3	1:A:749:PHE:CD2	2.50	0.46
1:A:261:SER:O	1:A:265:LYS:HB2	2.16	0.46
1:A:548:SER:N	1:A:573:GLN:NE2	2.46	0.46
1:B:241:GLN:NE2	1:B:241:GLN:HA	2.31	0.46
1:B:259:GLU:OE1	1:B:271:THR:N	2.43	0.46
1:A:492:LEU:HA	1:A:492:LEU:HD23	1.61	0.46
1:A:646:LYS:HD2	1:A:648:LYS:HE2	1.97	0.46
1:A:675:ILE:CD1	1:A:684:TRP:CD1	2.99	0.46
1:B:276:LEU:HD12	1:B:276:LEU:O	2.15	0.46
1:A:556:ARG:HH11	1:A:556:ARG:CG	2.18	0.46
1:A:694:VAL:N	1:A:695:PRO:HD2	2.30	0.46
1:A:507:PHE:CE1	1:A:542:HIS:ND1	2.79	0.45
1:B:270:MET:SD	1:B:275:PHE:HA	2.56	0.45
1:B:599:CYS:HA	5:B:771:HOH:O	2.16	0.45
1:A:516:ALA:CB	1:A:518:TYR:CZ	2.99	0.45
1:A:537:ASN:OD1	1:A:541:ARG:NE	2.41	0.45
1:A:548:SER:H	1:A:573:GLN:HE21	1.57	0.45
1:B:694:VAL:N	1:B:695:PRO:CD	2.79	0.45
1:A:311:HIS:HB2	1:A:576:ALA:HB1	1.97	0.45
1:A:349:ASN:O	1:A:350:GLN:HB2	2.15	0.45
1:A:539:PHE:O	1:A:542:HIS:HB3	2.16	0.45
1:B:497:ILE:CD1	1:B:497:ILE:N	2.79	0.45
1:B:702:PHE:O	1:B:718:GLN:HA	2.16	0.45
1:A:314:TYR:HB3	1:A:329:TYR:CE1	2.51	0.45
1:B:484:ASP:O	1:B:487:LYS:N	2.46	0.45
1:B:625:TRP:CD1	1:B:626:TRP:N	2.84	0.45
1:B:409:LEU:HD12	1:B:409:LEU:HA	1.52	0.45
1:B:520:MET:HE3	1:B:549:ARG:CB	2.36	0.45
1:B:530:ARG:HG3	1:B:530:ARG:NH1	2.23	0.45
1:A:252:LEU:HD23	1:A:256:GLU:CD	2.42	0.45
1:A:661:HIS:O	1:A:698:ALA:HA	2.17	0.45
1:B:388:SER:HA	1:B:438:LYS:HB3	1.99	0.45
1:B:396:GLU:OE1	1:B:396:GLU:HA	2.17	0.45
1:B:743:HIS:HA	1:B:744:PRO:HD3	1.59	0.45
1:A:291:HIS:HA	1:A:295:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ALA:CB	1:B:518:TYR:CZ	3.00	0.45
1:A:694:VAL:N	1:A:695:PRO:CD	2.79	0.45
1:B:227:THR:CG2	1:B:228:LEU:N	2.79	0.45
1:B:529:LEU:HD23	1:B:529:LEU:HA	1.74	0.45
1:B:661:HIS:O	1:B:698:ALA:HA	2.16	0.45
1:A:240:GLN:OE1	1:A:240:GLN:HA	2.16	0.45
1:A:314:TYR:CE1	1:A:315:LEU:HG	2.52	0.45
1:B:162:PHE:CZ	1:B:182:ARG:CA	2.99	0.45
1:B:495:MET:O	1:B:497:ILE:HD13	2.16	0.45
1:A:228:LEU:HD11	1:A:233:LEU:HA	1.99	0.44
1:B:305:TYR:CD1	1:B:305:TYR:N	2.84	0.44
1:A:314:TYR:CD1	1:A:315:LEU:HG	2.52	0.44
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.98	0.44
1:A:426:PRO:HG3	1:A:498:TYR:CE2	2.52	0.44
1:B:163:LYS:HA	1:B:166:LYS:HB2	1.99	0.44
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.52	0.44
1:A:228:LEU:CD1	1:A:233:LEU:CA	2.96	0.44
1:A:529:LEU:HA	1:A:529:LEU:HD23	1.65	0.44
1:A:681:ASN:N	1:A:682:PRO:CD	2.80	0.44
1:A:733:VAL:HB	1:A:748:LEU:HB2	2.00	0.44
1:B:561:ASN:OD1	1:B:578:ASN:N	2.30	0.44
1:A:227:THR:HG23	1:A:228:LEU:N	2.32	0.44
1:B:610:ASP:HA	1:B:611:PRO:HD3	1.54	0.44
1:A:694:VAL:HG12	1:A:694:VAL:O	2.17	0.44
1:B:730:TYR:C	1:B:731:ARG:HG2	2.42	0.44
1:A:657:ILE:HD13	1:A:671:GLN:HB3	1.99	0.44
1:A:715:PHE:HE2	1:A:718:GLN:HB2	1.81	0.44
1:B:165:LEU:CD1	1:B:204:PHE:CE2	3.00	0.44
1:B:212:ALA:O	1:B:215:ASP:HB2	2.18	0.44
1:A:542:HIS:CD2	1:A:546:CYS:HB2	2.52	0.44
1:B:184:ILE:HD12	1:B:184:ILE:HA	1.64	0.44
1:B:259:GLU:CD	1:B:271:THR:HG23	2.43	0.44
1:B:675:ILE:HD13	1:B:684:TRP:CD1	2.52	0.44
1:B:681:ASN:N	1:B:682:PRO:CD	2.81	0.44
1:A:622:GLN:HG3	1:A:623:GLY:N	2.32	0.44
1:A:241:GLN:N	1:A:241:GLN:HE21	2.15	0.43
1:A:651:ILE:CG2	1:A:652:VAL:N	2.80	0.43
1:B:210:GLN:HE21	1:B:210:GLN:HB2	1.55	0.43
