



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:51 AM EDT

PDB ID : 6V4A
Title : An open conformation of a Pentameic ligand-gated ion channel with additional N-terminal domain
Authors : Delarue, M.; Hu, H.D.
Deposited on : 2019-11-27
Resolution : 3.83 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.10.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

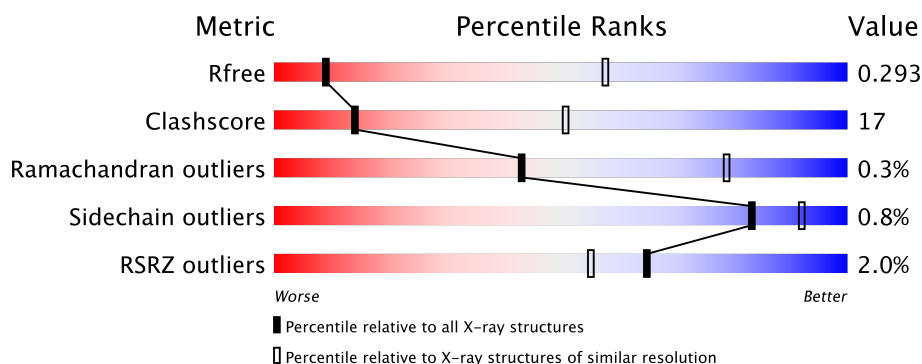
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.83 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}	111664	1018 (4.08-3.60)
Clashscore	122126	1087 (4.08-3.60)
Ramachandran outliers	120053	1050 (4.08-3.60)
Sidechain outliers	120020	1044 (4.08-3.60)
RSRZ outliers	108989	1002 (4.10-3.58)

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 on 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	642	<div> <div>2%</div> <div>64%</div> <div>25%</div> <div>8%</div> </div>
1	B	642	<div> <div>2%</div> <div>64%</div> <div>25%</div> <div>8%</div> </div>
1	C	642	<div> <div>%</div> <div>67%</div> <div>24%</div> <div>8%</div> </div>
1	D	642	<div> <div>2%</div> <div>67%</div> <div>24%</div> <div>8%</div> </div>
1	E	642	<div> <div>%</div> <div>67%</div> <div>23%</div> <div>8%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	P3A	E	702	-	-	-	X

2 Entry composition [i](#)

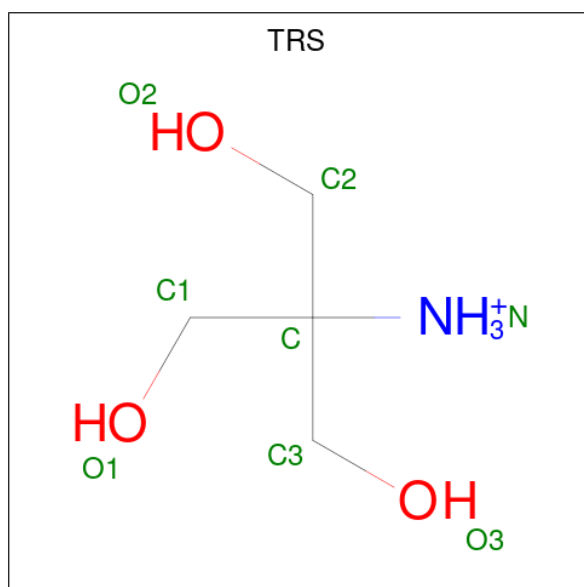
There are 3 unique types of molecules in this entry. The entry contains 23190 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Neur_chan_LBD domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4598	2966	752	869	11			
1	E	592	Total	C	N	O	S	0	0	0
			4604	2965	755	873	11			
1	D	592	Total	C	N	O	S	0	0	0
			4620	2976	758	875	11			
1	C	593	Total	C	N	O	S	0	0	0
			4628	2982	759	876	11			
1	B	589	Total	C	N	O	S	0	0	0
			4598	2966	752	869	11			

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



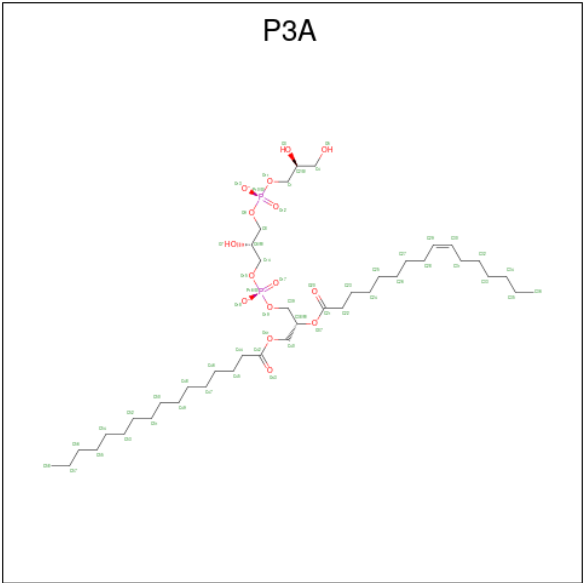
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is PHOSPHATIDYLGLYCEROL-PHOSPHOGLYCEROL (three-letter code: P3A) (formula: C₄₁H₇₈O₁₅P₂).

