



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:46 PM UTC

PDB ID : 1SJD / pdb_00001sjd
Title : x-ray structure of o-succinylbenzoate synthase complexed with n-succinyl phenylglycine
Authors : Thoden, J.B.; Taylor-Ringia, E.A.; Garrett, J.B.; Gerlt, J.A.; Holden, H.M.; Rayment, I.
Deposited on : 2004-03-03
Resolution : 1.87 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

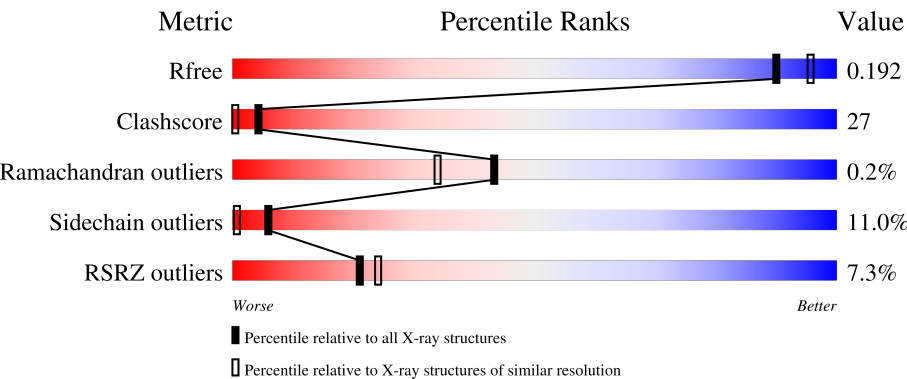
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	368	3% 58%33%8%
1	B	368	% 70%24%5%
1	C	368	2% 66%28%6%
1	D	368	23% 48%38%12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NPG	D	1500	-	-	X	-

2 Entry composition [i](#)

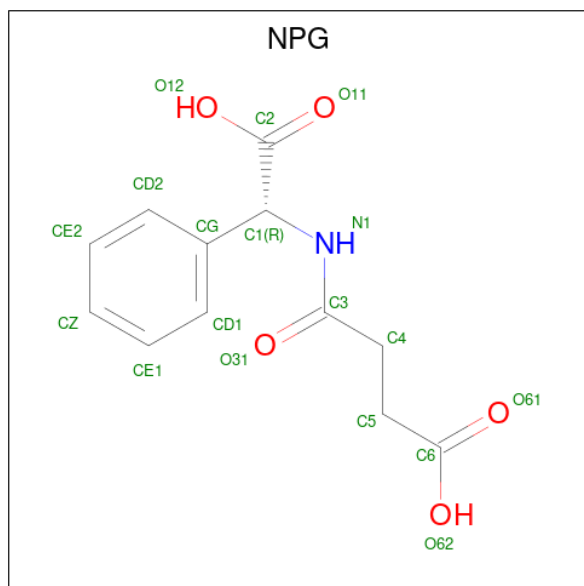
There are 3 unique types of molecules in this entry. The entry contains 12337 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-acylamino acid racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2765	1758	480	515	12			
1	B	368	Total	C	N	O	S	0	0	0
			2772	1761	481	518	12			
1	C	367	Total	C	N	O	S	0	0	0
			2765	1758	480	515	12			
1	D	367	Total	C	N	O	S	0	0	0
			2765	1758	480	515	12			

- Molecule 2 is N-SUCCINYL PHENYLGLYCINE (CCD ID: NPG) (formula: C₁₂H₁₃NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	12	1	5		
2	B	1	Total	C	N	O	0	0
			18	12	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			18	12	1	5		
2	C	1	Total	C	N	O	0	0
			18	12	1	5		
2	C	1	Total	C	N	O	0	0
			18	12	1	5		
2	D	1	Total	C	N	O	0	0
			18	12	1	5		

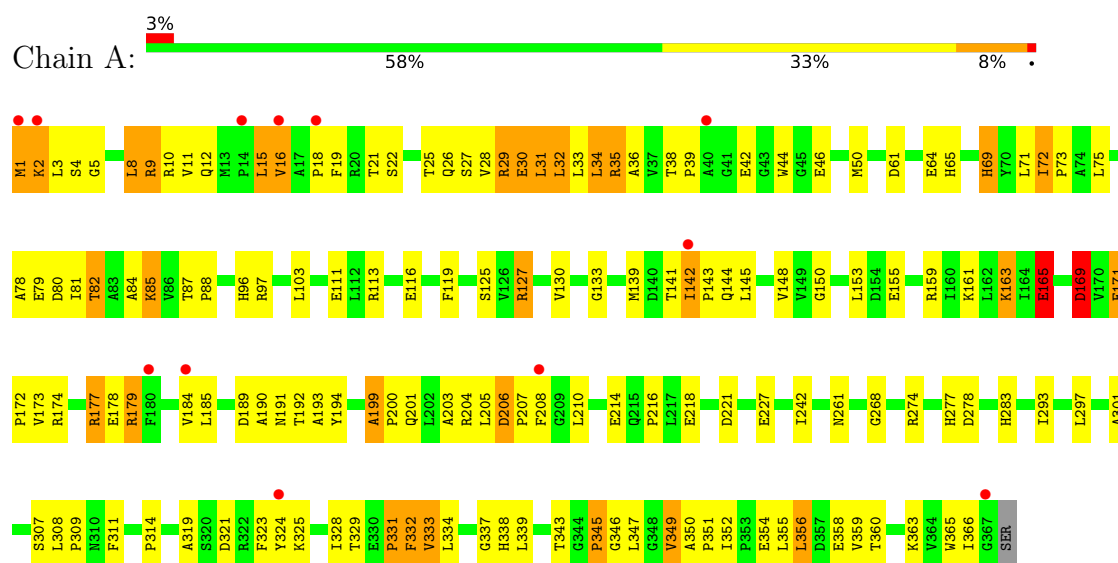
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	261	Total	O	0	0
			261	261		
3	B	375	Total	O	0	0
			375	375		
3	C	336	Total	O	0	0
			336	336		
3	D	190	Total	O	0	0
			190	190		

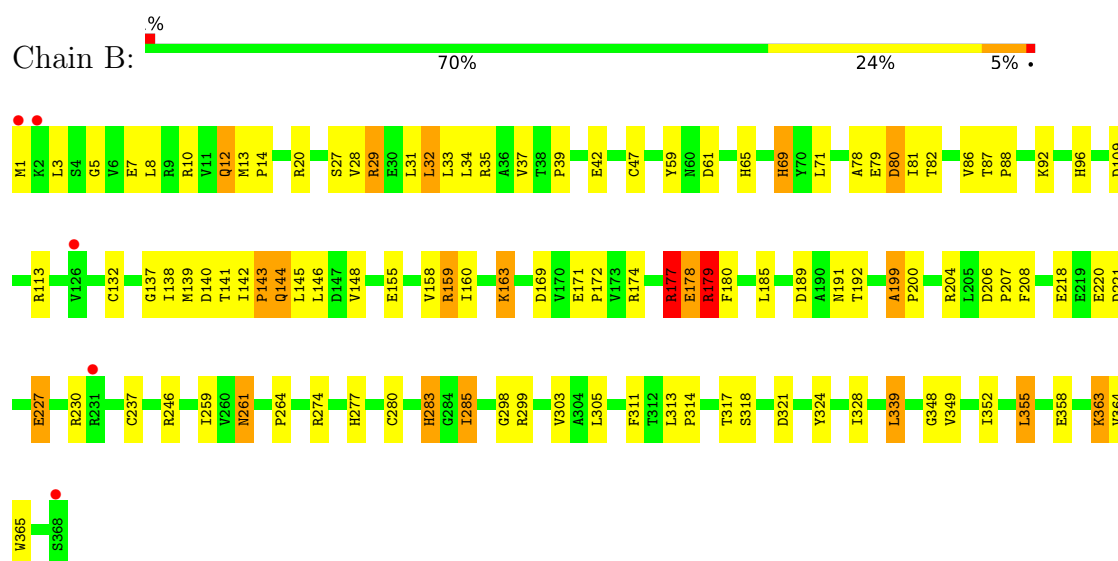
3 Residue-property plots

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: N-acylamino acid racemase



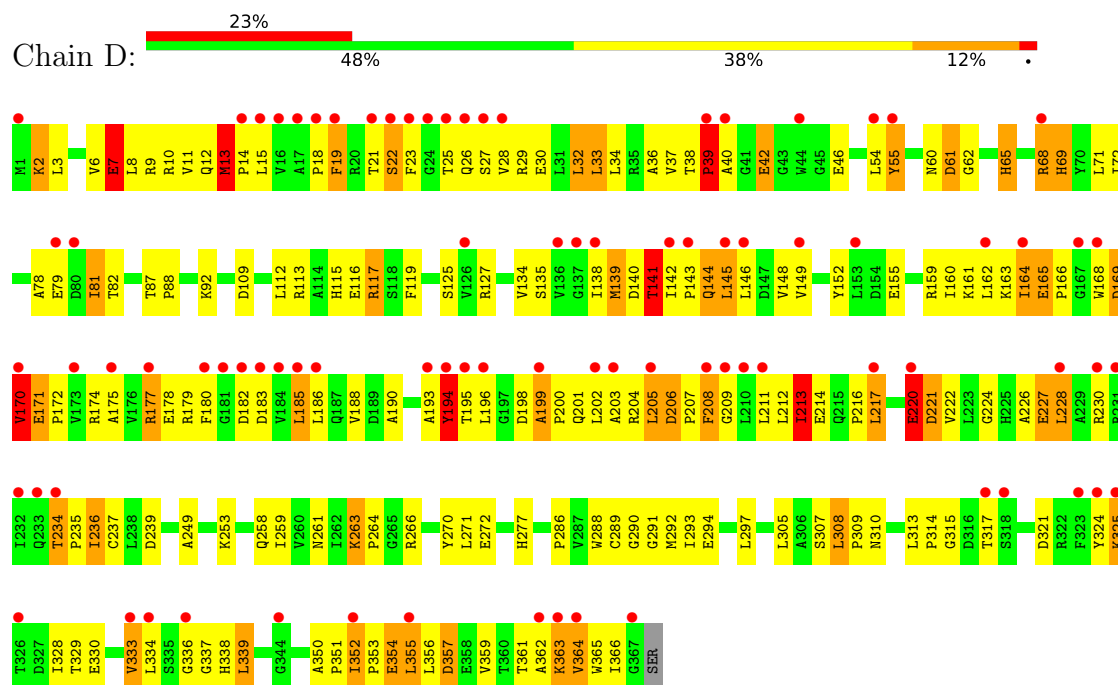
• Molecule 1: N-acylamino acid racemase



• Molecule 1: N-acylamino acid racemase



• Molecule 1: N-acylamino acid racemase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	215.20Å 215.20Å 257.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.87 50.00 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-1.87) 99.7 (50.00-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 1.87Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.196 , 0.241 0.193 , 0.192	Depositor DCC
R_{free} test set	18681 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 124.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k- 2/3*l,2/3*h-2/3*k+1/3*l 0.014 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3* k+1/3*l 0.011 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3* *k+1/3*l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12337	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.10	0/2821	1.57	29/3842 (0.8%)
1	B	1.10	0/2828	1.52	24/3850 (0.6%)
1	C	1.12	1/2821 (0.0%)	1.58	30/3842 (0.8%)
1	D	1.17	2/2821 (0.1%)	1.72	49/3842 (1.3%)
All	All	1.12	3/11291 (0.0%)	1.60	132/15376 (0.9%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	ILE	CA-CB	-5.86	1.51	1.54
1	D	7	GLU	N-CA	-5.45	1.39	1.46
1	D	220	GLU	CD-OE2	5.43	1.35	1.25