1:B:537:ASN:OD1	1:B:541:ARG:NE	2.40	0.43
1:B:573:GLN:H	1:B:573:GLN:CD	2.26	0.43
1:A:405:LEU:HD23	1:A:409:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ILE:HG21	1:A:498:TYR:CE1	2.53	0.43
1:A:646:LYS:HA	1:A:646:LYS:HD3	1.46	0.43
1:B:196:LEU:HB3	1:B:201:ILE:HD13	1.94	0.43
1:A:301:PRO:HB3	1:A:425:LEU:O	2.18	0.43
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.17	0.43
1:A:517:PHE:CD1	1:A:517:PHE:C	2.96	0.43
1:A:645:ASN:O	1:A:646:LYS:O	2.35	0.43
1:A:706:ASP:N	1:A:714:ASP:O	2.38	0.43
1:B:517:PHE:CD1	1:B:517:PHE:C	2.96	0.43
1:A:278:TYR:O	1:A:281:SER:OG	2.32	0.43
1:A:497:ILE:HG22	1:A:498:TYR:CE1	2.54	0.43
1:A:651:ILE:CD1	1:A:677:ASN:HD21	2.24	0.43
1:B:297:ASP:CG	1:B:300:GLN:HE21	2.26	0.43
1:B:613:THR:HG22	1:B:615:PHE:H	1.83	0.43
1:B:659:GLU:OE1	1:B:701:ARG:HD3	2.18	0.43
1:A:498:TYR:CD1	1:A:498:TYR:N	2.85	0.43
1:B:295:TYR:CD1	1:B:295:TYR:C	2.96	0.43
1:B:610:ASP:C	1:B:612:ASN:N	2.76	0.43
1:B:723:TRP:CD1	1:B:723:TRP:C	2.97	0.43
1:A:227:THR:CG2	1:A:228:LEU:N	2.79	0.43
1:A:556:ARG:NH1	1:A:556:ARG:CG	2.79	0.43
1:B:397:GLN:O	1:B:400:VAL:HB	2.19	0.43
1:B:441:LYS:NZ	1:B:493:SER:O	2.51	0.43
1:B:734:HIS:HE1	5:B:777:HOH:O	2.00	0.43
1:B:735:LEU:O	1:B:743:HIS:HB2	2.19	0.43
1:A:409:LEU:HD12	1:A:409:LEU:HA	1.66	0.43
1:B:233:LEU:O	1:B:236:PHE:HB3	2.19	0.43
1:B:342:LEU:N	1:B:342:LEU:CD1	2.82	0.43
1:B:701:ARG:HG3	1:B:720:THR:OG1	2.18	0.43
1:B:441:LYS:HG3	1:B:496:ILE:HB	2.01	0.42
1:A:518:TYR:CD1	1:A:518:TYR:C	2.97	0.42
1:B:610:ASP:C	1:B:612:ASN:H	2.27	0.42
1:A:207:MET:SD	1:A:210:GLN:HB2	2.59	0.42
1:B:291:HIS:HA	1:B:295:TYR:CE2	2.55	0.42
1:B:654:PRO:HD2	1:B:675:ILE:O	2.20	0.42
1:B:556:ARG:HG2	1:B:556:ARG:NH1	2.34	0.42
1:B:739:ASN:HB2	1:B:741:ASP:OD2	2.19	0.42
1:A:207:MET:HE1	1:A:210:GLN:CB	2.33	0.42
1:A:432:LYS:HB3	1:A:432:LYS:HE3	1.91	0.42
1:A:496:ILE:N	1:A:496:ILE:HD13	2.34	0.42
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ILE:O	1:B:412:ILE:HG22	2.18	0.42
1:B:675:ILE:HD13	1:B:684:TRP:NE1	2.34	0.42
1:A:306:LEU:HA	1:A:306:LEU:HD23	1.69	0.42
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	3.08	0.42
1:A:429:GLU:OE1	1:A:432:LYS:HE2	2.18	0.42
1:A:504:PHE:CZ	1:A:506:GLY:CA	2.99	0.42
1:B:651:ILE:HA	1:B:651:ILE:HD13	1.59	0.42
1:A:405:LEU:HD13	1:A:437:LEU:HD11	2.01	0.42
1:A:542:HIS:CD2	1:A:542:HIS:C	2.97	0.42
1:B:502:VAL:HG21	1:B:519:GLU:HB3	2.00	0.42
1:B:530:ARG:CG	1:B:530:ARG:NH1	2.80	0.42
1:A:610:ASP:HA	1:A:611:PRO:HD3	1.55	0.42
1:A:628:PRO:HA	1:A:692:VAL:O	2.19	0.42
1:B:182:ARG:O	1:B:185:PHE:HB3	2.20	0.42
1:B:191:SER:HB2	1:B:193:THR:HG23	2.01	0.42
1:A:267:GLN:O	1:A:269:GLN:HG3	2.20	0.42
1:A:289:LEU:HD12	1:A:289:LEU:C	2.45	0.42
1:A:556:ARG:C	1:A:558:ASP:H	2.27	0.42
1:A:558:ASP:O	1:A:559:SER:HB2	2.19	0.42
1:B:281:SER:C	1:B:283:ASP:N	2.77	0.42
1:B:509:SER:H	1:B:510:PRO:HD2	1.83	0.42
1:B:653:ASP:O	1:B:674:VAL:HG13	2.20	0.42
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.49	0.42
1:A:608:LEU:HD23	1:A:608:LEU:HA	1.88	0.42
1:B:211:ARG:NE	1:B:213:GLU:OE2	2.47	0.42
1:A:207:MET:SD	1:A:210:GLN:CB	3.09	0.41
1:A:638:GLY:O	1:A:681:ASN:HA	2.20	0.41
1:B:162:PHE:HZ	1:B:182:ARG:HB2	1.85	0.41