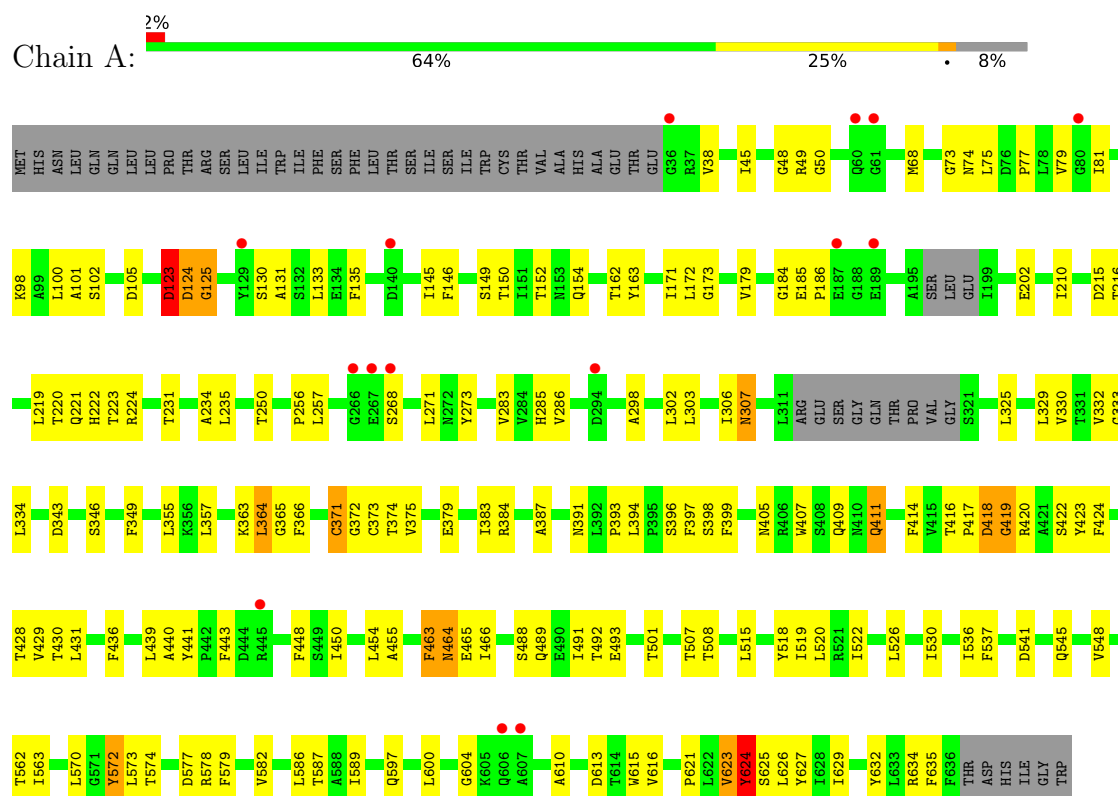


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			20	7	11	2		
3	A	1	Total	C	O	P	0	0
			21	8	11	2		
3	E	1	Total	C	O	P	0	0
			20	7	11	2		
3	C	1	Total	C	O	P	0	0
			20	7	11	2		
3	B	1	Total	C	O	P	0	0
			21	8	11	2		

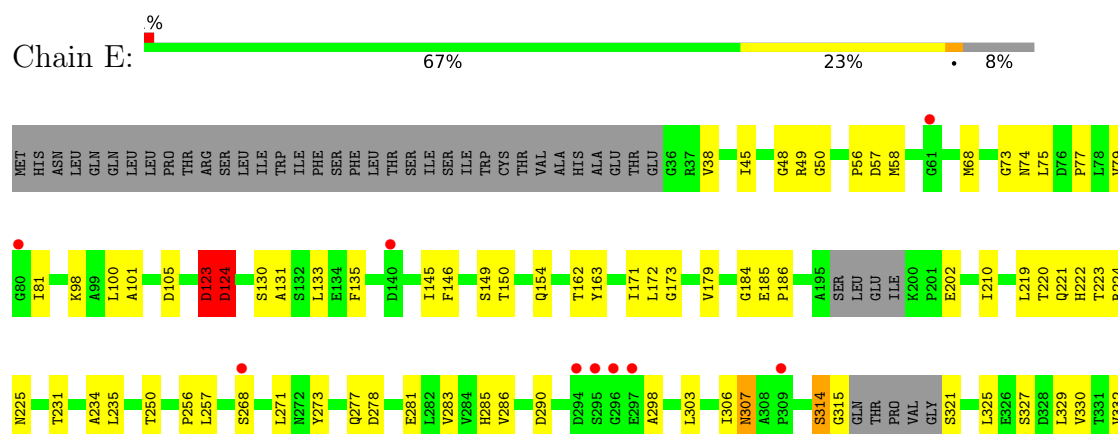
3 Residue-property plots [i](#)

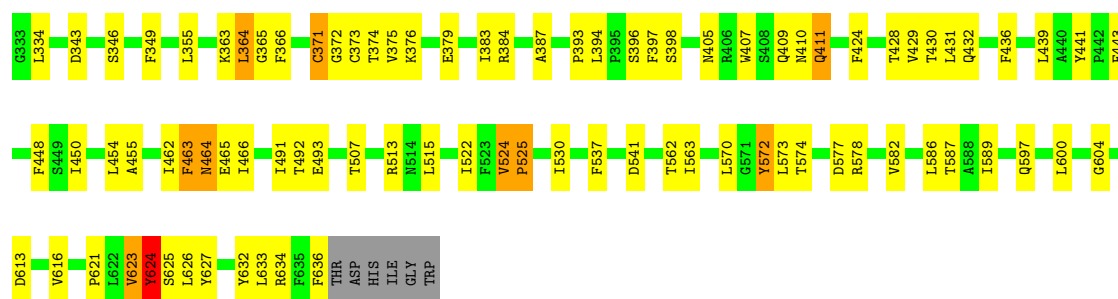
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