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	PRO	CA-C-N	13.13	138.27	120.54
1	D	39	PRO	C-N-CA	13.13	138.27	120.54
1	B	352	ILE	CA-C-O	8.44	124.13	119.15
1	A	242	ILE	N-CA-C	8.10	114.87	106.21
1	D	221	ASP	N-CA-C	7.84	121.58	110.68
1	D	6	VAL	CA-C-N	-7.75	112.20	123.05
1	D	6	VAL	C-N-CA	-7.75	112.20	123.05
1	D	55	TYR	N-CA-C	-7.67	102.25	111.69
1	D	72	ILE	CA-C-O	7.60	124.49	118.71
1	C	352	ILE	CA-C-N	7.59	129.33	119.84
1	C	352	ILE	C-N-CA	7.59	129.33	119.84
1	A	165	GLU	CB-CA-C	-7.33	98.62	109.97
1	D	290	GLY	CA-C-N	-7.13	117.26	122.18
1	D	290	GLY	C-N-CA	-7.13	117.26	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	HIS	CA-CB-CG	-7.02	106.78	113.80
1	A	19	PHE	CA-CB-CG	-7.01	106.79	113.80
1	A	221	ASP	N-CA-C	6.77	119.77	109.62
1	A	171	GLU	O-C-N	6.75	125.72	120.38
1	D	180	PHE	CA-CB-CG	-6.75	107.05	113.80
1	C	40	ALA	N-CA-C	6.72	118.69	111.36
1	A	130	VAL	O-C-N	6.71	125.92	121.69
1	D	314	PRO	N-CA-CB	6.68	109.28	103.27
1	C	93	PHE	CA-CB-CG	-6.66	107.14	113.80
1	B	314	PRO	CA-C-N	-6.62	114.76	122.77
1	B	314	PRO	C-N-CA	-6.62	114.76	122.77
1	B	208	PHE	CA-CB-CG	-6.62	107.18	113.80
1	D	308	LEU	CA-C-N	6.55	128.03	119.84
1	D	308	LEU	C-N-CA	6.55	128.03	119.84
1	B	13	MET	CA-C-N	6.54	126.30	119.76
1	B	13	MET	C-N-CA	6.54	126.30	119.76
1	D	206	ASP	CA-C-O	6.45	124.50	118.44
1	A	72	ILE	CA-C-O	6.44	123.01	118.69
1	D	183	ASP	CA-CB-CG	-6.30	106.30	112.60
1	A	206	ASP	CA-C-N	6.27	125.89	119.56
1	A	206	ASP	C-N-CA	6.27	125.89	119.56
1	D	333	VAL	N-CA-C	6.22	116.83	107.75
1	D	234	THR	O-C-N	6.22	126.59	121.31
1	C	308	LEU	CA-C-N	6.19	126.38	119.32
1	C	308	LEU	C-N-CA	6.19	126.38	119.32
1	A	325	LYS	N-CA-C	-6.19	104.45	111.07
1	B	285	ILE	CA-C-O	6.16	123.70	119.20
1	D	357	ASP	CA-CB-CG	-6.10	106.50	112.60
1	D	138	ILE	N-CA-CB	6.09	117.94	111.00
1	D	336	GLY	N-CA-C	-6.03	106.92	115.30
1	B	69	HIS	N-CA-C	6.03	120.63	113.28
1	C	36	ALA	CA-C-N	-6.02	115.25	123.14
1	C	36	ALA	C-N-CA	-6.02	115.25	123.14
1	A	199	ALA	CA-C-O	6.00	124.08	118.44
1	D	82	THR	N-CA-C	-5.99	100.19	109.24
1	A	71	LEU	N-CA-C	5.95	117.57	111.14
1	D	289	CYS	CA-C-N	5.94	126.60	120.60
1	D	289	CYS	C-N-CA	5.94	126.60	120.60
1	A	283	HIS	CA-CB-CG	-5.88	107.92	113.80
1	D	141	THR	N-CA-CB	-5.87	102.28	111.56
1	D	352	ILE	CA-C-N	5.83	125.30	119.24
1	D	352	ILE	C-N-CA	5.83	125.30	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	163	LYS	N-CA-CB	5.82	118.60	109.69
1	C	230	ARG	CD-NE-CZ	5.80	132.52	124.40
1	C	344	GLY	CA-C-N	5.78	125.69	119.85
1	C	344	GLY	C-N-CA	5.78	125.69	119.85
1	B	221	ASP	CA-CB-CG	-5.77	106.83	112.60
1	A	69	HIS	CA-CB-CG	-5.76	108.04	113.80
1	D	352	ILE	N-CA-C	-5.75	102.33	107.56
1	A	169	ASP	CA-C-N	5.69	127.94	120.60
1	A	169	ASP	C-N-CA	5.69	127.94	120.60
1	B	14	PRO	CB-CA-C	-5.69	103.64	111.21
1	D	208	PHE	N-CA-C	5.65	118.17	111.33
1	B	348	GLY	N-CA-C	-5.65	107.84	115.36
1	D	170	VAL	N-CA-CB	-5.65	103.41	110.47
1	C	72	ILE	CA-C-O	5.64	122.47	118.69
1	C	68	ARG	CB-CA-C	-5.62	102.06	110.88
1	D	206	ASP	O-C-N	5.62	125.74	120.51
1	C	206	ASP	CA-C-O	5.62	123.50	118.33
1	A	314	PRO	CA-C-N	-5.61	115.98	122.77
1	A	314	PRO	C-N-CA	-5.61	115.98	122.77
1	D	206	ASP	CA-C-N	5.61	125.07	119.24
1	D	206	ASP	C-N-CA	5.61	125.07	119.24
1	D	213	ILE	CB-CA-C	5.59	118.90	110.63
1	D	115	HIS	CA-CB-CG	-5.56	108.24	113.80
1	A	193	ALA	N-CA-C	5.56	119.68	113.01
1	B	143	PRO	N-CA-C	-5.54	105.55	113.47
1	A	221	ASP	CA-CB-CG	-5.50	107.10	112.60
1	A	332	PHE	CA-C-N	-5.50	115.94	123.14
1	A	332	PHE	C-N-CA	-5.50	115.94	123.14
1	C	91	ALA	N-CA-C	5.48	118.76	111.75
1	D	13	MET	CB-CA-C	5.48	116.29	108.68
1	A	96	HIS	CA-CB-CG	-5.47	108.33	113.80
1	C	332	PHE	CA-CB-CG	-5.46	108.34	113.80
1	D	199	ALA	CA-C-O	5.46	127.64	120.16
1	C	230	ARG	NE-CZ-NH1	5.44	126.94	121.50
1	C	354	GLU	CB-CA-C	5.43	119.85	110.84
1	D	170	VAL	N-CA-C	5.41	116.79	110.62
1	D	71	LEU	N-CA-C	5.40	116.86	110.97
1	C	18	PRO	N-CA-CB	5.39	107.85	103.32
1	B	155	GLU	CA-C-N	-5.38	114.66	122.29
1	B	155	GLU	C-N-CA	-5.38	114.66	122.29
1	B	199	ALA	CA-C-O	5.37	123.27	118.33
1	D	194	TYR	N-CA-C	5.36	118.43	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	40	ALA	N-CA-C	5.33	117.51	111.11
1	D	61	ASP	N-CA-C	5.33	117.17	111.36
1	A	119	PHE	N-CA-C	-5.31	105.38	111.07
1	D	140	ASP	N-CA-C	-5.28	106.84	113.28
1	D	19	PHE	CB-CA-C	5.28	119.40	110.79
1	A	333	VAL	N-CA-C	5.26	115.47	108.11
1	D	203	ALA	N-CA-C	-5.26	105.63	111.36
1	A	331	PRO	N-CA-CB	5.25	108.32	103.39
1	A	133	GLY	N-CA-C	-5.23	104.31	112.58
1	B	261	ASN	CA-C-N	-5.23	116.34	122.93
1	B	261	ASN	C-N-CA	-5.23	116.34	122.93
1	C	69	HIS	N-CA-C	5.22	119.36	112.89
1	C	171	GLU	O-C-N	5.18	124.47	120.38
1	A	345	PRO	N-CA-CB	5.16	108.80	103.38
1	D	65	HIS	CA-CB-CG	-5.14	108.66	113.80
1	C	130	VAL	CA-C-N	5.11	124.87	119.76
1	C	130	VAL	C-N-CA	5.11	124.87	119.76
1	C	193	ALA	N-CA-C	5.11	119.14	113.01
1	B	177	ARG	N-CA-C	-5.10	105.80	111.36
1	C	132	CYS	N-CA-C	5.10	117.72	109.40
1	D	222	VAL	N-CA-C	5.10	115.32	110.53
1	C	257	VAL	N-CA-C	5.09	115.08	108.35
1	B	69	HIS	CA-CB-CG	-5.07	108.73	113.80
1	C	342	PRO	N-CA-CB	5.07	107.83	103.31
1	B	179	ARG	N-CA-C	5.07	116.89	111.36
1	A	9	ARG	N-CA-CB	-5.07	101.83	111.00
1	C	309	PRO	N-CA-C	5.04	121.27	113.75
1	B	96	HIS	CA-CB-CG	-5.04	108.76	113.80
1	B	71	LEU	CA-C-N	-5.04	116.30	120.33
1	B	71	LEU	C-N-CA	-5.04	116.30	120.33
1	D	354	GLU	O-C-N	5.04	127.47	122.08
1	C	55	TYR	N-CA-C	-5.03	106.83	113.12
1	B	283	HIS	CA-CB-CG	-5.02	108.78	113.80
1	C	177	ARG	CA-C-O	5.01	125.73	120.42

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	2765	0	2805	134	1
1	B	2772	0	2810	90	0
1	C	2765	0	2805	113	0
1	D	2765	0	2805	270	1
2	A	18	0	11	1	0
2	B	36	0	21	1	0
2	C	36	0	21	7	0
2	D	18	0	11	12	0
3	A	261	0	0	9	1
3	B	375	0	0	8	0
3	C	336	0	0	11	0
3	D	190	0	0	7	1
All	All	12337	0	11289	606	2

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 27.