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.80	0.41
1:A:349:ASN:O	1:A:349:ASN:OD1	2.38	0.41
1:A:631:LEU:HG	1:A:633:VAL:HG23	2.02	0.41
1:A:371:ARG:O	1:A:375:ASP:N	2.47	0.41
1:A:411:PRO:O	1:A:434:LYS:NZ	2.52	0.41
1:A:573:GLN:NE2	1:A:573:GLN:N	2.61	0.41
1:B:311:HIS:CD2	1:B:312:ASN:HD22	2.37	0.41
1:B:497:ILE:N	1:B:497:ILE:HD12	2.36	0.41
1:A:401:MET:HE3	1:A:401:MET:HB3	1.82	0.41
1:B:176:VAL:HG12	1:B:177:ASP:N	2.36	0.41
1:B:296:GLN:HG3	1:B:596:ASN:CG	2.44	0.41
1:B:732:HIS:NE2	1:B:749:PHE:CD1	2.89	0.41
1:A:344:CYS:O	1:A:392:HIS:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LEU:HB2	1:B:389:LEU:HD23	2.01	0.41
1:A:426:PRO:HD3	1:A:498:TYR:CE2	2.55	0.41
1:A:651:ILE:CD1	1:A:677:ASN:ND2	2.80	0.41
1:B:205:TYR:CD1	1:B:205:TYR:C	2.99	0.41
1:B:333:LEU:HD21	1:B:340:LEU:HD11	2.02	0.41
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.74	0.41
1:A:665:ARG:HD3	1:A:693:THR:HG21	2.01	0.41
1:B:169:LEU:O	1:B:172:LEU:HD12	2.21	0.41
1:B:542:HIS:CD2	1:B:546:CYS:HB2	2.56	0.41
1:B:678:ASN:HA	5:B:879:HOH:O	2.20	0.41
1:A:610:ASP:O	1:A:613:THR:OG1	2.29	0.41
1:A:652:VAL:H	1:A:652:VAL:HG23	1.53	0.41
1:B:162:PHE:CE1	1:B:182:ARG:HA	2.56	0.41
1:A:228:LEU:CD1	1:A:233:LEU:N	2.84	0.41
1:A:297:ASP:O	1:A:305:TYR:OH	2.32	0.41
1:A:413:LEU:HD12	1:A:414:LEU:H	1.86	0.41
1:A:426:PRO:CG	1:A:498:TYR:CE2	3.04	0.41
1:B:162:PHE:HD1	1:B:162:PHE:HA	1.73	0.41
1:B:311:HIS:HB2	1:B:576:ALA:HB1	2.02	0.41
1:B:391:ASN:N	5:B:830:HOH:O	2.40	0.41
1:B:405:LEU:HD13	1:B:437:LEU:HD11	2.02	0.41
1:B:651:ILE:CG2	1:B:677:ASN:CA	2.98	0.41
1:B:701:ARG:HD3	1:B:701:ARG:HH11	1.74	0.41
1:B:739:ASN:ND2	5:B:890:HOH:O	2.53	0.41
1:A:216:ARG:HG3	1:A:216:ARG:NH1	2.34	0.41
1:A:425:LEU:HD23	1:A:498:TYR:HD2	1.86	0.41
1:B:578:ASN:C	1:B:580:GLN:H	2.29	0.41
1:B:729:GLY:C	1:B:751:LYS:HD2	2.46	0.41
1:B:730:TYR:CZ	1:B:751:LYS:HD3	2.56	0.41
1:A:228:LEU:HD13	1:A:232:ARG:HB2	2.03	0.40
1:A:626:TRP:CD1	1:A:626:TRP:C	2.98	0.40
1:A:709:SER:OG	1:A:710:SER:N	2.54	0.40
1:B:187:GLU:OE1	1:B:207:MET:HE1	2.22	0.40
1:B:492:LEU:HA	1:B:492:LEU:HD23	1.74	0.40
1:B:507:PHE:CZ	1:B:531:LEU:HD22	2.56	0.40
1:B:573:GLN:CD	1:B:573:GLN:N	2.79	0.40
1:B:590:LEU:HD23	1:B:590:LEU:HA	1.78	0.40
1:B:715:PHE:HB2	5:B:850:HOH:O	2.20	0.40
1:A:321:THR:HG22	1:A:360:PHE:HB2	2.04	0.40
1:A:345:TRP:CE3	1:A:392:HIS:HB3	2.56	0.40
1:B:227:THR:HG21	1:B:269:GLN:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LYS:HE2	1:B:496:ILE:O	2.20	0.40
1:A:606:ALA:C	1:A:608:LEU:N	2.80	0.40
1:B:165:LEU:HD13	1:B:204:PHE:CE2	2.56	0.40
1:B:595:ASP:OD1	1:B:596:ASN:N	2.52	0.40
1:B:610:ASP:O	1:B:613:THR:OG1	2.35	0.40
1:A:342:LEU:HB2	1:A:389:LEU:HD23	2.04	0.40
1:A:616:ASN:C	1:A:618:ARG:N	2.79	0.40
1:A:622:GLN:CA	1:B:445:LEU:CD1	3.00	0.40
1:B:162:PHE:O	1:B:166:LYS:N	2.39	0.40
1:B:198:ASP:O	1:B:201:ILE:N	2.47	0.40
1:B:300:GLN:CB	1:B:301:PRO:CD	2.99	0.40
1:B:651:ILE:HG21	1:B:677:ASN:CG	2.47	0.40
1:B:254:LEU:HD12	1:B:254:LEU:HA	1.79	0.40
1:B:638:GLY:O	1:B:681:ASN:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/624 (82%)	449 (88%)	51 (10%)	9 (2%)	6	19
1	B	557/624 (89%)	485 (87%)	65 (12%)	7 (1%)	9	26
All	All	1066/1248 (85%)	934 (88%)	116 (11%)	16 (2%)	8	23