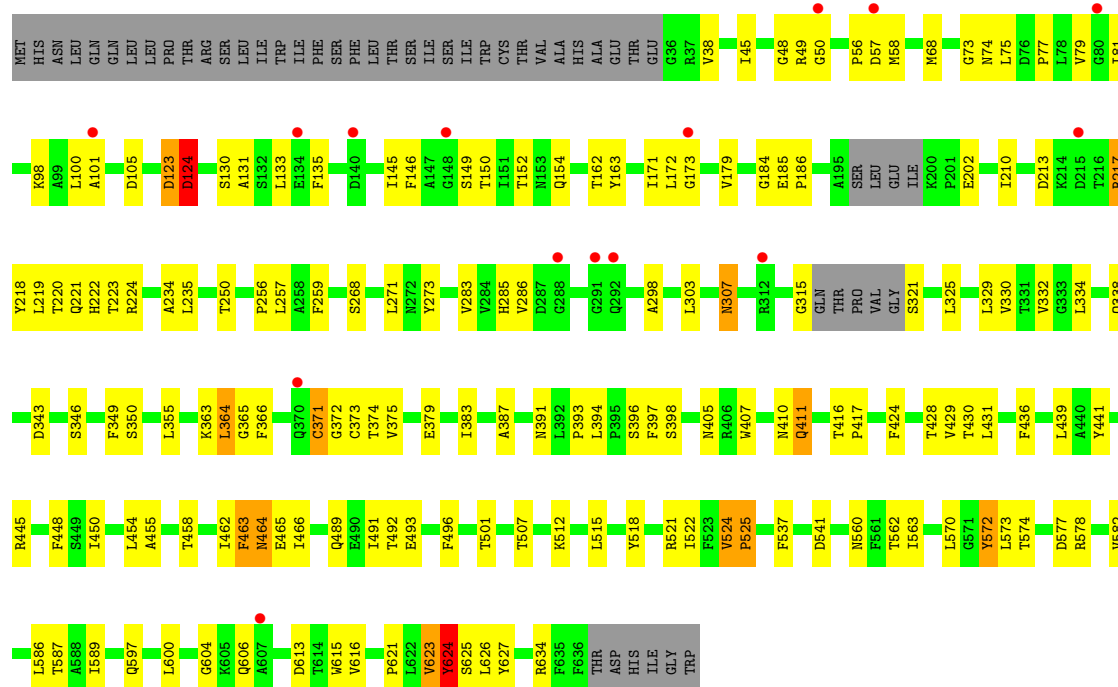


- Molecule 1: Neur_chan_LBD domain-containing protein

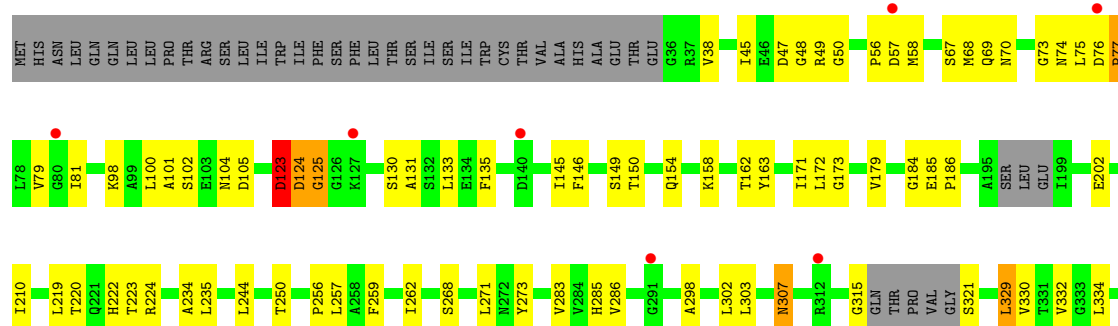


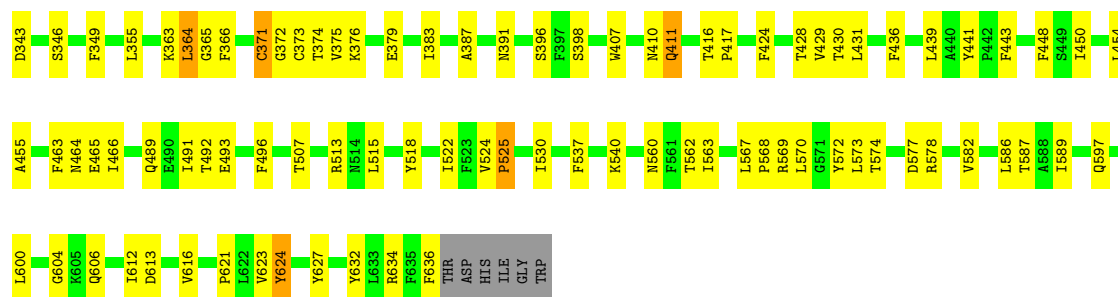


• Molecule 1: Neur_chan_LBD domain-containing protein

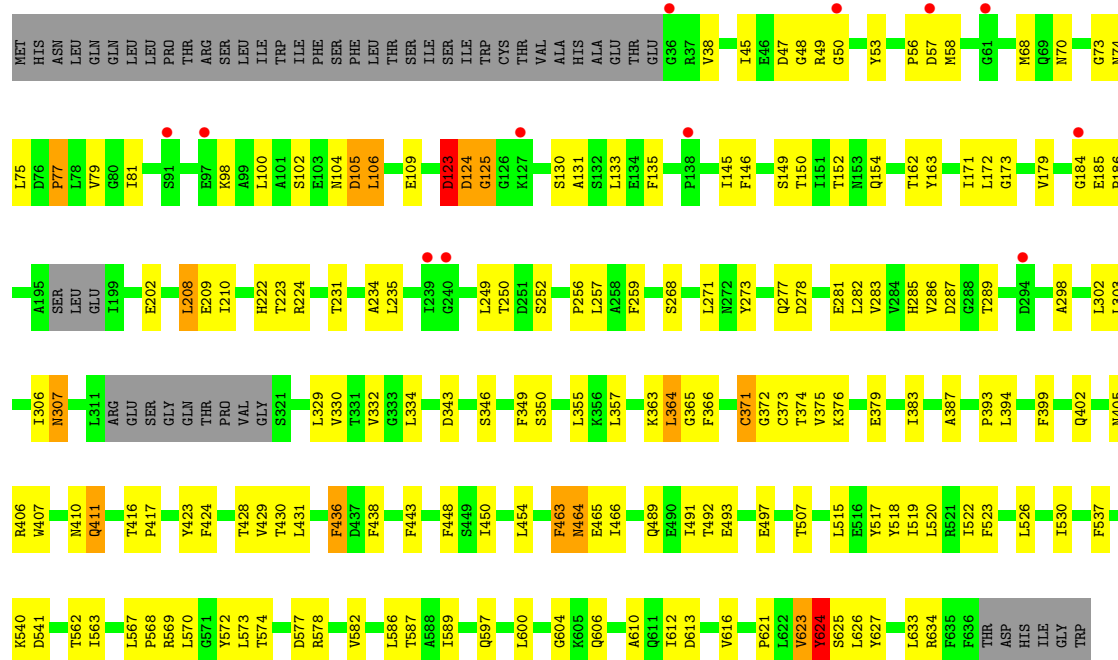


• Molecule 1: Neur_chan_LBD domain-containing protein





• Molecule 1: Neur_chan_LBD domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	141.06Å 116.03Å 169.63Å 90.00° 109.17° 90.00°	Depositor
Resolution (Å)	25.00 – 3.83 25.00 – 3.83	Depositor EDS
% Data completeness (in resolution range)	73.3 (25.00-3.83) 73.6 (25.00-3.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.85Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.256 , 0.291 0.256 , 0.293	Depositor DCC
R_{free} test set	1876 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	112.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 86.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23190	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: TRS, P3A

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	0.76	1/4702 (0.0%)	1.00	17/6402 (0.3%)
1	B	0.76	1/4702 (0.0%)	1.03	20/6402 (0.3%)
1	C	0.77	2/4732 (0.0%)	1.01	12/6441 (0.2%)
1	D	0.79	3/4724 (0.1%)	1.03	18/6430 (0.3%)
1	E	0.78	1/4707 (0.0%)	1.05	22/6409 (0.3%)
All	All	0.77	8/23567 (0.0%)	1.02	89/32084 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	525	PRO	N-CD	15.71	1.69	1.47
1	D	525	PRO	N-CD	15.34	1.69	1.47
1	C	77	PRO	N-CD	-11.69	1.31	1.47
1	C	525	PRO	N-CD	7.66	1.58	1.47
1	B	77	PRO	N-CD	-7.00	1.38	1.47
1	A	418	ASP	CA-C	6.32	1.69	1.52
1	D	615	TRP	CB-CG	5.72	1.60	1.50
1	D	124	ASP	C-O	5.47	1.33	1.23