All (606) 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:D:38:THR:HB	1:D:39:PRO:HD2	1.20	1.17
1:C:10:ARG:HD2	1:C:32:LEU:CD1	1.74	1.14
1:A:1:MET:HE3	1:A:38:THR:CG2	1.78	1.12
1:D:141:THR:HG23	1:D:143:PRO:HD2	1.16	1.12
1:A:1:MET:CE	1:A:38:THR:HG21	1.83	1.09
1:B:12:GLN:NE2	1:B:28:VAL:HG11	1.74	1.01
1:D:139:MET:HB2	1:D:168:TRP:CZ2	1.99	0.98
1:D:206:ASP:HB2	1:D:207:PRO:HD3	1.46	0.98
1:D:221:ASP:OD2	1:D:224:GLY:HA3	1.64	0.96
1:D:205:LEU:C	1:D:207:PRO:HD2	1.91	0.95
1:D:206:ASP:N	1:D:207:PRO:HD2	1.83	0.94
1:A:38:THR:HB	1:A:39:PRO:HD2	1.51	0.93
1:D:328:ILE:O	1:D:351:PRO:HA	1.70	0.92
1:D:236:ILE:N	1:D:236:ILE:HD13	1.84	0.91
1:C:141:THR:HG22	1:C:144:GLN:H	1.35	0.91
1:C:10:ARG:HD2	1:C:32:LEU:HD12	1.53	0.90
1:A:29:ARG:HD2	1:A:31:LEU:HD23	1.53	0.90
1:D:141:THR:CG2	1:D:143:PRO:HD2	1.99	0.90
1:D:213:ILE:HG22	1:D:234:THR:HG22	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ASP:O	3:D:1681:HOH:O	1.91	0.88
1:A:206:ASP:N	1:A:207:PRO:HD2	1.86	0.88
1:D:293:ILE:HD12	2:D:1500:NPG:HE2	1.55	0.88
1:A:1:MET:HE3	1:A:38:THR:HG21	0.91	0.88
1:D:206:ASP:N	1:D:207:PRO:CD	2.37	0.87
1:D:18:PRO:HA	1:D:26:GLN:O	1.74	0.87
1:D:109:ASP:O	1:D:113:ARG:HG3	1.74	0.87
1:D:201:GLN:O	1:D:204:ARG:HB2	1.76	0.86
1:A:144:GLN:O	1:A:148:VAL:HG23	1.74	0.85
1:A:199:ALA:HB3	1:A:200:PRO:HD3	1.58	0.85
1:D:213:ILE:HG22	1:D:234:THR:CG2	2.07	0.85
1:D:217:LEU:HD21	1:D:228:LEU:HD23	1.59	0.84
1:B:139:MET:HB3	1:B:144:GLN:HG2	1.59	0.84
1:A:8:LEU:HD12	1:A:366:ILE:HD13	1.59	0.83
1:C:141:THR:HG23	1:C:143:PRO:HD2	1.60	0.83
1:D:139:MET:HB2	1:D:168:TRP:CH2	2.12	0.83
1:D:171:GLU:OE1	1:D:174:ARG:NH1	2.11	0.83
1:C:220:GLU:HG2	3:C:1656:HOH:O	1.79	0.82
1:D:216:PRO:C	1:D:217:LEU:HD23	2.03	0.82
1:C:204:ARG:HH11	1:C:204:ARG:HG2	1.43	0.82
1:D:227:GLU:O	1:D:230:ARG:HB2	1.80	0.82
1:D:162:LEU:CD1	1:D:186:LEU:HD11	2.11	0.81
1:D:199:ALA:HB3	1:D:200:PRO:HD3	1.61	0.81
1:D:32:LEU:C	1:D:32:LEU:HD23	2.07	0.80
1:D:32:LEU:HD23	1:D:33:LEU:N	1.96	0.80
1:D:293:ILE:HG13	2:D:1500:NPG:HD2	1.63	0.80
1:C:109:ASP:O	1:C:113:ARG:HG3	1.80	0.80
1:D:228:LEU:HD12	1:D:228:LEU:O	1.81	0.80
1:D:363:LYS:HG2	1:D:364:VAL:N	1.97	0.80
1:A:201:GLN:O	1:A:204:ARG:HB2	1.82	0.79
1:B:199:ALA:HB3	1:B:200:PRO:HD3	1.63	0.79
1:B:78:ALA:HB3	1:B:81:ILE:HD11	1.64	0.79
1:C:8:LEU:CD2	1:C:64:GLU:HG3	2.11	0.79
1:D:162:LEU:HD11	1:D:186:LEU:HD11	1.65	0.79
1:A:82:THR:HG22	1:A:84:ALA:H	1.48	0.78
1:C:12:GLN:HG2	1:C:30:GLU:HG2	1.65	0.78
1:A:12:GLN:HG2	1:A:30:GLU:HG3	1.66	0.78
1:D:139:MET:CG	1:D:145:LEU:HB2	2.13	0.78
1:D:78:ALA:HB3	1:D:81:ILE:CD1	2.14	0.77
1:D:353:PRO:O	1:D:357:ASP:N	2.12	0.77
1:D:38:THR:HB	1:D:39:PRO:CD	2.10	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLU:OE2	3:C:1656:HOH:O	2.00	0.77
1:A:82:THR:HG22	1:A:84:ALA:N	1.98	0.77
1:C:10:ARG:HD2	1:C:32:LEU:HD11	1.66	0.77
1:D:148:VAL:HG12	1:D:152:TYR:CE1	2.21	0.76
1:D:21:THR:HG22	1:D:23:PHE:H	1.50	0.76
1:D:293:ILE:HD12	2:D:1500:NPG:CE2	2.15	0.76
1:D:21:THR:HG22	1:D:22:SER:N	2.01	0.76
1:A:113:ARG:HA	1:A:345:PRO:HB2	1.68	0.75
1:D:21:THR:HG21	1:D:23:PHE:CE1	2.21	0.75
1:C:87:THR:HB	1:C:88:PRO:HD3	1.69	0.74
1:D:226:ALA:O	3:D:1660:HOH:O	2.03	0.74
1:D:334:LEU:HD12	1:D:339:LEU:CD1	2.16	0.74
1:D:38:THR:CB	1:D:39:PRO:HD2	1.99	0.74
1:D:228:LEU:HD12	1:D:228:LEU:C	2.11	0.74
1:D:169:ASP:HB2	1:D:170:VAL:HG23	1.70	0.74
1:D:141:THR:HG22	1:D:144:GLN:HB2	1.70	0.74
1:D:55:TYR:OH	1:D:266:ARG:HD3	1.87	0.73
1:D:194:TYR:N	1:D:194:TYR:CD1	2.56	0.73
1:A:21:THR:HG22	1:A:163:LYS:HE2	1.71	0.72
1:B:142:ILE:N	1:B:143:PRO:CD	2.53	0.72
1:B:206:ASP:HB2	1:B:207:PRO:HD3	1.72	0.72
1:A:203:ALA:HB3	3:A:1414:HOH:O	1.89	0.72
1:D:146:LEU:HD22	1:D:179:ARG:HG2	1.72	0.71
1:A:206:ASP:N	1:A:207:PRO:CD	2.53	0.71
1:A:8:LEU:HD12	1:A:366:ILE:CD1	2.19	0.71
1:C:10:ARG:CD	1:C:32:LEU:CD1	2.61	0.71
1:C:68:ARG:HD3	3:C:1709:HOH:O	1.91	0.71
1:B:10:ARG:NH2	1:B:61:ASP:OD1	2.21	0.71
1:C:39:PRO:HG2	3:C:1623:HOH:O	1.89	0.71
1:D:363:LYS:CB	1:D:363:LYS:NZ	2.53	0.71
1:D:194:TYR:CE2	1:D:202:LEU:HD21	2.26	0.71
1:A:64:GLU:OE2	3:A:1429:HOH:O	2.08	0.71
1:C:38:THR:HB	1:C:39:PRO:HD2	1.72	0.71
1:D:334:LEU:HD12	1:D:339:LEU:HD13	1.71	0.70
1:A:33:LEU:HD13	1:A:297:LEU:HD12	1.73	0.70
1:B:1:MET:HB2	3:B:1339:HOH:O	1.92	0.70
1:D:171:GLU:OE1	1:D:171:GLU:HA	1.89	0.70
1:B:141:THR:CB	1:B:143:PRO:HD2	2.21	0.70
1:C:141:THR:HG23	1:C:143:PRO:CD	2.21	0.70
1:D:21:THR:CG2	1:D:22:SER:N	2.55	0.69
1:D:213:ILE:CG1	1:D:216:PRO:HG3	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:LYS:HD2	1:D:3:LEU:N	2.07	0.69
1:D:236:ILE:N	1:D:236:ILE:CD1	2.54	0.69
1:A:8:LEU:HD23	1:A:32:LEU:CD2	2.22	0.68
1:D:291:GLY:O	2:D:1500:NPG:N1	2.27	0.68
1:B:12:GLN:NE2	1:B:28:VAL:CG1	2.52	0.68
1:D:32:LEU:C	1:D:32:LEU:CD2	2.66	0.68
1:B:141:THR:OG1	1:B:143:PRO:HD2	1.94	0.67
1:C:50:MET:HE2	3:C:1475:HOH:O	1.94	0.67
1:B:171:GLU:CD	1:B:174:ARG:HH21	2.02	0.67
1:D:363:LYS:HB3	1:D:363:LYS:HZ3	1.60	0.67
1:C:206:ASP:N	1:C:207:PRO:CD	2.57	0.67
1:C:8:LEU:CD2	1:C:64:GLU:CG	2.73	0.66
1:C:205:LEU:C	1:C:207:PRO:HD2	2.21	0.66
1:D:352:ILE:O	1:D:355:LEU:HB2	1.95	0.65
1:D:21:THR:CG2	1:D:22:SER:H	2.10	0.65
1:A:329:THR:HG21	1:A:349:VAL:CG1	2.27	0.65
1:A:205:LEU:C	1:A:207:PRO:HD2	2.20	0.65
1:B:185:LEU:N	1:B:185:LEU:CD1	2.59	0.65
1:D:353:PRO:HA	1:D:356:LEU:HB3	1.76	0.65
1:A:163:LYS:HE3	1:A:191:ASN:OD1	1.97	0.65
1:C:7:GLU:CD	1:C:35:ARG:HH12	2.04	0.65
1:C:8:LEU:HD23	1:C:64:GLU:HG3	1.79	0.65
1:A:65:HIS:HD2	1:B:59:TYR:OH	1.79	0.65
1:D:141:THR:HG22	1:D:144:GLN:H	1.62	0.64
1:C:64:GLU:O	1:C:68:ARG:HG3	1.97	0.64
1:D:8:LEU:HD13	1:D:366:ILE:CD1	2.27	0.64
1:D:33:LEU:O	1:D:34:LEU:HD23	1.97	0.64
1:D:12:GLN:O	1:D:14:PRO:HD3	1.97	0.64
1:D:352:ILE:HB	1:D:355:LEU:HD22	1.79	0.64
1:C:252:ILE:HA	3:C:1573:HOH:O	1.96	0.64
1:A:78:ALA:HB3	1:A:81:ILE:HD11	1.79	0.64
1:A:206:ASP:HB2	1:A:207:PRO:HD3	1.79	0.64
1:B:159:ARG:HG2	1:B:160:ILE:N	2.12	0.64
1:A:35:ARG:HG3	1:A:44:TRP:CE2	2.33	0.64
1:A:10:ARG:NH2	1:A:61:ASP:OD1	2.24	0.64
1:D:15:LEU:HD23	1:D:324:TYR:HE2	1.64	0.63
1:D:36:ALA:O	1:D:42:GLU:HB3	1.98	0.63
1:C:48:VAL:HB	1:C:292:MET:HG3	1.81	0.63
1:D:217:LEU:HD21	1:D:228:LEU:CD2	2.28	0.63
1:D:171:GLU:HB2	3:D:1513:HOH:O	1.98	0.63
1:D:338:HIS:O	1:D:339:LEU:HD12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:GLN:O	1:C:204:ARG:HB2	1.99	0.63
1:D:2:LYS:HD2	1:D:2:LYS:C	2.24	0.62
1:D:217:LEU:HD23	1:D:217:LEU:N	2.14	0.62
1:A:8:LEU:HD23	1:A:32:LEU:HD21	1.81	0.62
1:A:8:LEU:CD2	1:A:32:LEU:HD21	2.29	0.62
1:B:227:GLU:OE1	1:B:230:ARG:NH1	2.32	0.62
1:C:366:ILE:HD12	1:C:366:ILE:N	2.14	0.62
1:D:213:ILE:HG12	1:D:216:PRO:HG3	1.82	0.62
1:A:329:THR:HB	1:A:349:VAL:HG13	1.81	0.62
1:B:42:GLU:OE1	3:B:1666:HOH:O	2.16	0.61
1:D:206:ASP:HB2	1:D:207:PRO:CD	2.28	0.61
1:B:283:HIS:CE1	1:C:253:LYS:HE2	2.35	0.61
1:A:274:ARG:NH1	1:A:278:ASP:OD2	2.33	0.61
1:D:8:LEU:HD13	1:D:366:ILE:HD11	1.82	0.61
1:D:139:MET:HG2	1:D:145:LEU:HB2	1.81	0.61
1:D:7:GLU:CD	1:D:9:ARG:HH12	2.09	0.61
1:A:29:ARG:CD	1:A:31:LEU:HD23	2.30	0.61
1:A:35:ARG:HG3	1:A:44:TRP:CZ2	2.36	0.61
1:D:68:ARG:CG	1:D:68:ARG:HH11	2.14	0.60
1:A:171:GLU:N	1:A:172:PRO:HD2	2.15	0.60
1:D:143:PRO:O	1:D:144:GLN:C	2.44	0.60
1:A:65:HIS:HE1	3:B:1659:HOH:O	1.85	0.60
1:B:163:LYS:HE2	1:B:191:ASN:OD1	2.02	0.60
1:C:2:LYS:O	1:C:39:PRO:HD3	2.01	0.60
1:D:139:MET:HB2	1:D:168:TRP:HZ2	1.62	0.60
1:B:227:GLU:HA	1:B:230:ARG:NH1	2.17	0.60
1:A:38:THR:HB	1:A:39:PRO:CD	2.29	0.59
1:C:206:ASP:N	1:C:207:PRO:HD2	2.17	0.59
1:D:199:ALA:HB3	1:D:200:PRO:CD	2.29	0.59
1:C:142:ILE:N	1:C:143:PRO:HD2	2.18	0.59
1:D:194:TYR:CG	1:D:202:LEU:HD11	2.37	0.59
1:C:8:LEU:HD22	1:C:64:GLU:HG2	1.84	0.59
1:D:32:LEU:C	1:D:33:LEU:HD23	2.27	0.59
1:D:8:LEU:HD11	1:D:366:ILE:HD12	1.85	0.59
1:D:9:ARG:HG3	1:D:9:ARG:HH11	1.66	0.59
1:D:352:ILE:HB	1:D:355:LEU:CD2	2.33	0.59
1:A:32:LEU:O	1:A:33:LEU:HD23	2.03	0.59
1:D:174:ARG:HA	1:D:208:PHE:CE2	2.38	0.59
1:A:22:SER:HA	1:A:165:GLU:OE2	2.02	0.59
3:A:1360:HOH:O	1:B:65:HIS:HE1	1.84	0.59
1:B:364:VAL:CG2	3:B:1615:HOH:O	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LEU:CD1	1:D:366:ILE:HD12	2.33	0.59
1:C:87:THR:N	1:C:88:PRO:HD2	2.18	0.58
1:A:165:GLU:OE2	3:A:1352:HOH:O	2.17	0.58
1:D:355:LEU:O	1:D:359:VAL:HG22	2.02	0.58
1:A:169:ASP:O	1:A:172:PRO:HD2	2.02	0.58
1:C:87:THR:HB	1:C:88:PRO:CD	2.32	0.58
1:D:293:ILE:HG22	1:D:293:ILE:O	2.03	0.58
1:D:190:ALA:HB1	1:D:193:ALA:HB3	1.86	0.58
1:A:16:VAL:HB	1:A:323:PHE:O	2.04	0.58
1:D:7:GLU:HB2	1:D:365:TRP:HE3	1.68	0.58
1:B:148:VAL:HA	3:B:1634:HOH:O	2.04	0.58
1:D:160:ILE:O	1:D:186:LEU:HA	2.03	0.58
1:D:264:PRO:HG2	1:D:270:TYR:CE2	2.39	0.58
1:A:338:HIS:O	1:A:339:LEU:HD12	2.04	0.57
1:D:166:PRO:HD3	1:D:194:TYR:CZ	2.38	0.57
1:C:141:THR:CG2	1:C:144:GLN:H	2.13	0.57
1:B:140:ASP:HB2	1:B:144:GLN:OE1	2.04	0.57
1:C:8:LEU:HD22	1:C:64:GLU:CG	2.33	0.57