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	VAL
1	A	646	LYS
1	A	712	LYS
1	B	173	ASN

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Mol	Chain	Res	Type
1	B	645	ASN
1	A	644	VAL
1	B	647	ASN
1	B	649	ASN
1	A	219	GLU
1	A	263	THR
1	B	512	THR
1	A	579	PHE
1	A	713	ASN
1	B	417	PRO
1	A	744	PRO
1	B	648	LYS

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	444/545 (82%)	372 (84%)	72 (16%)	2	7
1	B	492/545 (90%)	408 (83%)	84 (17%)	2	5
All	All	936/1090 (86%)	780 (83%)	156 (17%)	2	6

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	PHE
1	A	207	MET
1	A	209	THR
1	A	210	GLN
1	A	211	ARG
1	A	219	GLU
1	A	220	GLU
1	A	227	THR
1	A	228	LEU
1	A	231	GLU
1	A	242	ARG

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Mol	Chain	Res	Type
1	A	252	LEU
1	A	253	SER
1	A	254	LEU
1	A	257	ARG
1	A	277	MET
1	A	293	ARG
1	A	296	GLN
1	A	300	GLN
1	A	309	SER
1	A	310	SER
1	A	344	CYS
1	A	362	SER
1	A	381	SER
1	A	388	SER
1	A	396	GLU
1	A	409	LEU
1	A	414	LEU
1	A	418	LEU
1	A	424	SER
1	A	432	LYS
1	A	436	LEU
1	A	438	LYS
1	A	441	LYS
1	A	487	LYS
1	A	489	VAL
1	A	497	ILE
1	A	502	VAL
1	A	513	SER
1	A	526	SER
1	A	530	ARG
1	A	535	SER
1	A	539	PHE
1	A	556	ARG
1	A	563	SER
1	A	573	GLN
1	A	610	ASP
1	A	612	ASN
1	A	617	SER
1	A	621	THR
1	A	632	ARG
1	A	643	LYS
1	A	644	VAL

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Mol	Chain	Res	Type
1	A	646	LYS
1	A	648	LYS
1	A	651	ILE
1	A	652	VAL
1	A	655	LYS
1	A	657	ILE
1	A	671	GLN
1	A	676	THR
1	A	677	ASN
1	A	685	ASP
1	A	710	SER
1	A	711	SER
1	A	727	LYS
1	A	728	GLN
1	A	738	LYS
1	A	743	HIS
1	A	745	SER
1	A	753	SER
1	A	756	ASP
1	B	159	LYS
1	B	160	MET
1	B	162	PHE
1	B	165	LEU
1	B	166	LYS
1	B	171	GLU
1	B	172	LEU
1	B	176	VAL
1	B	178	ASP
1	B	184	ILE
1	B	186	ARG
1	B	194	ASP
1	B	201	ILE
1	B	210	GLN
1	B	211	ARG
1	B	227	THR
1	B	230	VAL
1	B	234	VAL
1	B	238	GLN
1	B	242	ARG
1	B	253	SER
1	B	254	LEU
1	B	257	ARG