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	124	ASP	N-CA-C	10.12	138.34	111.00
1	D	124	ASP	N-CA-C	9.15	135.72	111.00
1	C	76	ASP	C-N-CD	-8.60	101.69	120.60
1	C	77	PRO	N-CA-CB	-8.40	93.22	103.30
1	B	541	ASP	N-CA-C	-8.23	88.79	111.00
1	E	525	PRO	CA-N-CD	-8.17	100.06	111.50
1	D	525	PRO	CA-N-CD	-8.10	100.16	111.50
1	D	525	PRO	N-CA-CB	7.79	112.65	103.30
1	B	497	GLU	CA-CB-CG	7.68	130.31	113.40
1	E	525	PRO	N-CA-CB	7.65	112.48	103.30
1	B	106	LEU	N-CA-CB	7.53	125.46	110.40
1	C	77	PRO	CA-N-CD	7.44	122.12	111.70
1	D	624	TYR	N-CA-CB	7.42	123.96	110.60
1	A	371	CYS	CA-CB-SG	-7.40	100.67	114.00
1	B	371	CYS	CA-CB-SG	-7.38	100.72	114.00
1	E	464	ASN	CB-CA-C	-7.27	95.87	110.40
1	C	371	CYS	CA-CB-SG	-7.21	101.02	114.00
1	C	540	LYS	N-CA-C	7.17	130.35	111.00
1	D	371	CYS	CA-CB-SG	-7.05	101.31	114.00
1	E	371	CYS	CA-CB-SG	-7.03	101.34	114.00
1	B	624	TYR	N-CA-CB	6.93	123.08	110.60
1	E	624	TYR	N-CA-CB	6.91	123.03	110.60
1	B	104	ASN	N-CA-C	6.81	129.40	111.00
1	E	314	SER	N-CA-C	6.63	128.91	111.00
1	C	623	VAL	N-CA-C	-6.57	93.27	111.00
1	E	623	VAL	N-CA-C	-6.53	93.38	111.00
1	E	541	ASP	N-CA-C	-6.47	93.53	111.00
1	D	623	VAL	N-CA-C	-6.47	93.53	111.00
1	D	541	ASP	N-CA-C	-6.39	93.75	111.00
1	E	314	SER	N-CA-CB	-6.33	101.00	110.50
1	A	623	VAL	N-CA-C	-6.27	94.06	111.00
1	B	105	ASP	CB-CA-C	-6.26	97.88	110.40
1	C	298	ALA	N-CA-C	-6.25	94.11	111.00
1	E	298	ALA	N-CA-C	-6.20	94.27	111.00
1	D	298	ALA	N-CA-C	-6.18	94.30	111.00
1	B	623	VAL	N-CA-C	-6.18	94.31	111.00
1	A	298	ALA	N-CA-C	-6.18	94.31	111.00
1	B	298	ALA	N-CA-C	-6.16	94.37	111.00
1	E	124	ASP	CB-CA-C	-6.08	98.24	110.40
1	E	327	SER	N-CA-CB	-6.05	101.42	110.50
1	A	624	TYR	N-CA-CB	6.00	121.40	110.60
1	A	625	SER	N-CA-C	5.99	127.16	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	524	VAL	C-N-CD	5.96	140.92	128.40
1	E	524	VAL	C-N-CD	5.95	140.89	128.40
1	C	364	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	418	ASP	CA-C-O	5.95	132.59	120.10
1	E	364	LEU	CA-CB-CG	5.94	128.97	115.30
1	D	464	ASN	CB-CA-C	-5.94	98.52	110.40
1	A	541	ASP	N-CA-C	-5.93	94.99	111.00
1	A	419	GLY	N-CA-C	-5.92	98.31	113.10
1	D	217	ARG	CB-CG-CD	5.92	126.98	111.60
1	B	364	LEU	CA-CB-CG	5.90	128.87	115.30
1	A	418	ASP	CA-C-N	-5.87	104.45	116.20
1	D	364	LEU	CA-CB-CG	5.86	128.78	115.30
1	B	307	ASN	N-CA-C	5.83	126.73	111.00
1	C	307	ASN	N-CA-C	5.80	126.67	111.00
1	E	463	PHE	N-CA-C	-5.76	95.44	111.00
1	A	364	LEU	CA-CB-CG	5.75	128.52	115.30
1	D	124	ASP	CB-CA-C	-5.68	99.03	110.40
1	A	411	GLN	N-CA-C	-5.67	95.70	111.00
1	D	625	SER	N-CA-C	5.67	126.30	111.00
1	D	307	ASN	N-CA-C	5.66	126.28	111.00
1	A	307	ASN	N-CA-C	5.63	126.19	111.00
1	E	411	GLN	N-CA-C	-5.61	95.85	111.00
1	E	625	SER	N-CA-C	5.61	126.15	111.00
1	B	464	ASN	CB-CA-C	-5.60	99.19	110.40
1	D	634	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	E	123	ASP	N-CA-C	5.55	125.99	111.00
1	E	307	ASN	N-CA-C	5.51	125.88	111.00
1	B	634	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	C	123	ASP	N-CA-C	5.46	125.73	111.00
1	E	464	ASN	N-CA-C	5.45	125.71	111.00
1	B	411	GLN	N-CA-C	-5.43	96.34	111.00
1	D	411	GLN	N-CA-C	-5.41	96.39	111.00
1	E	384	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	123	ASP	N-CA-C	5.39	125.56	111.00
1	B	520	LEU	CA-CB-CG	5.39	127.69	115.30
1	C	411	GLN	N-CA-C	-5.38	96.48	111.00
1	B	625	SER	N-CA-C	5.35	125.44	111.00
1	B	208	LEU	CB-CG-CD2	5.32	120.04	111.00
1	A	520	LEU	CA-CB-CG	5.30	127.50	115.30
1	B	633	LEU	CA-CB-CG	5.29	127.47	115.30
1	B	463	PHE	N-CA-C	-5.28	96.73	111.00
1	D	463	PHE	N-CA-C	-5.22	96.91	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	PHE	N-CA-C	-5.18	97.02	111.00
1	A	123	ASP	N-CA-C	5.16	124.92	111.00
1	A	384	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	464	ASN	CB-CA-C	-5.12	100.16	110.40
1	C	634	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ASP	Peptide
1	B	123	ASP	Peptide
1	C	123	ASP	Peptide
1	D	123	ASP	Peptide
1	E	123	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4598	0	4490	158	0
1	B	4598	0	4490	192	0
1	C	4628	0	4517	150	0
1	D	4620	0	4506	152	0
1	E	4604	0	4484	145	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
2	D	8	0	12	0	0
2	E	8	0	12	0	0
3	A	41	0	28	0	0
3	B	21	0	15	0	0
3	C	20	0	13	0	0
3	E	20	0	13	0	0
All	All	23190	0	22616	768	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 17.