1:B:142:ILE:N	1:B:143:PRO:HD2	2.19	0.57
1:B:227:GLU:HA	1:B:230:ARG:HH11	1.70	0.57
1:C:217:LEU:HB2	1:C:225:HIS:CE1	2.39	0.57
1:C:171:GLU:N	1:C:172:PRO:HD2	2.20	0.57
1:C:220:GLU:CG	3:C:1656:HOH:O	2.43	0.57
1:D:7:GLU:CD	1:D:9:ARG:NH1	2.63	0.57
1:D:214:GLU:C	1:D:216:PRO:HD3	2.30	0.57
1:B:171:GLU:HB2	1:B:172:PRO:HD3	1.87	0.57
1:D:205:LEU:C	1:D:207:PRO:CD	2.71	0.57
1:D:363:LYS:NZ	1:D:363:LYS:HB3	2.19	0.57
1:A:12:GLN:NE2	1:A:28:VAL:HG11	2.20	0.56
1:C:9:ARG:NH2	1:C:360:THR:OG1	2.38	0.56
1:D:8:LEU:CD1	1:D:366:ILE:CD1	2.83	0.56
1:A:159:ARG:HD2	1:A:159:ARG:C	2.30	0.56
1:B:141:THR:HB	1:B:143:PRO:HD2	1.85	0.56
1:D:141:THR:CG2	1:D:144:GLN:HB2	2.34	0.56
1:D:141:THR:HG22	1:D:144:GLN:CB	2.35	0.56
1:D:249:ALA:O	1:D:253:LYS:HG3	2.05	0.56
1:A:1:MET:CE	1:A:38:THR:CG2	2.59	0.56
1:D:21:THR:HG21	1:D:23:PHE:CD1	2.39	0.56
2:C:1164:NPG:O62	3:C:1728:HOH:O	2.18	0.56
1:D:185:LEU:CD1	1:D:185:LEU:N	2.68	0.56
1:D:7:GLU:OE1	1:D:9:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:LYS:CB	1:D:363:LYS:HZ3	2.18	0.56
1:B:141:THR:OG1	1:B:144:GLN:HB3	2.05	0.56
1:B:199:ALA:HB3	1:B:200:PRO:CD	2.34	0.56
1:D:196:LEU:O	1:D:199:ALA:HB2	2.06	0.56
1:A:85:LYS:C	1:A:88:PRO:HD2	2.31	0.55
1:C:75:LEU:HD11	1:C:103:LEU:HD13	1.87	0.55
1:A:169:ASP:C	1:A:172:PRO:HD2	2.32	0.55
1:C:308:LEU:HB3	1:C:309:PRO:HD2	1.89	0.55
1:A:139:MET:HG3	1:A:145:LEU:HA	1.87	0.55
1:D:142:ILE:HB	1:D:143:PRO:HD3	1.87	0.55
1:D:171:GLU:HB2	1:D:172:PRO:HD3	1.89	0.55
1:B:321:ASP:HA	1:B:324:TYR:O	2.07	0.55
1:D:194:TYR:N	1:D:194:TYR:HD1	2.05	0.55
1:D:139:MET:HG3	1:D:145:LEU:CA	2.37	0.54
1:A:87:THR:HB	1:A:88:PRO:HD3	1.89	0.54
1:B:185:LEU:N	1:B:185:LEU:HD12	2.22	0.54
1:D:68:ARG:HH11	1:D:68:ARG:HG3	1.70	0.54
1:A:356:LEU:HD22	1:A:360:THR:OG1	2.08	0.54
1:C:141:THR:CG2	1:C:143:PRO:CD	2.84	0.54
1:D:171:GLU:CB	1:D:172:PRO:CD	2.85	0.54
1:D:354:GLU:HG3	1:D:355:LEU:N	2.20	0.54
1:B:163:LYS:HE3	1:B:189:ASP:OD2	2.08	0.54
1:C:96:HIS:O	1:C:100:LYS:HG3	2.07	0.54
1:C:190:ALA:HB3	1:C:216:PRO:HA	1.90	0.54
1:C:249:ALA:O	1:C:253:LYS:HG3	2.07	0.54
1:C:112:LEU:HB3	1:C:117:ARG:O	2.08	0.54
1:D:199:ALA:CB	1:D:200:PRO:HD3	2.36	0.54
1:A:331:PRO:HD3	3:A:1261:HOH:O	2.08	0.53
1:A:12:GLN:HE21	1:A:28:VAL:HG11	1.73	0.53
1:B:12:GLN:HE21	1:B:28:VAL:CG1	2.21	0.53
1:C:38:THR:CB	1:C:39:PRO:HD2	2.38	0.53
1:D:239:ASP:OD2	1:D:263:LYS:HE3	2.09	0.53
1:D:25:THR:HG22	1:D:26:GLN:N	2.24	0.53
1:B:261:ASN:C	1:B:261:ASN:OD1	2.51	0.53
1:C:293:ILE:HG13	2:C:1400:NPG:HD2	1.90	0.53
1:B:283:HIS:ND1	1:C:253:LYS:HE2	2.24	0.53
1:D:141:THR:HB	1:D:144:GLN:OE1	2.09	0.53
1:C:30:GLU:HB3	3:C:1704:HOH:O	2.08	0.53
1:D:37:VAL:HG21	1:D:365:TRP:CH2	2.44	0.53
1:A:169:ASP:O	1:A:173:VAL:HG23	2.09	0.53
1:A:33:LEU:CD2	1:A:46:GLU:HG3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ARG:HG2	1:C:204:ARG:NH1	2.16	0.52
1:D:164:ILE:HB	1:D:168:TRP:O	2.08	0.52
1:D:333:VAL:HG12	1:D:334:LEU:O	2.08	0.52
1:B:109:ASP:O	1:B:113:ARG:HG3	2.09	0.52
1:C:75:LEU:CD1	1:C:103:LEU:HD13	2.39	0.52
1:C:50:MET:CE	3:C:1475:HOH:O	2.56	0.52
1:D:293:ILE:CD1	2:D:1500:NPG:CE2	2.87	0.52
1:D:293:ILE:CD1	2:D:1500:NPG:HE2	2.35	0.52
2:A:1200:NPG:HD1	2:A:1200:NPG:O12	2.08	0.52
1:C:9:ARG:NH2	1:C:356:LEU:HD13	2.24	0.52
1:D:148:VAL:O	1:D:149:VAL:C	2.52	0.52
1:A:30:GLU:HG2	3:A:1300:HOH:O	2.10	0.52
1:A:334:LEU:HD12	1:A:339:LEU:CD1	2.40	0.52
1:A:349:VAL:CG1	1:A:350:ALA:N	2.72	0.52
1:D:228:LEU:C	1:D:228:LEU:CD1	2.81	0.52
1:D:334:LEU:CD1	1:D:339:LEU:HD13	2.40	0.52
1:A:206:ASP:OD1	3:A:1444:HOH:O	2.19	0.52
1:D:352:ILE:HD12	1:D:355:LEU:HD23	1.91	0.52
1:D:148:VAL:CG1	1:D:152:TYR:CE1	2.92	0.52
1:A:142:ILE:O	1:A:143:PRO:C	2.51	0.51
1:B:174:ARG:O	1:B:178:GLU:HB2	2.11	0.51
1:C:192:THR:HB	1:C:218:GLU:HA	1.92	0.51
1:D:127:ARG:NH2	1:D:308:LEU:O	2.44	0.51
1:D:195:THR:O	1:D:198:ASP:HB2	2.10	0.51
1:A:8:LEU:HD23	1:A:32:LEU:HD22	1.92	0.51
1:D:164:ILE:HG12	1:D:188:VAL:HB	1.92	0.51
1:A:192:THR:HB	1:A:218:GLU:HA	1.93	0.51
1:D:216:PRO:HB2	1:D:217:LEU:HD23	1.91	0.51
1:D:33:LEU:C	1:D:34:LEU:HD23	2.35	0.51
1:D:139:MET:HG3	1:D:145:LEU:N	2.25	0.51
1:D:159:ARG:HD2	1:D:159:ARG:C	2.35	0.51
1:D:171:GLU:CB	1:D:172:PRO:HD3	2.41	0.51
1:D:235:PRO:C	1:D:236:ILE:HD13	2.35	0.51
1:A:206:ASP:CB	1:A:207:PRO:HD3	2.41	0.51
1:C:59:TYR:OH	1:D:65:HIS:HD2	1.93	0.51
1:C:65:HIS:HD2	2:C:1164:NPG:C2	2.23	0.51
1:A:29:ARG:HD2	1:A:31:LEU:CD2	2.35	0.51
1:B:39:PRO:HG2	3:B:1409:HOH:O	2.11	0.51
1:D:135:SER:OG	1:D:161:LYS:HE2	2.12	0.50
1:A:199:ALA:N	1:A:200:PRO:CD	2.75	0.50
1:A:329:THR:HG21	1:A:349:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:VAL:HB	1:D:365:TRP:HH2	1.75	0.50
1:D:185:LEU:N	1:D:185:LEU:HD13	2.25	0.50
1:D:328:ILE:O	1:D:351:PRO:CA	2.52	0.50
1:D:142:ILE:HG22	1:D:146:LEU:HD12	1.94	0.50
1:A:142:ILE:N	1:A:143:PRO:HD2	2.27	0.50
1:A:293:ILE:HG22	1:A:293:ILE:O	2.12	0.50
1:D:293:ILE:CG1	2:D:1500:NPG:HD2	2.39	0.50
1:B:199:ALA:N	1:B:200:PRO:HD2	2.26	0.50
1:C:10:ARG:CD	1:C:32:LEU:HD11	2.36	0.50
1:D:195:THR:O	1:D:198:ASP:N	2.38	0.50
1:C:87:THR:CB	1:C:88:PRO:CD	2.90	0.49
1:D:363:LYS:NZ	1:D:363:LYS:HB2	2.26	0.49
1:D:213:ILE:HG13	1:D:216:PRO:HG3	1.94	0.49
1:A:9:ARG:CG	1:A:360:THR:HG23	2.42	0.49
1:A:171:GLU:N	1:A:172:PRO:CD	2.75	0.49
1:D:193:ALA:HB3	1:D:194:TYR:CE1	2.48	0.49
1:D:199:ALA:CB	1:D:200:PRO:CD	2.89	0.49
1:D:308:LEU:CB	1:D:309:PRO:HD2	2.41	0.49
1:A:161:LYS:HE3	1:A:189:ASP:HB2	1.93	0.49
1:D:9:ARG:HH11	1:D:9:ARG:CG	2.26	0.49
1:D:235:PRO:HB3	1:D:258:GLN:NE2	2.28	0.49
1:A:11:VAL:HB	1:A:31:LEU:HD12	1.94	0.49
1:D:227:GLU:HA	1:D:230:ARG:NH1	2.27	0.49
1:A:352:ILE:O	1:A:355:LEU:N	2.45	0.49
1:B:137:GLY:HA2	1:B:163:LYS:HB2	1.93	0.49
1:C:159:ARG:HD2	1:C:159:ARG:C	2.37	0.49
1:A:139:MET:HG3	1:A:145:LEU:CA	2.43	0.49
1:B:146:LEU:O	1:B:180:PHE:HZ	1.96	0.49
1:D:263:LYS:NZ	2:D:1500:NPG:O11	2.44	0.49
1:A:169:ASP:O	1:A:172:PRO:HG2	2.12	0.49
1:D:141:THR:O	1:D:168:TRP:HH2	1.95	0.49
1:D:350:ALA:HB1	1:D:351:PRO:HD2	1.95	0.49
1:A:65:HIS:CE1	1:A:69:HIS:CD2	3.01	0.48
1:A:218:GLU:OE2	1:B:246:ARG:NE	2.46	0.48
1:D:277:HIS:CD2	1:D:310:ASN:HB3	2.48	0.48
1:B:5:GLY:HA3	1:B:365:TRP:CZ2	2.48	0.48
1:A:33:LEU:HD21	1:A:46:GLU:HG3	1.96	0.48
1:A:28:VAL:HG12	1:A:29:ARG:N	2.28	0.48
2:B:1163:NPG:H41	3:B:1403:HOH:O	2.14	0.48
1:D:353:PRO:O	1:D:354:GLU:C	2.51	0.48
1:D:10:ARG:NH2	1:D:61:ASP:OD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:PHE:HA	3:D:1603:HOH:O	2.13	0.48
1:D:288:TRP:HB3	1:D:313:LEU:HB2	1.95	0.48
1:D:293:ILE:HG13	2:D:1500:NPG:CD2	2.40	0.48
1:D:334:LEU:HG	1:D:337:GLY:HA2	1.95	0.48
1:C:365:TRP:CD1	1:C:365:TRP:C	2.92	0.48
1:B:204:ARG:O	1:B:207:PRO:HD2	2.14	0.48
1:A:190:ALA:HB3	1:A:216:PRO:HA	1.95	0.48
1:C:141:THR:CG2	1:C:143:PRO:HD2	2.39	0.48
1:D:46:GLU:OE2	1:D:294:GLU:HB3	2.14	0.48
1:D:194:TYR:CB	1:D:202:LEU:HD11	2.43	0.48
1:D:194:TYR:CD2	1:D:202:LEU:HD21	2.49	0.48
1:D:321:ASP:HA	1:D:324:TYR:O	2.14	0.48
1:C:95:GLY:O	1:C:100:LYS:HE3	2.14	0.48
1:A:141:THR:OG1	1:A:144:GLN:HB2	2.13	0.47
1:D:8:LEU:O	1:D:363:LYS:HA	2.14	0.47
1:D:261:ASN:C	1:D:261:ASN:OD1	2.57	0.47
1:D:293:ILE:N	2:D:1500:NPG:O62	2.40	0.47
1:D:37:VAL:HG21	1:D:365:TRP:CZ3	2.49	0.47
1:A:261:ASN:OD1	1:A:261:ASN:C	2.57	0.47
1:B:264:PRO:HG3	1:B:305:LEU:HD22	1.95	0.47
1:C:293:ILE:HG13	2:C:1400:NPG:CD2	2.44	0.47
1:D:87:THR:N	1:D:88:PRO:HD2	2.30	0.47
1:A:87:THR:N	1:A:88:PRO:HD2	2.30	0.47
1:A:206:ASP:CB	1:A:207:PRO:CD	2.92	0.47
1:A:97:ARG:O	1:A:268:GLY:HA2	2.15	0.47
1:D:315:GLY:C	1:D:317:THR:H	2.22	0.47
1:B:171:GLU:N	1:B:172:PRO:HD2	2.30	0.47
1:D:190:ALA:O	1:D:193:ALA:HB2	2.14	0.47
1:A:32:LEU:C	1:A:33:LEU:HD23	2.40	0.47
1:A:127:ARG:NH2	1:A:308:LEU:O	2.48	0.47
1:B:78:ALA:HB3	1:B:81:ILE:CD1	2.41	0.47
1:B:142:ILE:HB	1:B:143:PRO:HD3	1.97	0.47
1:C:35:ARG:HD2	1:C:42:GLU:OE1	2.14	0.47
1:D:33:LEU:HD13	1:D:297:LEU:HD12	1.96	0.47
1:D:68:ARG:CG	1:D:68:ARG:NH1	2.76	0.47
1:D:87:THR:HB	1:D:88:PRO:HD3	1.97	0.47
1:D:141:THR:CG2	1:D:144:GLN:H	2.27	0.47
1:C:87:THR:CB	1:C:88:PRO:HD3	2.43	0.47
1:C:353:PRO:O	1:C:354:GLU:C	2.58	0.47
1:D:112:LEU:HB3	1:D:117:ARG:O	2.15	0.47
1:C:142:ILE:N	1:C:143:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:ALA:N	1:D:200:PRO:HD2	2.30	0.46
1:D:171:GLU:HB2	1:D:172:PRO:CD	2.46	0.46
1:C:21:THR:HG22	1:C:163:LYS:HE2	1.96	0.46
1:D:141:THR:HG23	1:D:142:ILE:N	2.30	0.46
1:D:148:VAL:HG12	1:D:152:TYR:CD1	2.51	0.46
1:D:166:PRO:HD3	1:D:194:TYR:CE1	2.51	0.46
1:A:179:ARG:NH2	3:A:1441:HOH:O	2.25	0.46
1:B:10:ARG:NH2	1:B:61:ASP:HA	2.30	0.46
1:D:211:LEU:O	1:D:212:LEU:HB3	2.15	0.46
1:D:363:LYS:HB2	1:D:363:LYS:HZ2	1.80	0.46
1:D:162:LEU:HD12	1:D:186:LEU:HD11	1.96	0.46
1:D:177:ARG:HD2	1:D:182:ASP:HA	1.98	0.46
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.76	0.46
3:A:1456:HOH:O	1:B:220:GLU:HG2	2.14	0.46
1:C:7:GLU:CD	1:C:35:ARG:NH1	2.71	0.46