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Mol	Chain	Res	Type
1	B	261	SER
1	B	262	GLU
1	B	263	THR
1	B	293	ARG
1	B	296	GLN
1	B	298	MET
1	B	300	GLN
1	B	309	SER
1	B	310	SER
1	B	331	ARG
1	B	344	CYS
1	B	362	SER
1	B	388	SER
1	B	409	LEU
1	B	414	LEU
1	B	423	THR
1	B	432	LYS
1	B	436	LEU
1	B	441	LYS
1	B	486	LEU
1	B	488	LEU
1	B	489	VAL
1	B	497	ILE
1	B	502	VAL
1	B	508	SER
1	B	526	SER
1	B	530	ARG
1	B	535	SER
1	B	545	SER
1	B	550	ILE
1	B	563	SER
1	B	573	GLN
1	B	577	LEU
1	B	613	THR
1	B	614	THR
1	B	617	SER
1	B	618	ARG
1	B	621	THR
1	B	646	LYS
1	B	648	LYS
1	B	651	ILE
1	B	652	VAL

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Mol	Chain	Res	Type
1	B	655	LYS
1	B	657	ILE
1	B	659	GLU
1	B	665	ARG
1	B	671	GLN
1	B	675	ILE
1	B	676	THR
1	B	677	ASN
1	B	685	ASP
1	B	687	GLU
1	B	689	GLU
1	B	709	SER
1	B	710	SER
1	B	715	PHE
1	B	727	LYS
1	B	738	LYS
1	B	743	HIS
1	B	753	SER
1	B	755	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	291	HIS
1	A	312	ASN
1	A	349	ASN
1	A	573	GLN
1	A	612	ASN
1	A	639	GLN
1	A	645	ASN
1	A	718	GLN
1	A	728	GLN
1	A	743	HIS
1	A	755	GLN
1	B	210	GLN
1	B	241	GLN
1	B	291	HIS
1	B	312	ASN
1	B	319	GLN
1	B	349	ASN
1	B	542	HIS

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Mol	Chain	Res	Type
1	B	573	GLN
1	B	639	GLN
1	B	718	GLN
1	B	728	GLN
1	B	734	HIS
1	B	739	ASN
1	B	743	HIS
1	B	755	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	IP2	B	1	2	20,20,20	2.19	8 (40%)	32,32,32	2.00	11 (34%)
3	ACT	B	5	-	3,3,3	1.03	0	3,3,3	1.00	0
3	ACT	A	5	-	3,3,3	0.97	0	3,3,3	0.91	0
4	IP2	A	1	2	20,20,20	2.16	9 (45%)	32,32,32	1.63	8 (25%)

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
4	IP2	B	1	2	-	1/10/34/34	0/1/1/1
4	IP2	A	1	2	-	1/10/34/34	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	IP2	P4-O4	4.65	1.67	1.59
4	A	1	IP2	P4-O4	4.25	1.67	1.59
4	B	1	IP2	P4-O41	4.12	1.63	1.50
4	A	1	IP2	P5-O51	3.88	1.62	1.50
4	A	1	IP2	P4-O41	3.82	1.62	1.50
4	B	1	IP2	P5-O51	3.72	1.62	1.50
4	A	1	IP2	C5-C4	2.75	1.57	1.52
4	B	1	IP2	P5-O5	2.58	1.64	1.59
4	A	1	IP2	P5-O5	2.43	1.63	1.59
4	B	1	IP2	P5-O52	2.33	1.63	1.54
4	A	1	IP2	C6-C5	2.30	1.58	1.52
4	B	1	IP2	P5-O53	2.28	1.63	1.54
4	B	1	IP2	P4-O42	2.22	1.63	1.54
4	A	1	IP2	P5-O53	2.19	1.62	1.54
4	B	1	IP2	P4-O43	2.18	1.62	1.54
4	A	1	IP2	P4-O43	2.08	1.62	1.54
4	A	1	IP2	P5-O52	2.05	1.62	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	IP2	C3-C2-C1	4.65	119.00	110.83
4	B	1	IP2	O1-C1-C2	-4.24	100.39	110.38
4	B	1	IP2	C1-C6-C5	3.81	118.32	109.68
4	A	1	IP2	O2-C2-C1	-3.61	101.86	110.38
4	B	1	IP2	O2-C2-C1	-3.30	102.60	110.38
4	A	1	IP2	C1-C6-C5	3.19	116.92	109.68
4	A	1	IP2	C3-C2-C1	-3.10	105.39	110.83
4	B	1	IP2	O3-C3-C2	-2.89	103.55	110.38
4	B	1	IP2	O5-C5-C4	-2.76	102.89	108.76
4	B	1	IP2	C2-C3-C4	2.71	115.84	109.68
4	A	1	IP2	C6-C5-C4	2.71	117.82	111.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	IP2	P4-O4-C4	2.50	130.12	123.43
4	A	1	IP2	O4-C4-C5	2.48	114.04	108.76
4	B	1	IP2	O4-C4-C3	2.45	113.93	108.73
4	B	1	IP2	O3-C3-C4	-2.39	103.82	109.94
4	B	1	IP2	P5-O5-C5	2.34	129.67	123.43
4	A	1	IP2	O4-C4-C3	2.24	113.48	108.73
4	A	1	IP2	P4-O4-C4	2.06	128.93	123.43
4	A	1	IP2	O3-C3-C2	2.05	115.21	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