All (768) 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:525:PRO:CD	1:D:525:PRO:N	1.69	1.43
1:C:416:THR:CG2	1:C:417:PRO:HD2	1.49	1.43
1:E:525:PRO:CD	1:E:525:PRO:N	1.69	1.41
1:D:416:THR:CG2	1:D:417:PRO:HD2	1.52	1.39
1:B:416:THR:CG2	1:B:417:PRO:HD2	1.54	1.37
1:C:101:ALA:HB3	1:C:105:ASP:OD2	1.19	1.29
1:C:416:THR:CG2	1:C:417:PRO:CD	2.10	1.29
1:C:416:THR:HG22	1:C:417:PRO:CD	1.64	1.27
1:A:101:ALA:HB3	1:A:105:ASP:OD2	1.20	1.27
1:D:101:ALA:HB3	1:D:105:ASP:OD2	1.20	1.27
1:B:416:THR:CG2	1:B:417:PRO:CD	2.13	1.26
1:E:101:ALA:HB3	1:E:105:ASP:OD2	1.21	1.26
1:D:416:THR:CG2	1:D:417:PRO:CD	2.15	1.23
1:D:416:THR:HG22	1:D:417:PRO:CD	1.68	1.19
1:B:416:THR:HG22	1:B:417:PRO:CD	1.71	1.18
1:A:515:LEU:O	1:A:515:LEU:HD23	1.45	1.16
1:B:402:GLN:HE22	1:B:406:ARG:HB2	1.03	1.11
1:B:350:SER:OG	1:B:430:THR:HG22	1.52	1.10
1:C:568:PRO:O	1:C:570:LEU:HG	1.51	1.10
1:B:568:PRO:O	1:B:570:LEU:HG	1.47	1.10
1:A:416:THR:OG1	1:A:417:PRO:CD	2.02	1.08
1:B:515:LEU:O	1:B:515:LEU:HD23	1.50	1.06
1:D:350:SER:OG	1:D:430:THR:HG22	1.54	1.05
1:C:416:THR:HG23	1:C:417:PRO:CD	1.87	1.03
1:B:145:ILE:CD1	1:B:172:LEU:HD11	1.88	1.02
1:C:464:ASN:OD1	1:C:465:GLU:N	1.92	1.02
1:B:416:THR:HG22	1:B:417:PRO:HD2	1.08	1.02
1:B:145:ILE:HD11	1:B:172:LEU:HD11	1.37	1.02
1:E:56:PRO:O	1:E:57:ASP:OD1	1.75	1.02
1:B:416:THR:HG23	1:B:417:PRO:CD	1.86	1.02
1:D:416:THR:HG22	1:D:417:PRO:HD2	1.05	1.02
1:A:416:THR:OG1	1:A:417:PRO:HD2	1.62	1.00
1:B:123:ASP:HB2	1:B:124:ASP:OD1	1.61	1.00
1:C:123:ASP:HB2	1:C:124:ASP:OD1	1.61	0.99
1:E:450:ILE:HB	1:E:507:THR:HG23	1.40	0.99
1:D:123:ASP:HB2	1:D:124:ASP:OD1	1.63	0.99
1:C:416:THR:HG22	1:C:417:PRO:HD2	0.99	0.99
1:D:416:THR:HG23	1:D:417:PRO:HD2	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:ASP:HB2	1:E:124:ASP:OD1	1.62	0.98
1:B:568:PRO:HG2	1:B:570:LEU:HD21	1.45	0.98
1:E:464:ASN:OD1	1:E:465:GLU:N	1.94	0.98
1:A:123:ASP:HB2	1:A:124:ASP:OD1	1.63	0.98
1:D:464:ASN:OD1	1:D:465:GLU:N	1.97	0.98
1:D:522:ILE:HD12	1:D:563:ILE:HG22	1.46	0.98
1:B:464:ASN:OD1	1:B:465:GLU:N	1.96	0.96
1:D:416:THR:HG23	1:D:417:PRO:CD	1.91	0.96
1:A:573:LEU:HD13	1:A:578:ARG:HG3	1.48	0.95
1:A:464:ASN:OD1	1:A:465:GLU:N	1.98	0.95
1:D:101:ALA:CB	1:D:105:ASP:OD2	2.14	0.95
1:E:79:VAL:HG12	1:E:131:ALA:HB1	1.50	0.94
1:B:573:LEU:HD13	1:B:578:ARG:HG3	1.48	0.94
1:A:634:ARG:NH2	1:A:635:PHE:CE1	2.35	0.94
1:C:101:ALA:CB	1:C:105:ASP:OD2	2.14	0.93
1:E:101:ALA:CB	1:E:105:ASP:OD2	2.16	0.91
1:B:402:GLN:NE2	1:B:406:ARG:HB2	1.83	0.91
1:A:101:ALA:CB	1:A:105:ASP:OD2	2.15	0.90
1:A:79:VAL:HG12	1:A:131:ALA:HB1	1.53	0.90
1:B:626:LEU:HD12	1:B:627:TYR:N	1.87	0.90
1:C:621:PRO:HA	1:C:624:TYR:HB2	1.54	0.89
1:B:518:TYR:O	1:B:522:ILE:HG13	1.73	0.89
1:D:56:PRO:O	1:D:57:ASP:OD1	1.91	0.89
1:B:416:THR:HG23	1:B:417:PRO:HD2	1.45	0.89