1:D:143:PRO:O	1:D:144:GLN:O	2.34	0.46
1:D:325:LYS:HB3	3:D:1601:HOH:O	2.15	0.46
1:A:75:LEU:HD12	1:A:103:LEU:HD21	1.98	0.46
1:D:171:GLU:O	1:D:172:PRO:C	2.58	0.46
1:D:350:ALA:HB1	1:D:351:PRO:CD	2.44	0.46
1:D:87:THR:HB	1:D:88:PRO:CD	2.46	0.45
2:D:1500:NPG:O12	2:D:1500:NPG:HD1	2.17	0.45
1:A:356:LEU:C	1:A:356:LEU:CD2	2.89	0.45
1:C:38:THR:O	1:C:39:PRO:C	2.58	0.45
1:C:141:THR:HG22	1:C:144:GLN:N	2.17	0.45
1:D:37:VAL:CG2	1:D:365:TRP:CH2	2.99	0.45
1:B:237:CYS:HA	1:B:259:ILE:O	2.16	0.45
1:D:18:PRO:CA	1:D:26:GLN:O	2.57	0.45
1:A:18:PRO:HA	1:A:26:GLN:O	2.16	0.45
1:A:174:ARG:HA	1:A:208:PHE:CE2	2.52	0.45
1:B:192:THR:HB	1:B:218:GLU:HA	1.99	0.45
1:C:191:ASN:C	1:C:192:THR:HG23	2.41	0.45
1:D:216:PRO:HB2	1:D:217:LEU:CD2	2.47	0.45
1:A:38:THR:CB	1:A:39:PRO:CD	2.90	0.45
1:B:185:LEU:N	1:B:185:LEU:HD13	2.32	0.45
1:C:137:GLY:HA2	1:C:163:LYS:HG2	1.99	0.45
1:D:11:VAL:HG13	1:D:359:VAL:HB	1.99	0.45
1:A:150:GLY:O	1:A:153:LEU:HB2	2.17	0.45
1:C:308:LEU:CB	1:C:309:PRO:CD	2.95	0.45
1:C:321:ASP:HA	1:C:324:TYR:O	2.16	0.45
1:A:36:ALA:O	1:A:42:GLU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:N	1:A:88:PRO:CD	2.79	0.45
1:B:179:ARG:HG2	1:B:180:PHE:CE1	2.52	0.45
1:C:13:MET:HA	1:C:14:PRO:HD3	1.84	0.45
1:C:165:GLU:O	1:C:166:PRO:C	2.58	0.45
1:C:328:ILE:O	1:C:351:PRO:HA	2.16	0.45
1:D:7:GLU:HG3	1:D:363:LYS:HG3	1.98	0.45
1:D:169:ASP:O	1:D:172:PRO:HD2	2.16	0.45
1:D:352:ILE:CB	1:D:355:LEU:HD22	2.46	0.45
1:B:12:GLN:HE22	1:B:28:VAL:HG11	1.71	0.45
1:D:30:GLU:O	1:D:60:ASN:ND2	2.46	0.45
1:A:72:ILE:N	1:A:73:PRO:CD	2.79	0.45
1:C:72:ILE:HB	1:C:73:PRO:HD3	1.99	0.45
1:C:141:THR:HG23	1:C:143:PRO:CG	2.47	0.45
1:D:25:THR:CG2	1:D:26:GLN:N	2.80	0.45
1:D:174:ARG:O	1:D:178:GLU:HB2	2.17	0.45
1:B:177:ARG:HA	1:B:177:ARG:HD3	1.79	0.44
1:D:141:THR:CG2	1:D:142:ILE:N	2.79	0.44
1:B:35:ARG:HD2	1:B:42:GLU:OE2	2.17	0.44
1:C:67:LEU:HA	1:C:71:LEU:HB2	1.99	0.44
1:B:29:ARG:HD2	1:B:31:LEU:HD21	1.98	0.44
1:A:22:SER:CB	1:A:165:GLU:HG3	2.47	0.44
1:C:50:MET:HE3	1:C:50:MET:HB2	1.65	0.44
1:C:87:THR:N	1:C:88:PRO:CD	2.81	0.44
1:A:329:THR:CG2	1:A:349:VAL:CG1	2.93	0.44
1:C:141:THR:HG22	1:C:143:PRO:N	2.32	0.44
1:D:21:THR:HG22	1:D:23:PHE:N	2.26	0.44
1:D:65:HIS:O	1:D:69:HIS:HD2	2.01	0.44
1:D:190:ALA:O	1:D:193:ALA:CB	2.66	0.44
1:B:179:ARG:O	1:B:179:ARG:HG3	2.09	0.44
1:D:13:MET:HE2	1:D:324:TYR:CD1	2.53	0.44
1:D:139:MET:HG2	1:D:145:LEU:HD12	1.98	0.44
1:D:139:MET:HG3	1:D:145:LEU:HB2	1.99	0.44
1:D:264:PRO:CG	1:D:270:TYR:CE2	2.99	0.44
1:A:125:SER:OG	1:A:307:SER:OG	2.29	0.44
1:A:319:ALA:HB1	1:A:332:PHE:O	2.17	0.44
1:B:113:ARG:NH2	1:B:349:VAL:O	2.51	0.44
1:B:139:MET:HG3	1:B:145:LEU:HA	1.99	0.44
1:D:146:LEU:HD22	1:D:179:ARG:CG	2.45	0.44
1:D:209:GLY:HA3	3:D:1612:HOH:O	2.16	0.44
1:A:199:ALA:N	1:A:200:PRO:HD2	2.33	0.44
1:D:144:GLN:O	1:D:148:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:CYS:HA	1:D:259:ILE:O	2.18	0.44
1:A:2:LYS:O	1:A:39:PRO:HD3	2.17	0.44
1:B:37:VAL:HB	1:B:365:TRP:HH2	1.83	0.44
1:B:339:LEU:HD12	1:B:339:LEU:HA	1.87	0.44
1:C:32:LEU:HD12	1:C:32:LEU:HA	1.84	0.44
1:C:34:LEU:O	1:C:44:TRP:HA	2.18	0.44
1:D:134:VAL:HG11	1:D:152:TYR:HB3	2.00	0.44
1:B:364:VAL:HG23	3:B:1615:HOH:O	2.16	0.43
1:D:329:THR:O	1:D:330:GLU:C	2.60	0.43
1:A:72:ILE:N	1:A:73:PRO:HD2	2.33	0.43
1:D:55:TYR:OH	1:D:239:ASP:OD1	2.29	0.43
1:D:169:ASP:HB2	1:D:170:VAL:H	1.43	0.43
1:A:328:ILE:O	1:A:351:PRO:HA	2.18	0.43
1:C:163:LYS:HE3	1:C:191:ASN:OD1	2.18	0.43
1:A:337:GLY:C	1:A:338:HIS:HD2	2.26	0.43
1:B:80:ASP:C	1:B:81:ILE:HG12	2.43	0.43
1:C:163:LYS:HA	1:C:163:LYS:HD2	1.70	0.43
1:D:361:THR:O	1:D:362:ALA:HB2	2.17	0.43
1:B:171:GLU:OE2	1:B:174:ARG:NH2	2.51	0.43
1:A:33:LEU:C	1:A:34:LEU:HD23	2.44	0.43
1:D:363:LYS:HG2	1:D:364:VAL:H	1.82	0.43
1:D:185:LEU:HA	1:D:185:LEU:HD12	1.75	0.43
1:B:82:THR:O	1:B:86:VAL:HG23	2.19	0.43
1:C:293:ILE:HG13	2:C:1400:NPG:HE2	2.00	0.43
1:D:139:MET:HE3	1:D:148:VAL:HG21	2.01	0.43
1:D:171:GLU:CD	1:D:174:ARG:NH1	2.76	0.43
1:D:352:ILE:CD1	1:D:355:LEU:HD23	2.49	0.43
1:D:363:LYS:C	1:D:364:VAL:HG22	2.44	0.43
1:C:171:GLU:N	1:C:172:PRO:CD	2.80	0.42
1:D:142:ILE:N	1:D:143:PRO:HD2	2.34	0.42
1:A:301:ALA:HB2	1:A:347:LEU:CD2	2.49	0.42
1:B:199:ALA:CB	1:B:200:PRO:CD	2.95	0.42
1:C:293:ILE:HG13	2:C:1400:NPG:CE2	2.49	0.42
1:D:356:LEU:O	1:D:359:VAL:HG23	2.19	0.42
1:B:20:ARG:HG2	1:B:138:ILE:HB	2.02	0.42
1:B:227:GLU:CD	1:B:230:ARG:HH11	2.25	0.42
1:A:2:LYS:O	1:A:2:LYS:HG3	2.19	0.42
1:C:85:LYS:C	1:C:88:PRO:HD2	2.44	0.42
1:A:337:GLY:C	1:A:338:HIS:CD2	2.97	0.42
1:A:355:LEU:O	1:A:358:GLU:HB2	2.20	0.42
1:D:9:ARG:NH1	1:D:9:ARG:CG	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:MET:CG	1:D:145:LEU:CB	2.93	0.42
1:A:356:LEU:CD2	1:A:360:THR:OG1	2.67	0.42
1:B:206:ASP:N	1:B:207:PRO:CD	2.82	0.42
1:D:194:TYR:HB3	1:D:198:ASP:HB2	2.02	0.42
1:D:258:GLN:O	1:D:286:PRO:HD2	2.20	0.42
1:D:263:LYS:HD3	1:D:292:MET:SD	2.60	0.42
1:B:355:LEU:HD12	1:B:355:LEU:HA	1.77	0.42
1:C:86:VAL:O	1:C:90:LEU:HG	2.19	0.42
1:D:78:ALA:HB3	1:D:81:ILE:HD11	1.94	0.42
1:D:141:THR:HG22	1:D:144:GLN:N	2.32	0.42
1:B:7:GLU:HB3	1:B:35:ARG:HB3	2.02	0.42
1:B:199:ALA:N	1:B:200:PRO:CD	2.82	0.42
1:B:299:ARG:HD3	1:B:318:SER:O	2.20	0.42
1:C:139:MET:HB2	1:C:168:TRP:CH2	2.54	0.42
1:D:21:THR:HG21	1:D:23:PHE:CZ	2.54	0.42
1:D:212:LEU:C	1:D:212:LEU:HD12	2.44	0.42
1:C:308:LEU:HB3	1:C:309:PRO:CD	2.50	0.42
1:D:125:SER:HB2	1:D:307:SER:OG	2.20	0.42
1:D:165:GLU:HG2	1:D:166:PRO:N	2.35	0.42
1:A:142:ILE:HB	1:A:143:PRO:HD3	2.02	0.42
1:A:355:LEU:O	1:A:359:VAL:HG22	2.20	0.42
1:B:65:HIS:O	1:B:69:HIS:HD2	2.03	0.42
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.88	0.42
1:D:328:ILE:HG13	1:D:329:THR:HG23	2.02	0.42
1:C:354:GLU:HB3	3:C:1435:HOH:O	2.20	0.41
1:D:354:GLU:HG3	1:D:355:LEU:H	1.85	0.41
1:D:139:MET:CB	1:D:145:LEU:HB2	2.50	0.41
1:D:190:ALA:HB1	1:D:194:TYR:CE1	2.55	0.41
1:D:363:LYS:O	1:D:364:VAL:HG22	2.20	0.41
1:A:308:LEU:CB	1:A:309:PRO:HD2	2.49	0.41
1:B:163:LYS:CE	1:B:191:ASN:OD1	2.68	0.41
1:B:280:CYS:HB3	1:B:285:ILE:O	2.20	0.41
1:C:7:GLU:OE1	1:C:35:ARG:NH1	2.54	0.41
1:C:185:LEU:N	1:C:185:LEU:HD23	2.35	0.41
1:D:170:VAL:HA	1:D:205:LEU:CD2	2.50	0.41
1:A:82:THR:CG2	1:A:84:ALA:H	2.26	0.41
1:A:142:ILE:N	1:A:143:PRO:CD	2.84	0.41
1:A:163:LYS:HA	1:A:163:LYS:HD2	1.83	0.41
1:A:356:LEU:C	1:A:356:LEU:HD23	2.46	0.41
1:B:87:THR:HB	1:B:88:PRO:HD3	2.01	0.41
1:C:206:ASP:HB2	1:C:207:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ALA:O	1:D:178:GLU:HB3	2.20	0.41
1:D:227:GLU:HA	1:D:230:ARG:HH11	1.85	0.41
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.72	0.41
1:A:113:ARG:HG3	1:A:346:GLY:HA3	2.01	0.41
1:B:132:CYS:SG	1:B:317:THR:O	2.74	0.41
1:B:299:ARG:O	1:B:303:VAL:HG23	2.20	0.41
1:C:125:SER:HA	1:C:308:LEU:HD12	2.03	0.41
1:D:334:LEU:HD12	1:D:334:LEU:HA	1.78	0.41
1:A:210:LEU:H	1:A:210:LEU:HG	1.67	0.41
1:B:163:LYS:HE3	1:B:189:ASP:CG	2.46	0.41
1:C:141:THR:HG23	1:C:143:PRO:HG2	2.03	0.41
2:C:1164:NPG:HE2	1:D:62:GLY:HA2	2.02	0.41
1:D:271:LEU:HA	1:D:271:LEU:HD23	1.74	0.41
1:D:334:LEU:CD1	1:D:339:LEU:CD1	2.94	0.41
1:A:5:GLY:HA3	1:A:365:TRP:CZ2	2.56	0.41
1:B:298:GLY:O	1:B:299:ARG:C	2.64	0.41
1:D:2:LYS:O	1:D:39:PRO:HD3	2.20	0.41
1:D:196:LEU:O	1:D:199:ALA:CB	2.68	0.41
1:A:25:THR:HG22	1:A:26:GLN:N	2.36	0.41
1:A:277:HIS:CD2	1:A:311:PHE:CE1	3.08	0.41
1:B:32:LEU:HB3	1:B:47:CYS:HB3	2.03	0.41
1:C:10:ARG:HD3	1:C:64:GLU:OE2	2.21	0.41
1:C:139:MET:HB2	1:C:168:TRP:CZ2	2.56	0.41
1:C:352:ILE:O	1:C:355:LEU:N	2.54	0.41
1:D:13:MET:HE2	1:D:324:TYR:CG	2.56	0.41
1:D:81:ILE:O	1:D:81:ILE:HG22	2.21	0.41
1:D:220:GLU:HA	3:D:1589:HOH:O	2.20	0.41
1:A:3:LEU:HD12	1:A:3:LEU:HA	1.61	0.41
1:A:321:ASP:HA	1:A:324:TYR:O	2.21	0.41
1:B:8:LEU:O	1:B:363:LYS:HA	2.21	0.41
1:B:33:LEU:C	1:B:34:LEU:HD12	2.46	0.41
1:A:189:ASP:HA	1:A:214:GLU:HB3	2.02	0.40
1:B:29:ARG:HD2	1:B:31:LEU:HG	2.03	0.40
1:D:15:LEU:HD23	1:D:324:TYR:CE2	2.51	0.40
1:D:142:ILE:HD13	1:D:142:ILE:HA	1.82	0.40
1:D:264:PRO:HG3	1:D:305:LEU:HD22	2.03	0.40
1:A:29:ARG:HH22	1:A:50:MET:HA	1.85	0.40
1:B:132:CYS:O	1:B:158:VAL:HG22	2.21	0.40
1:B:277:HIS:CD2	1:B:311:PHE:CE1	3.09	0.40
1:D:33:LEU:N	1:D:33:LEU:HD23	2.37	0.40
1:D:139:MET:CB	1:D:168:TRP:CH2	2.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ILE:CD1	2:D:1500:NPG:CD2	3.00	0.40
1:A:169:ASP:OD1	1:A:194:TYR:OH	2.39	0.40
1:A:177:ARG:HD3	1:A:177:ARG:HA	1.85	0.40
1:C:258:GLN:HE21	1:C:258:GLN:HB3	1.68	0.40
1:C:288:TRP:HB3	1:C:313:LEU:HB2	2.03	0.40
1:D:271:LEU:O	1:D:272:GLU:C	2.64	0.40
1:A:87:THR:CB	1:A:88:PRO:HD3	2.51	0.40
1:C:3:LEU:H	1:C:81:ILE:HD13	1.86	0.40
1:C:142:ILE:O	1:C:145:LEU:HB3	2.22	0.40
1:D:239:ASP:CG	1:D:263:LYS:HE3	2.47	0.40
1:C:29:ARG:HG2	1:C:324:TYR:OH	2.22	0.40
1:C:352:ILE:HA	1:C:353:PRO:HD3	1.59	0.40
1:D:12:GLN:HG2	1:D:28:VAL:CG1	2.52	0.40