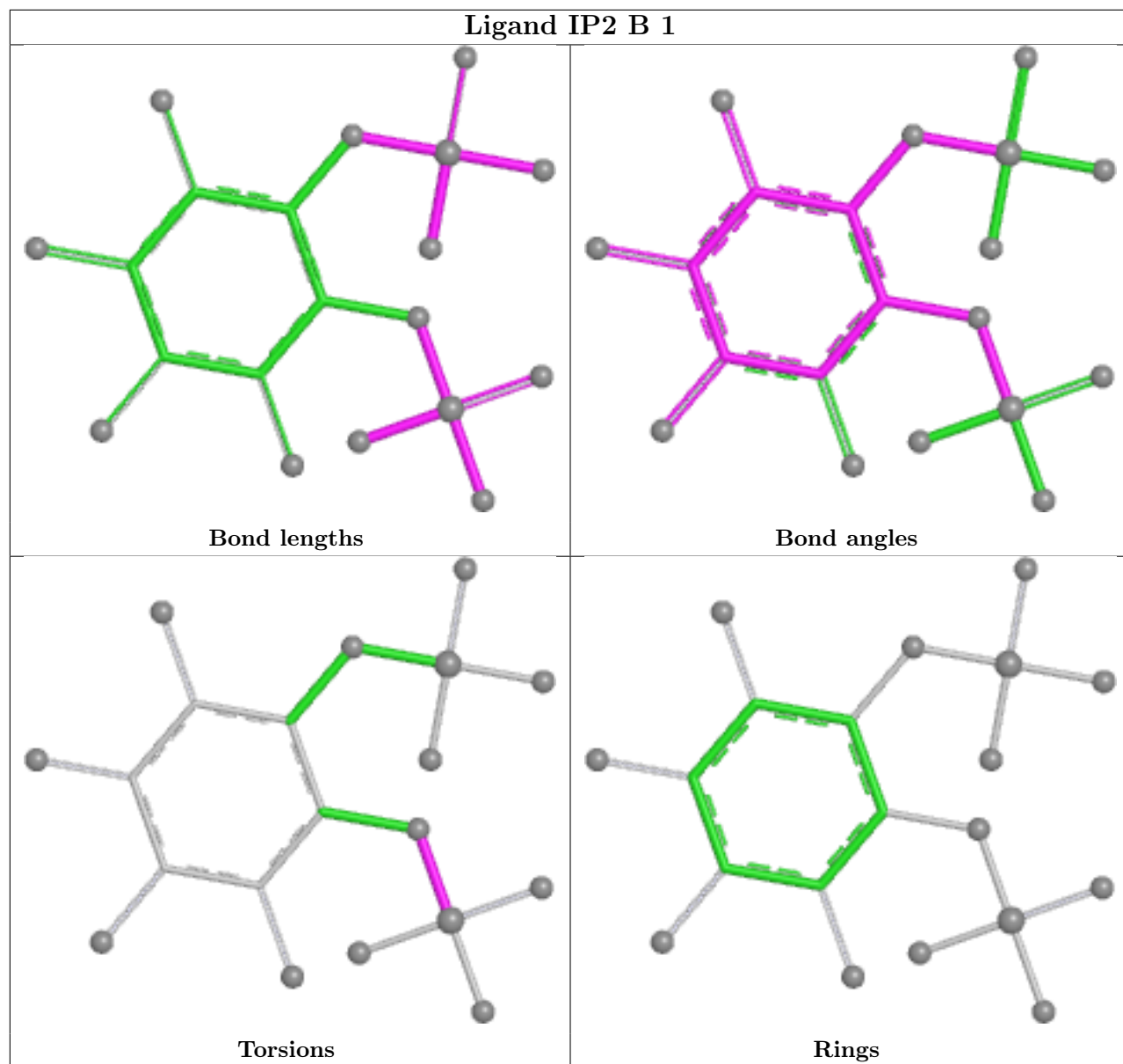
Mol	Chain	Res	Type	Atoms
4	A	1	IP2	C6-C5-O5-P5
4	B	1	IP2	C5-O5-P5-O53