1:D:621:PRO:HA	1:D:624:TYR:HB2	1.54	0.89
1:D:79:VAL:HG12	1:D:131:ALA:HB1	1.55	0.89
1:E:621:PRO:HA	1:E:624:TYR:HB2	1.54	0.88
1:B:56:PRO:O	1:B:57:ASP:OD1	1.91	0.88
1:A:536:ILE:HD11	1:A:548:VAL:HG12	1.55	0.87
1:A:621:PRO:HA	1:A:624:TYR:HB2	1.57	0.87
1:B:79:VAL:HG12	1:B:131:ALA:HB1	1.56	0.87
1:B:621:PRO:HA	1:B:624:TYR:HB2	1.57	0.87
1:C:56:PRO:O	1:C:57:ASP:OD1	1.91	0.86
1:C:573:LEU:HD13	1:C:578:ARG:HG3	1.56	0.86
1:E:573:LEU:HD13	1:E:578:ARG:HG3	1.55	0.85
1:A:626:LEU:HD12	1:A:627:TYR:N	1.90	0.85
1:B:416:THR:HG23	1:B:417:PRO:HD3	1.58	0.85
1:D:573:LEU:HD13	1:D:578:ARG:HG3	1.56	0.85
1:A:79:VAL:CG1	1:A:131:ALA:HB1	2.07	0.85
1:D:626:LEU:HD12	1:D:627:TYR:N	1.93	0.84
1:E:626:LEU:HD12	1:E:627:TYR:N	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HG13	1:A:75:LEU:HD11	1.59	0.84
1:C:79:VAL:HG12	1:C:131:ALA:HB1	1.57	0.84
1:B:540:LYS:HE2	1:B:613:ASP:OD2	1.76	0.84
1:B:79:VAL:CG1	1:B:131:ALA:HB1	2.09	0.83
1:C:568:PRO:HG2	1:C:570:LEU:HD21	1.59	0.83
1:B:522:ILE:HD11	1:B:523:PHE:CD1	2.14	0.83
1:C:79:VAL:CG1	1:C:131:ALA:HB1	2.09	0.82
1:D:79:VAL:CG1	1:D:131:ALA:HB1	2.09	0.82
1:B:249:LEU:HD21	1:B:282:LEU:HD13	1.62	0.82
1:C:416:THR:HG23	1:C:417:PRO:HD3	1.59	0.81
1:E:45:ILE:HG13	1:E:75:LEU:HD11	1.61	0.81
1:A:330:VAL:O	1:A:463:PHE:HA	1.80	0.81
1:B:330:VAL:O	1:B:463:PHE:HA	1.80	0.81
1:B:45:ILE:HG13	1:B:75:LEU:HD11	1.62	0.81
1:B:540:LYS:HZ2	1:B:610:ALA:HB1	1.46	0.80
1:B:522:ILE:HG22	1:B:563:ILE:HG22	1.62	0.80
1:D:515:LEU:HD12	1:D:518:TYR:HB2	1.64	0.80
1:A:416:THR:OG1	1:A:417:PRO:HD3	1.81	0.79
1:B:252:SER:HB2	1:B:281:GLU:HG3	1.63	0.78
1:A:634:ARG:NH2	1:A:635:PHE:HE1	1.80	0.78
1:C:330:VAL:O	1:C:463:PHE:HA	1.83	0.78
1:E:330:VAL:O	1:E:463:PHE:HA	1.82	0.78
1:C:524:VAL:HG13	1:C:525:PRO:HD3	1.66	0.78
1:B:522:ILE:HD11	1:B:523:PHE:CE1	2.18	0.78
1:C:70:ASN:ND2	1:C:75:LEU:O	2.16	0.77
1:D:330:VAL:O	1:D:463:PHE:HA	1.83	0.77
1:D:398:SER:HB2	1:C:410:ASN:OD1	1.84	0.76
1:B:402:GLN:HE22	1:B:406:ARG:CB	1.91	0.76
1:A:45:ILE:CG1	1:A:75:LEU:HD11	2.14	0.76
1:E:573:LEU:O	1:E:573:LEU:HD12	1.86	0.75
1:B:45:ILE:CG1	1:B:75:LEU:HD11	2.16	0.75
1:E:290:ASP:O	1:E:290:ASP:OD1	2.04	0.75
1:C:416:THR:HG23	1:C:417:PRO:HD2	1.47	0.74
1:E:45:ILE:CG1	1:E:75:LEU:HD11	2.17	0.74
1:A:202:GLU:H	1:A:307:ASN:HD22	1.36	0.74
1:D:573:LEU:HD12	1:D:573:LEU:O	1.86	0.74
1:C:573:LEU:O	1:C:573:LEU:HD12	1.88	0.73
1:D:416:THR:HG23	1:D:417:PRO:HD3	1.68	0.73
1:A:573:LEU:HD13	1:A:578:ARG:CG	2.18	0.73
1:C:567:LEU:HD13	1:C:570:LEU:HD12	1.71	0.73
1:D:350:SER:HG	1:D:430:THR:HG22	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:ILE:CD1	1:D:563:ILE:HG22	2.18	0.72
1:E:443:PHE:CD1	1:E:515:LEU:HD21	2.24	0.72
1:A:634:ARG:NH2	1:A:635:PHE:CZ	2.58	0.72
1:C:416:THR:HG22	1:C:417:PRO:N	2.04	0.72