All (2) 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:111:GLU:OE2	1:D:117:ARG:NH2[17_555]	1.85	0.35
3:A:1310:HOH:O	3:D:1604:HOH:O[17_555]	1.97	0.23

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/368 (99%)	350 (96%)	15 (4%)	0	100	100
1	B	366/368 (100%)	358 (98%)	8 (2%)	0	100	100
1	C	365/368 (99%)	349 (96%)	15 (4%)	1 (0%)	36	26
1	D	365/368 (99%)	334 (92%)	29 (8%)	2 (0%)	24	13
All	All	1461/1472 (99%)	1391 (95%)	67 (5%)	3 (0%)	43	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	144	GLN
1	C	353	PRO
1	D	39	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/291 (100%)	254 (88%)	36 (12%)	4	0
1	B	291/291 (100%)	268 (92%)	23 (8%)	11	2
1	C	290/291 (100%)	263 (91%)	27 (9%)	8	1
1	D	290/291 (100%)	248 (86%)	42 (14%)	3	0
All	All	1161/1164 (100%)	1033 (89%)	128 (11%)	6	1

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	4	SER
1	A	8	LEU
1	A	15	LEU
1	A	16	VAL
1	A	27	SER
1	A	29	ARG
1	A	30	GLU
1	A	31	LEU
1	A	32	LEU
1	A	34	LEU
1	A	35	ARG
1	A	79	GLU
1	A	80	ASP
1	A	82	THR
1	A	85	LYS

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Mol	Chain	Res	Type
1	A	116	GLU
1	A	127	ARG
1	A	142	ILE
1	A	155	GLU
1	A	163	LYS
1	A	165	GLU
1	A	169	ASP
1	A	177	ARG
1	A	178	GLU
1	A	179	ARG
1	A	184	VAL
1	A	185	LEU
1	A	227	GLU
1	A	333	VAL
1	A	343	THR
1	A	349	VAL
1	A	354	GLU
1	A	356	LEU
1	A	363	LYS
1	B	3	LEU
1	B	12	GLN
1	B	27	SER
1	B	29	ARG
1	B	32	LEU
1	B	79	GLU
1	B	80	ASP
1	B	92	LYS
1	B	144	GLN
1	B	159	ARG
1	B	163	LYS
1	B	169	ASP
1	B	177	ARG
1	B	178	GLU
1	B	179	ARG
1	B	227	GLU
1	B	274	ARG
1	B	313	LEU
1	B	328	ILE
1	B	339	LEU
1	B	355	LEU
1	B	358	GLU
1	B	363	LYS

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Mol	Chain	Res	Type
1	C	1	MET
1	C	2	LYS
1	C	8	LEU
1	C	12	GLN
1	C	31	LEU
1	C	103	LEU
1	C	113	ARG
1	C	119	PHE
1	C	126	VAL
1	C	141	THR
1	C	142	ILE
1	C	174	ARG
1	C	177	ARG
1	C	185	LEU
1	C	204	ARG
1	C	213	ILE
1	C	217	LEU
1	C	227	GLU
1	C	233	GLN
1	C	261	ASN
1	C	274	ARG
1	C	293	ILE
1	C	354	GLU
1	C	356	LEU
1	C	361	THR
1	C	363	LYS
1	C	364	VAL
1	D	2	LYS
1	D	7	GLU
1	D	13	MET
1	D	22	SER
1	D	27	SER
1	D	29	ARG
1	D	32	LEU
1	D	33	LEU
1	D	42	GLU
1	D	54	LEU
1	D	68	ARG
1	D	79	GLU
1	D	81	ILE
1	D	92	LYS
1	D	116	GLU

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Mol	Chain	Res	Type
1	D	117	ARG
1	D	119	PHE
1	D	139	MET
1	D	141	THR
1	D	145	LEU
1	D	155	GLU
1	D	164	ILE
1	D	165	GLU
1	D	169	ASP
1	D	170	VAL
1	D	171	GLU
1	D	177	ARG
1	D	185	LEU
1	D	194	TYR
1	D	205	LEU
1	D	213	ILE
1	D	217	LEU
1	D	220	GLU
1	D	227	GLU
1	D	228	LEU
1	D	236	ILE
1	D	263	LYS
1	D	325	LYS
1	D	339	LEU
1	D	355	LEU
1	D	363	LYS
1	D	364	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	65	HIS
1	A	69	HIS
1	A	258	GLN
1	A	283	HIS
1	B	12	GLN
1	B	65	HIS
1	B	258	GLN
1	C	12	GLN
1	C	69	HIS
1	C	258	GLN

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Mol	Chain	Res	Type
1	D	65	HIS
1	D	69	HIS
1	D	258	GLN
1	D	283	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
2	NPG	D	1500	-	18,18,18	1.31	2 (11%)	21,23,23	1.38	4 (19%)
2	NPG	C	1164	-	18,18,18	1.36	2 (11%)	21,23,23	2.69	8 (38%)
2	NPG	A	1200	-	18,18,18	1.32	2 (11%)	21,23,23	1.52	5 (23%)
2	NPG	C	1400	-	18,18,18	1.35	2 (11%)	21,23,23	1.21	3 (14%)
2	NPG	B	1300	-	18,18,18	1.30	2 (11%)	21,23,23	2.23	8 (38%)
2	NPG	B	1163	-	18,18,18	1.34	2 (11%)	21,23,23	2.73	9 (42%)

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
2	NPG	D	1500	-	-	5/17/17/17	0/1/1/1
2	NPG	C	1164	-	-	6/17/17/17	0/1/1/1
2	NPG	A	1200	-	-	6/17/17/17	0/1/1/1
2	NPG	C	1400	-	-	7/17/17/17	0/1/1/1
2	NPG	B	1300	-	-	6/17/17/17	0/1/1/1
2	NPG	B	1163	-	-	4/17/17/17	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1163	NPG	CG-C1	-3.56	1.47	1.52
2	C	1164	NPG	CG-C1	-3.41	1.47	1.52
2	A	1200	NPG	C3-N1	3.20	1.40	1.34
2	C	1400	NPG	C3-N1	3.15	1.40	1.34
2	D	1500	NPG	C3-N1	2.89	1.40	1.34
2	A	1200	NPG	CG-C1	-2.84	1.48	1.52
2	B	1300	NPG	CG-C1	-2.70	1.48	1.52
2	B	1300	NPG	C3-N1	2.61	1.39	1.34
2	C	1400	NPG	CG-C1	-2.58	1.48	1.52
2	D	1500	NPG	CG-C1	-2.57	1.48	1.52
2	C	1164	NPG	C3-N1	2.49	1.39	1.34
2	B	1163	NPG	C3-N1	2.10	1.38	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1164	NPG	CG-C1-C2	9.87	128.34	109.44
2	B	1163	NPG	CG-C1-C2	8.13	125.00	109.44
2	B	1300	NPG	C4-C3-N1	-5.47	106.24	115.86
2	B	1163	NPG	C5-C4-C3	-4.61	103.18	112.67
2	B	1163	NPG	CD1-CG-C1	-4.55	113.49	120.78
2	B	1300	NPG	C4-C5-C6	-3.36	104.74	113.67
2	B	1300	NPG	O31-C3-C4	3.24	127.89	122.02
2	B	1300	NPG	CG-C1-C2	3.16	115.49	109.44
2	A	1200	NPG	O12-C2-O11	-3.05	117.17	124.08
2	B	1163	NPG	CG-C1-N1	-2.95	105.30	112.75
2	B	1300	NPG	O12-C2-C1	2.92	120.88	113.62
2	B	1300	NPG	O62-C6-C5	2.83	122.94	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1400	NPG	CG-C1-C2	2.80	114.81	109.44
2	B	1300	NPG	O12-C2-O11	-2.79	117.75	124.08
2	A	1200	NPG	C4-C3-N1	2.77	120.74	115.86
2	C	1164	NPG	CD1-CG-C1	-2.70	116.46	120.78
2	C	1164	NPG	O62-C6-C5	2.62	122.28	114.00
2	B	1300	NPG	O61-C6-C5	-2.58	114.89	123.09
2	A	1200	NPG	C5-C4-C3	-2.58	107.36	112.67
2	C	1400	NPG	O12-C2-O11	-2.53	118.34	124.08
2	B	1163	NPG	CD2-CG-CD1	2.53	121.44	118.30
2	C	1400	NPG	O12-C2-C1	2.50	119.84	113.62
2	B	1163	NPG	CD2-CG-C1	2.41	124.65	120.78
2	C	1164	NPG	O31-C3-C4	2.39	126.34	122.02
2	D	1500	NPG	CG-C1-C2	2.38	113.99	109.44
2	D	1500	NPG	C4-C5-C6	-2.36	107.40	113.67
2	D	1500	NPG	O12-C2-C1	2.30	119.33	113.62
2	C	1164	NPG	CD2-CG-CD1	2.23	121.07	118.30
2	C	1164	NPG	CG-C1-N1	-2.23	107.12	112.75
2	D	1500	NPG	O12-C2-O11	-2.20	119.10	124.08
2	B	1163	NPG	O12-C2-O11	-2.20	119.10	124.08
2	C	1164	NPG	C4-C3-N1	-2.17	112.04	115.86
2	A	1200	NPG	O12-C2-C1	2.16	118.99	113.62
2	B	1163	NPG	C4-C5-C6	-2.14	107.99	113.67
2	B	1163	NPG	O62-C6-C5	2.08	120.56	114.00
2	A	1200	NPG	C4-C5-C6	-2.04	108.25	113.67
2	C	1164	NPG	O62-C6-O61	-2.02	118.12	123.33

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1300	NPG	C4-C3-N1-C1
2	B	1300	NPG	O31-C3-N1-C1
2	D	1500	NPG	C3-C4-C5-C6
2	D	1500	NPG	C4-C3-N1-C1
2	D	1500	NPG	O31-C3-N1-C1
2	C	1164	NPG	C4-C3-N1-C1
2	C	1164	NPG	O31-C3-N1-C1
2	A	1200	NPG	N1-C3-C4-C5
2	B	1163	NPG	C3-C4-C5-C6
2	C	1400	NPG	N1-C3-C4-C5
2	A	1200	NPG	O31-C3-C4-C5
2	C	1400	NPG	O31-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	D	1500	NPG	C2-C1-CG-CD1
2	D	1500	NPG	C2-C1-CG-CD2
2	C	1164	NPG	N1-C1-C2-O12
2	A	1200	NPG	C2-C1-CG-CD1
2	C	1400	NPG	C2-C1-CG-CD1
2	B	1300	NPG	C2-C1-CG-CD1
2	C	1164	NPG	C2-C1-N1-C3
2	A	1200	NPG	C2-C1-CG-CD2
2	C	1164	NPG	C4-C5-C6-O61
2	B	1300	NPG	C2-C1-CG-CD2
2	C	1400	NPG	C2-C1-CG-CD2
2	B	1300	NPG	C4-C5-C6-O62
2	C	1164	NPG	C4-C5-C6-O62
2	B	1163	NPG	C2-C1-N1-C3
2	B	1300	NPG	C4-C5-C6-O61
2	A	1200	NPG	C4-C5-C6-O61
2	A	1200	NPG	C4-C5-C6-O62
2	B	1163	NPG	C4-C5-C6-O61
2	C	1400	NPG	C4-C5-C6-O62
2	C	1400	NPG	CG-C1-N1-C3
2	B	1163	NPG	C4-C5-C6-O62
2	C	1400	NPG	C4-C5-C6-O61

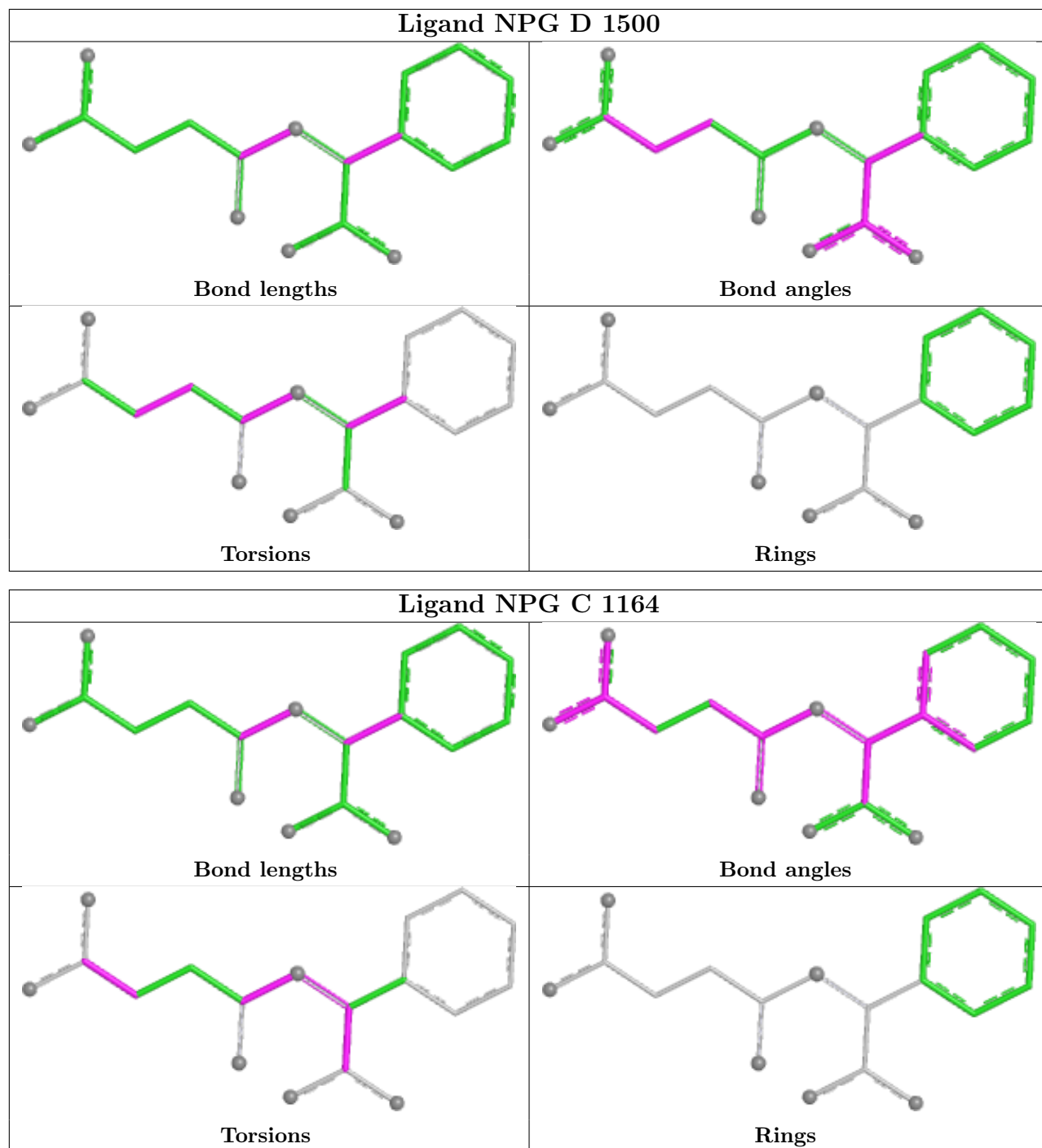
There are no ring outliers.