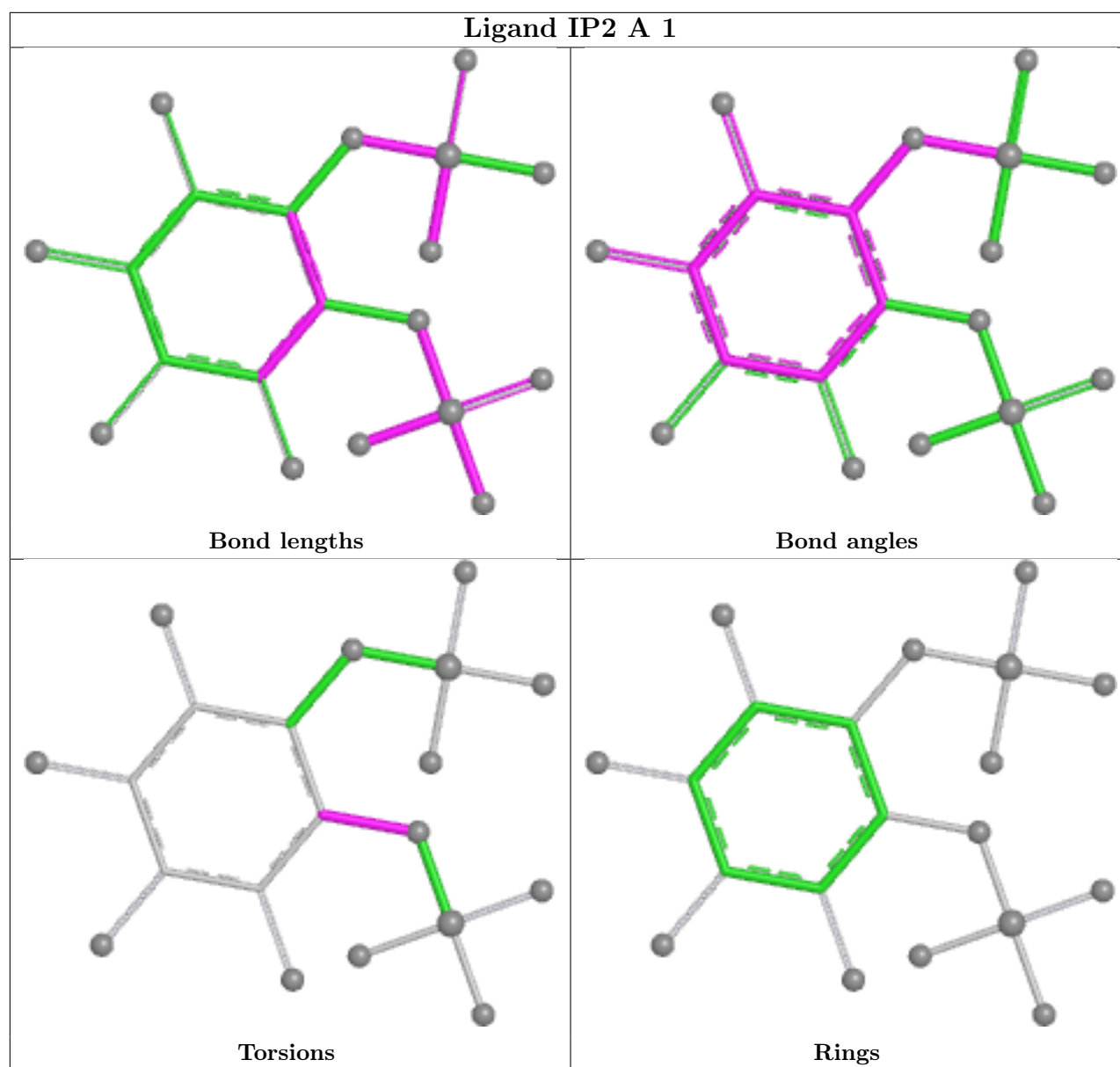
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	IP2	4	0
4	A	1	IP2	3	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 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	508/624 (81%)	-0.48	13 (2%)	57 49	4, 22, 77, 127	14 (2%)
1	B	558/624 (89%)	-0.47	15 (2%)	56 48	4, 23, 74, 118	23 (4%)
All	All	1066/1248 (85%)	-0.48	28 (2%)	57 49	4, 23, 76, 127	37 (3%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	LYS	6.2
1	B	514	GLY	5.7
1	B	649	ASN	5.0
1	A	201	ILE	4.7
1	A	647	ASN	4.2
1	A	203	THR	3.8
1	B	164	GLU	3.7
1	A	202	GLU	3.4
1	B	170	LYS	3.3
1	B	160	MET	3.2
1	A	645	ASN	3.1
1	A	207	MET	3.0
1	B	510	PRO	3.0
1	A	710	SER	3.0
1	A	200	GLU	2.9
1	B	647	ASN	2.9
1	A	711	SER	2.8
1	B	648	LYS	2.8
1	A	712	LYS	2.7
1	B	158	ASN	2.7
1	B	508	SER	2.6
1	B	645	ASN	2.6
1	B	710	SER	2.3
1	B	266	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	708	ASP	2.2
1	A	420	GLY	2.2
1	B	484	ASP	2.0
1	B	756	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

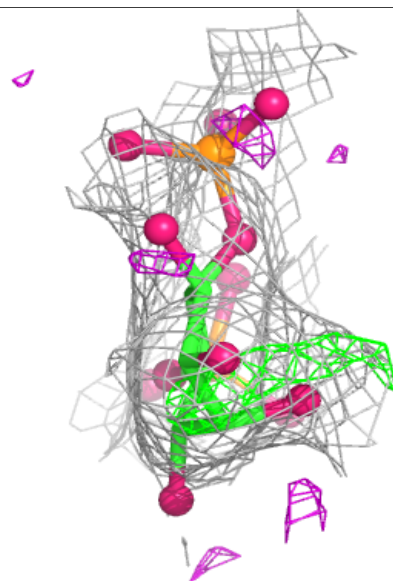
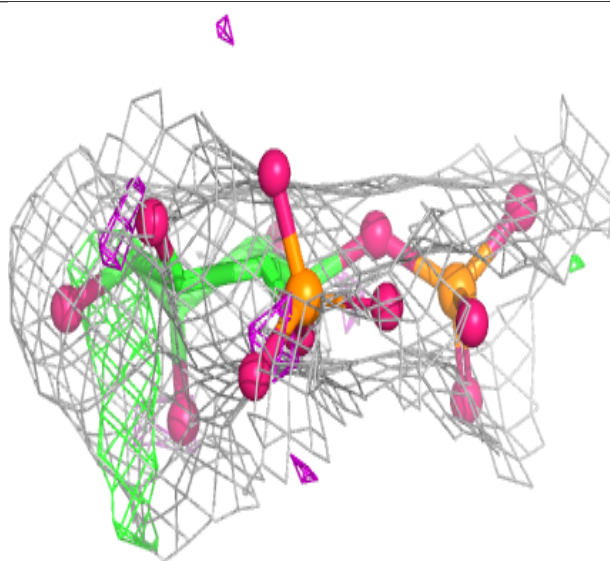
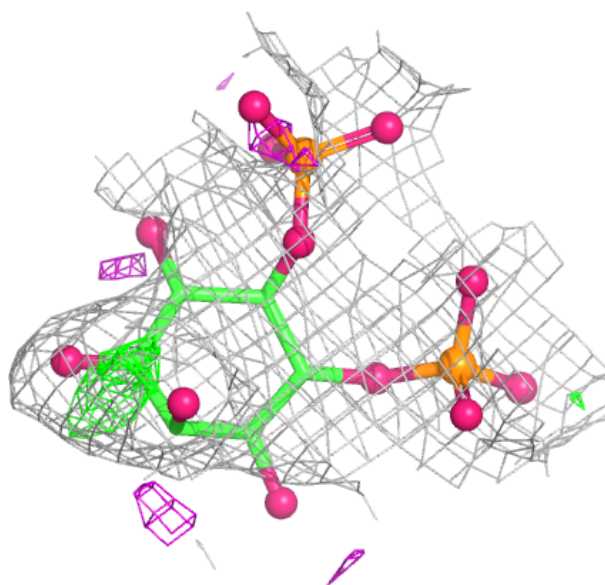
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IP2	A	1	20/20	0.84	0.16	70,97,136,136	0
4	IP2	B	1	20/20	0.84	0.12	53,74,108,110	0
3	ACT	A	5	4/4	0.92	0.11	36,38,38,39	0
2	CA	A	2	1/1	0.92	0.05	59,59,59,59	0
2	CA	B	3	1/1	0.92	0.04	74,74,74,74	0
2	CA	A	3	1/1	0.94	0.07	66,66,66,66	0
3	ACT	B	5	4/4	0.97	0.06	25,26,27,29	0
2	CA	B	2	1/1	0.99	0.02	37,37,37,37	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.

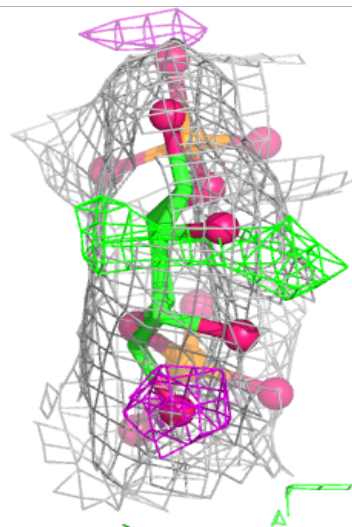
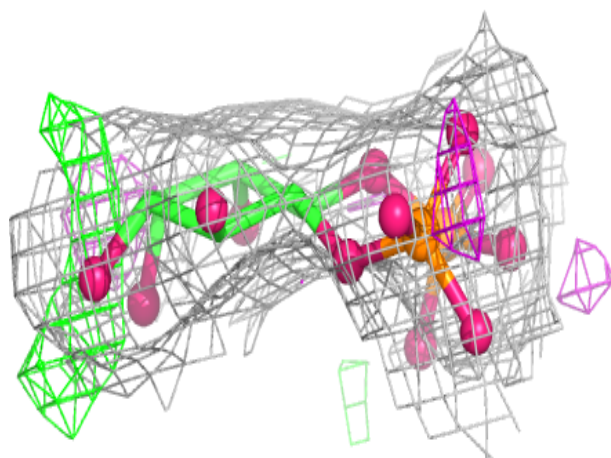
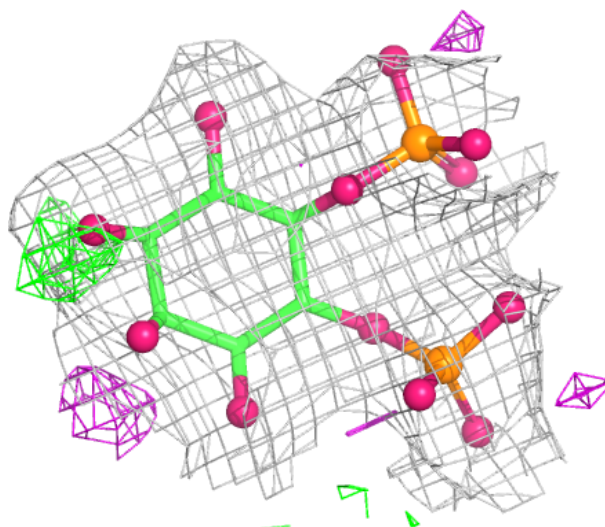
Electron density around IP2 A 1:

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



Electron density around IP2 B 1:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.