5 monomers are involved in 21 short contacts:

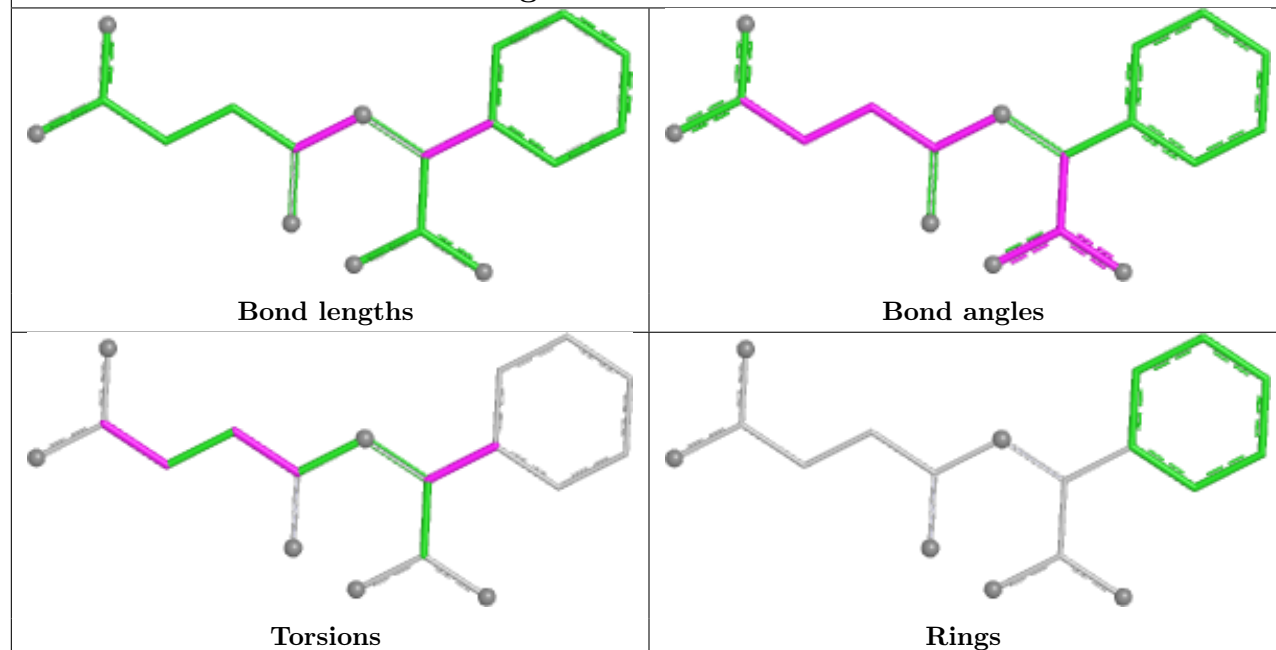
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1500	NPG	12	0
2	C	1164	NPG	3	0
2	A	1200	NPG	1	0
2	C	1400	NPG	4	0
2	B	1163	NPG	1	0

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 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

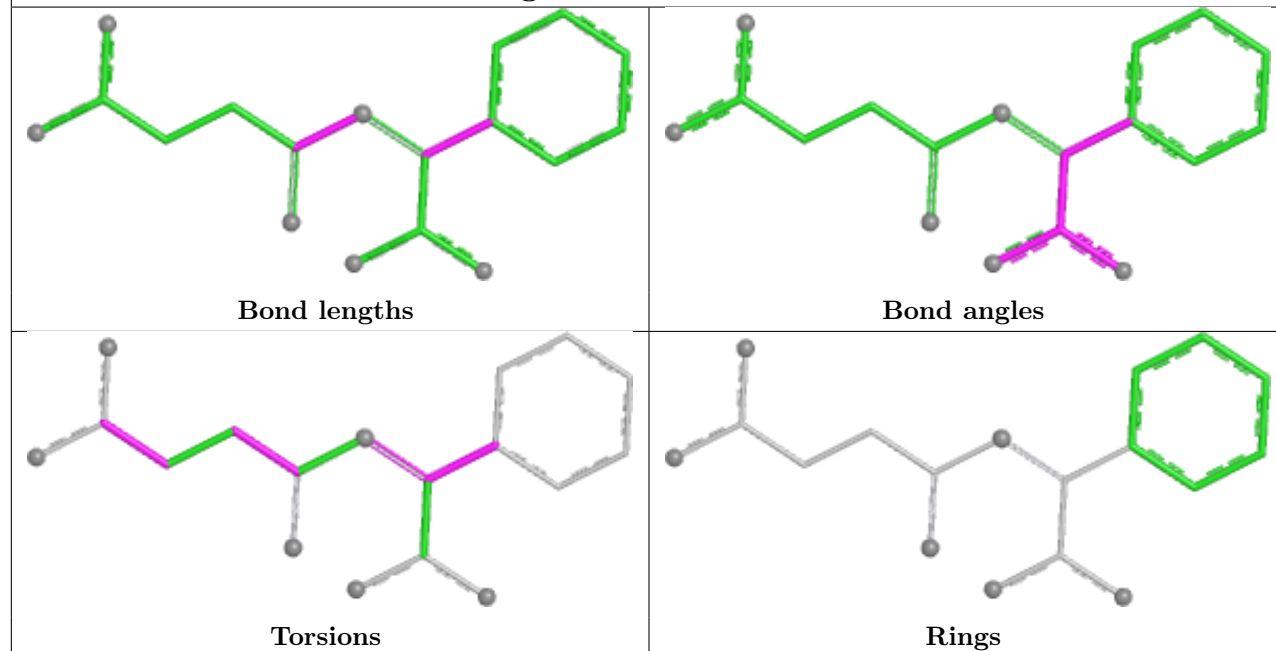
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

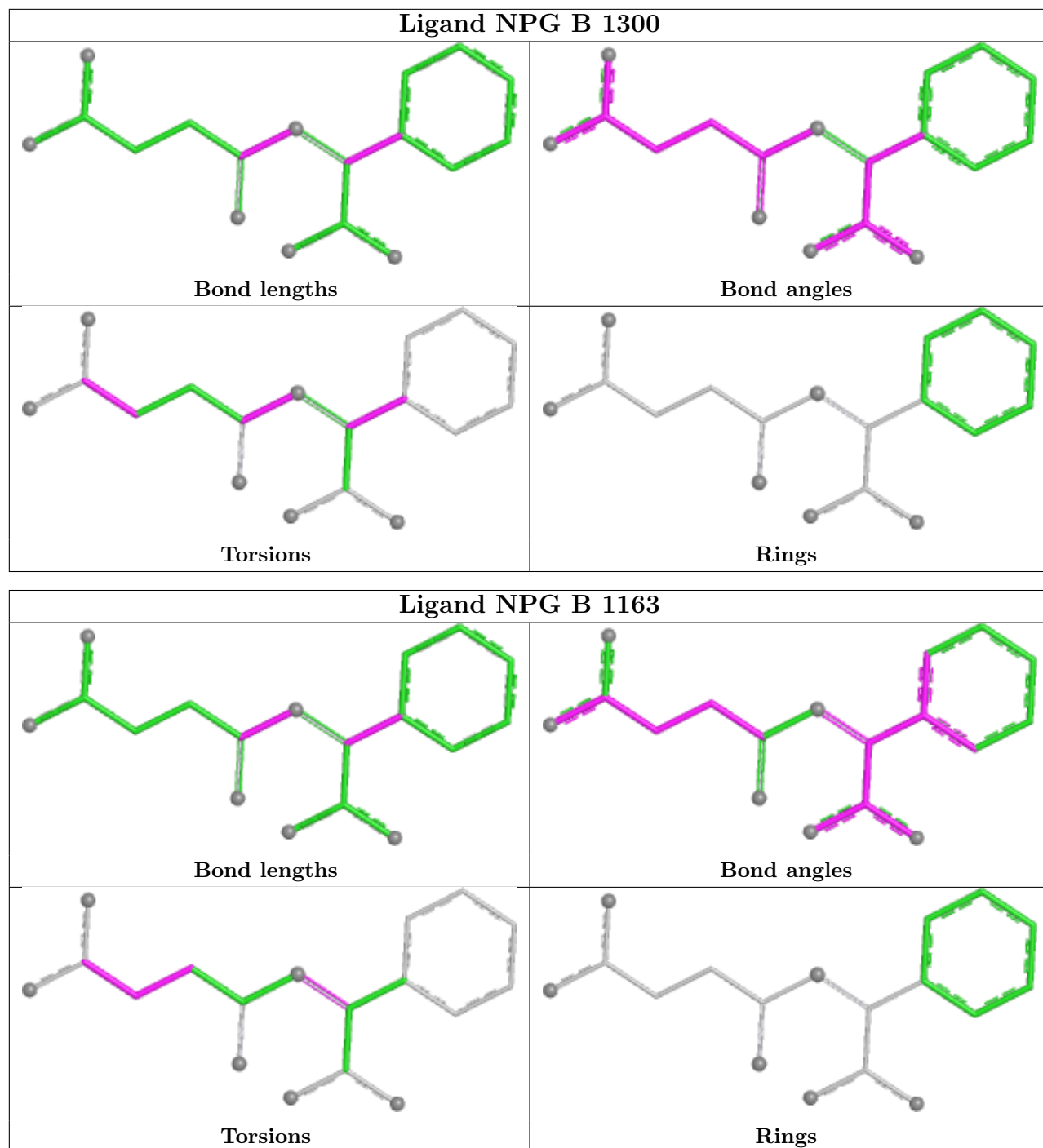


Ligand NPG A 1200



Ligand NPG C 1400





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	367/368 (99%)	0.09	12 (3%) 49 54	17, 37, 69, 96	0
1	B	368/368 (100%)	-0.42	5 (1%) 73 79	17, 27, 55, 91	0
1	C	367/368 (99%)	-0.18	6 (1%) 70 75	19, 30, 61, 97	0
1	D	367/368 (99%)	0.92	84 (22%) 2 2	15, 46, 89, 100	0
All	All	1469/1472 (99%)	0.10	107 (7%) 21 24	15, 33, 78, 100	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	184	VAL	5.6
1	D	208	PHE	5.2
1	D	142	ILE	5.1
1	D	196	LEU	5.1
1	D	17	ALA	5.0
1	D	19	PHE	5.0
1	D	324	TYR	4.9
1	D	23	PHE	4.8
1	D	193	ALA	4.8
1	D	40	ALA	4.6
1	D	145	LEU	4.6
1	D	232	ILE	4.6
1	D	39	PRO	4.5
1	D	22	SER	4.5
1	D	209	GLY	4.3
1	B	1	MET	4.3
1	A	367	GLY	4.2
1	D	205	LEU	4.2
1	D	234	THR	4.0
1	D	333	VAL	4.0
1	D	168	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	210	LEU	3.8
1	D	367	GLY	3.7
1	D	195	THR	3.6
1	D	170	VAL	3.6
1	D	186	LEU	3.6
1	C	81	ILE	3.5
1	D	164	ILE	3.5
1	D	181	GLY	3.5
1	D	325	LYS	3.5
1	D	21	THR	3.4
1	D	228	LEU	3.4
1	D	24	GLY	3.3
1	D	137	GLY	3.3
1	D	1	MET	3.3
1	D	44	TRP	3.3
1	D	54	LEU	3.1
1	D	180	PHE	3.1
1	D	26	GLN	3.1
1	D	55	TYR	3.0
1	D	231	ARG	3.0
1	A	142	ILE	3.0
1	D	185	LEU	3.0
1	D	352	ILE	2.9
1	D	138	ILE	2.8
1	B	231	ARG	2.8
1	D	177	ARG	2.7
1	A	40	ALA	2.7
1	D	217	LEU	2.7
1	C	141	THR	2.6
1	D	317	THR	2.6
1	D	230	ARG	2.6
1	D	14	PRO	2.6
1	D	16	VAL	2.6
1	D	25	THR	2.6
1	D	18	PRO	2.6
1	D	153	LEU	2.6
1	B	126	VAL	2.6
1	D	28	VAL	2.6
1	D	326	THR	2.6
1	D	146	LEU	2.5
1	C	367	GLY	2.5
1	C	40	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	175	ALA	2.5
1	D	143	PRO	2.5
1	D	173	VAL	2.5
1	D	363	LYS	2.5
1	D	149	VAL	2.5
1	D	211	LEU	2.4
1	D	80	ASP	2.4
1	B	368	SER	2.4
1	A	2	LYS	2.4
1	D	194	TYR	2.4
1	A	16	VAL	2.4
1	D	126	VAL	2.4
1	D	362	ALA	2.3
1	A	1	MET	2.3
1	A	184	VAL	2.3
1	D	79	GLU	2.3
1	D	202	LEU	2.3
1	A	180	PHE	2.3
1	D	355	LEU	2.3
1	B	2	LYS	2.3
1	D	199	ALA	2.3
1	D	203	ALA	2.3
1	C	80	ASP	2.3
1	D	15	LEU	2.2
1	D	344	GLY	2.2
1	A	324	TYR	2.2
1	C	2	LYS	2.2
1	A	18	PRO	2.2
1	D	68	ARG	2.2
1	D	220	GLU	2.2
1	D	233	GLN	2.2
1	D	318	SER	2.2
1	A	208	PHE	2.1
1	D	183	ASP	2.1
1	D	167	GLY	2.1
1	D	162	LEU	2.1
1	D	136	VAL	2.1
1	D	336	GLY	2.1
1	A	14	PRO	2.1
1	D	334	LEU	2.1
1	D	27	SER	2.1
1	D	323	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	182	ASP	2.0
1	D	364	VAL	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](#)

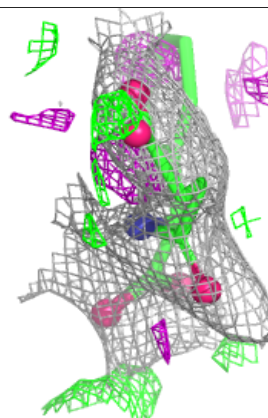
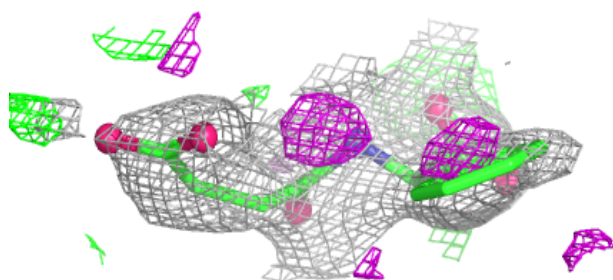
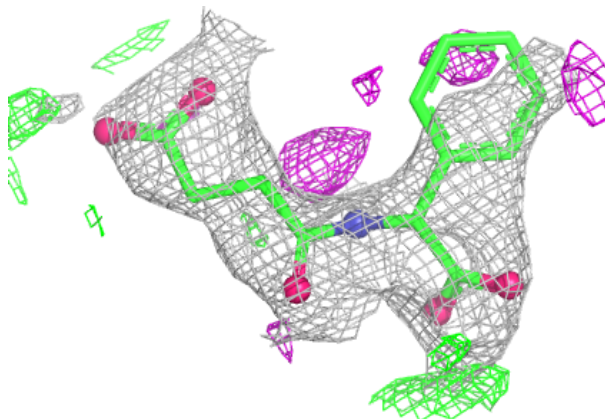
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	NPG	D	1500	18/18	0.81	0.22	50,84,100,100	0
2	NPG	C	1164	18/18	0.89	0.17	29,79,100,100	0
2	NPG	B	1300	18/18	0.93	0.13	29,44,65,67	0
2	NPG	B	1163	18/18	0.93	0.13	24,54,100,100	0
2	NPG	A	1200	18/18	0.94	0.12	30,53,98,100	0
2	NPG	C	1400	18/18	0.97	0.07	23,33,47,48	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.

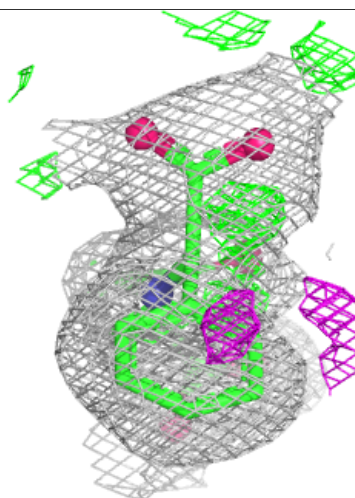
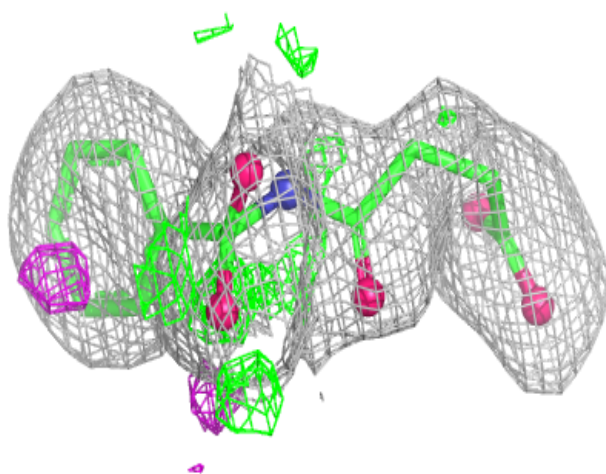
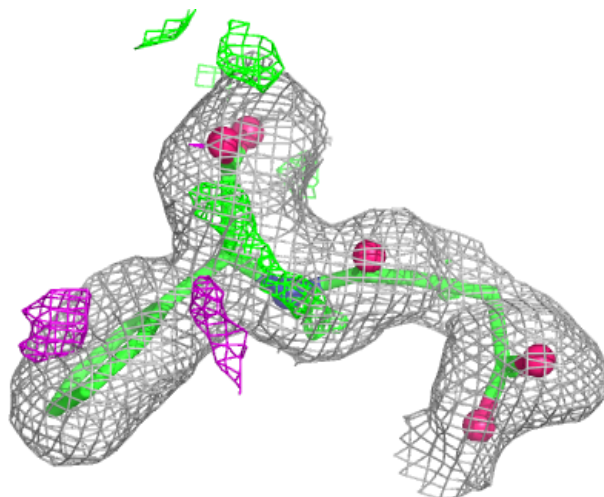
Electron density around NPG D 1500:

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



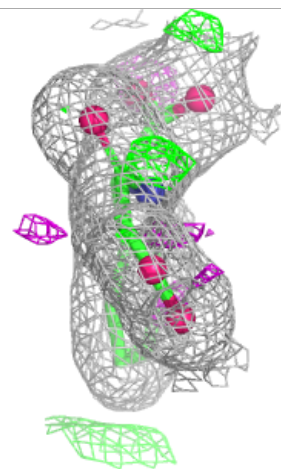
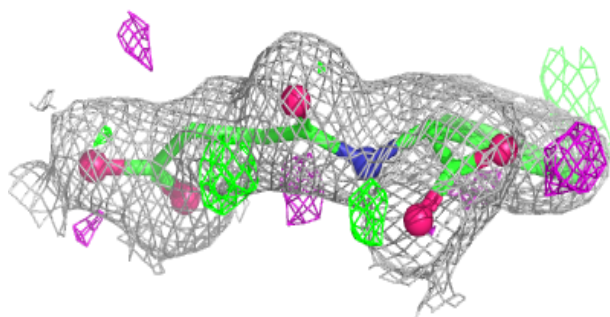
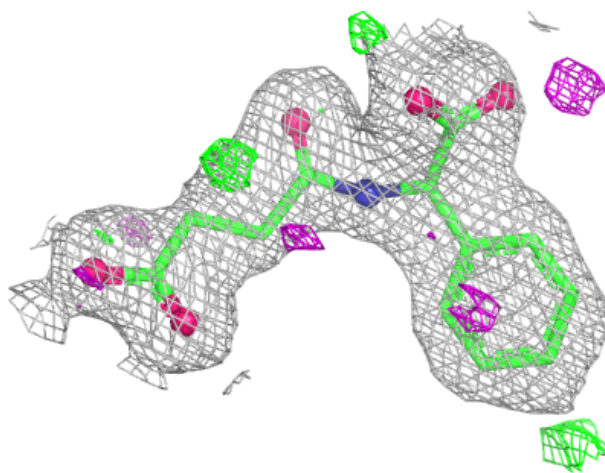
Electron density around NPG C 1164:

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



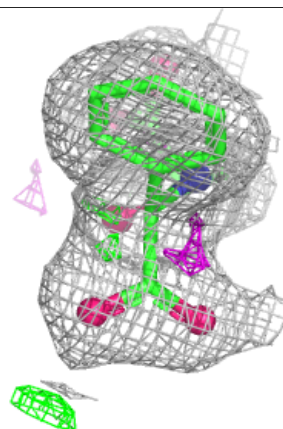
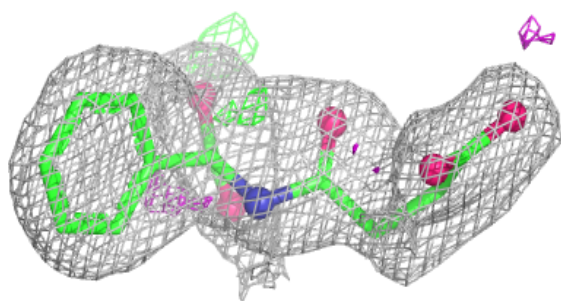
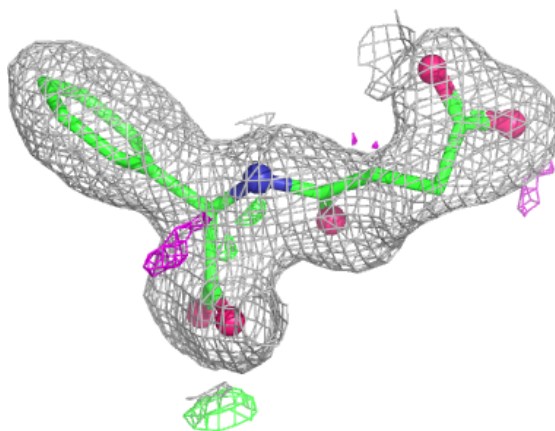
Electron density around NPG B 1300:

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



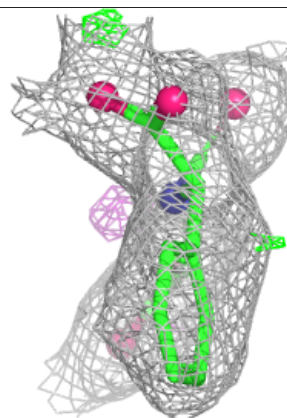
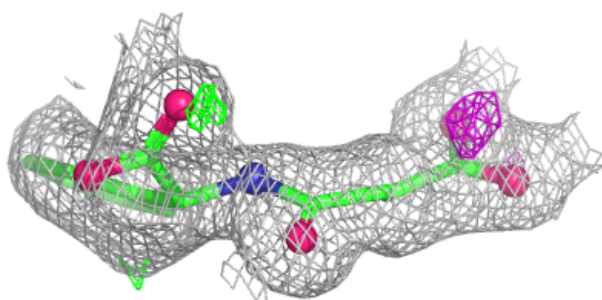
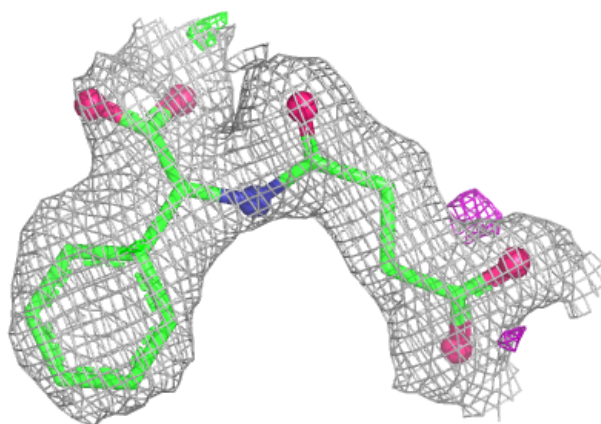
Electron density around NPG B 1163:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



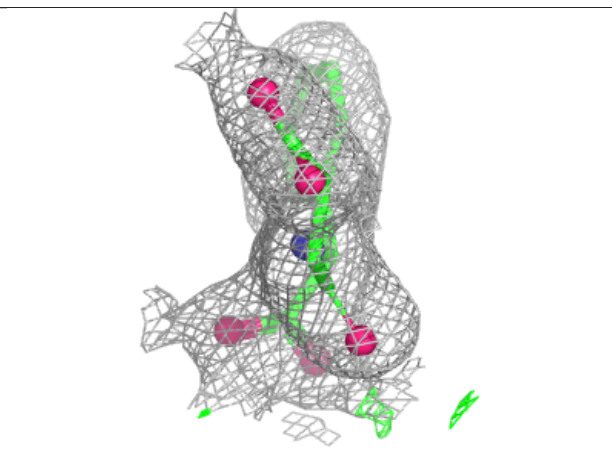
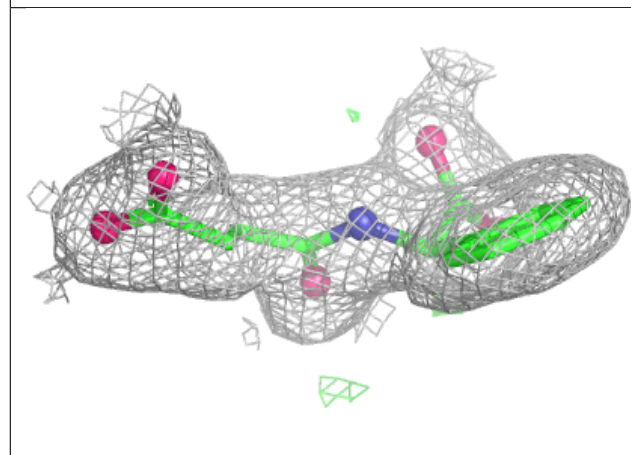
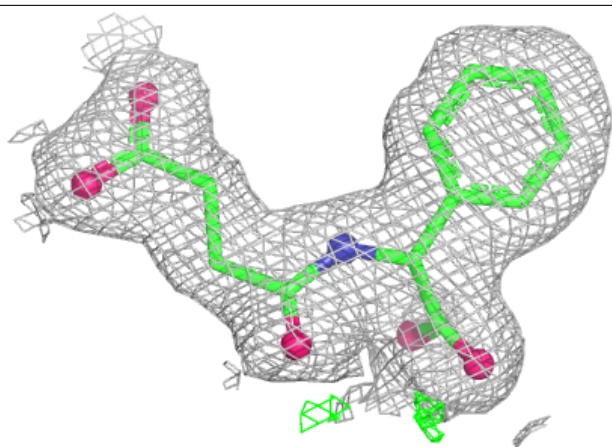
Electron density around NPG A 1200:

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



Electron density around NPG C 1400:

$2mF_o-DF_c$ (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.