1:E:202:GLU:H	1:E:307:ASN:HD22	1.38	0.72
1:B:573:LEU:HD13	1:B:578:ARG:CG	2.19	0.71
1:D:202:GLU:H	1:D:307:ASN:HD22	1.38	0.71
1:A:515:LEU:O	1:A:515:LEU:CD2	2.31	0.71
1:B:573:LEU:HD12	1:B:573:LEU:O	1.89	0.71
1:D:355:LEU:HD23	1:D:397:PHE:HE2	1.56	0.71
1:C:123:ASP:CB	1:C:124:ASP:OD1	2.39	0.71
1:D:560:ASN:O	1:D:563:ILE:HG13	1.90	0.71
1:A:215:ASP:OD1	1:A:216:THR:N	2.23	0.70
1:C:202:GLU:H	1:C:307:ASN:HD22	1.38	0.70
1:C:398:SER:HB2	1:B:410:ASN:OD1	1.91	0.70
1:A:573:LEU:O	1:A:573:LEU:HD12	1.90	0.70
1:E:234:ALA:HB3	1:E:271:LEU:HD12	1.73	0.70
1:E:355:LEU:HD23	1:E:397:PHE:HE2	1.55	0.70
1:C:443:PHE:CD1	1:C:515:LEU:HD21	2.26	0.70
1:E:633:LEU:HD12	1:E:634:ARG:N	2.06	0.70
1:D:623:VAL:HA	1:D:626:LEU:CD2	2.22	0.69
1:A:536:ILE:CG2	1:A:545:GLN:HG3	2.21	0.69
1:B:123:ASP:CB	1:B:124:ASP:OD1	2.39	0.69
1:D:597:GLN:NE2	1:D:613:ASP:OD1	2.25	0.69
1:B:515:LEU:O	1:B:515:LEU:CD2	2.36	0.69
1:A:234:ALA:HB3	1:A:271:LEU:HD12	1.74	0.69
1:B:234:ALA:HB3	1:B:271:LEU:HD12	1.74	0.69
1:C:597:GLN:NE2	1:C:613:ASP:OD1	2.25	0.69
1:B:597:GLN:NE2	1:B:613:ASP:OD1	2.25	0.69
1:D:522:ILE:HD12	1:D:563:ILE:CG2	2.22	0.69
1:D:213:ASP:O	1:D:217:ARG:HD2	1.91	0.69
1:D:416:THR:HG22	1:D:417:PRO:N	2.03	0.69
1:C:374:THR:HG23	1:C:375:VAL:HG23	1.76	0.68
1:D:407:TRP:HB2	1:D:428:THR:HB	1.76	0.68
1:B:568:PRO:O	1:B:570:LEU:CG	2.35	0.68
1:D:234:ALA:HB3	1:D:271:LEU:HD12	1.74	0.68
1:A:536:ILE:HG23	1:A:545:GLN:HG3	1.75	0.67
1:B:416:THR:HG22	1:B:417:PRO:N	2.06	0.67
1:C:234:ALA:HB3	1:C:271:LEU:HD12	1.74	0.67
1:A:123:ASP:CB	1:A:124:ASP:OD1	2.40	0.67
1:E:524:VAL:HG23	1:E:525:PRO:CD	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:THR:HG23	1:A:375:VAL:HG23	1.77	0.67
1:B:202:GLU:H	1:B:307:ASN:HD22	1.41	0.67
1:E:450:ILE:HB	1:E:507:THR:CG2	2.22	0.67
1:E:123:ASP:CB	1:E:124:ASP:OD1	2.42	0.67
1:B:374:THR:HG23	1:B:375:VAL:HG23	1.76	0.66
1:B:623:VAL:HA	1:B:626:LEU:CD2	2.25	0.66
1:D:524:VAL:HG23	1:D:525:PRO:CD	2.25	0.66
1:C:407:TRP:HB2	1:C:428:THR:HB	1.78	0.66
1:C:524:VAL:CG1	1:C:525:PRO:HD3	2.26	0.66
1:A:355:LEU:HD23	1:A:397:PHE:HE2	1.61	0.66
1:A:407:TRP:HB2	1:A:428:THR:HB	1.78	0.66
1:D:374:THR:HG23	1:D:375:VAL:HG23	1.78	0.66
1:B:249:LEU:HD21	1:B:282:LEU:CD1	2.26	0.66
1:E:407:TRP:HB2	1:E:428:THR:HB	1.79	0.65
1:B:567:LEU:HD13	1:B:570:LEU:HD12	1.76	0.65
1:D:355:LEU:HD23	1:D:397:PHE:CE2	2.31	0.65
1:E:623:VAL:HA	1:E:626:LEU:CD2	2.27	0.65
1:E:524:VAL:HG23	1:E:525:PRO:HD3	1.77	0.65
1:C:329:LEU:HD23	1:C:464:ASN:HD21	1.61	0.65
1:C:524:VAL:HG13	1:C:525:PRO:CD	2.26	0.65
1:A:536:ILE:CG2	1:A:545:GLN:CG	2.74	0.65
1:D:524:VAL:HG23	1:D:525:PRO:HD3	1.78	0.65
1:E:374:THR:HG23	1:E:375:VAL:HG23	1.77	0.65
1:E:355:LEU:HD23	1:E:397:PHE:CE2	2.32	0.65
1:B:568:PRO:HG2	1:B:570:LEU:CD2	2.25	0.65
1:C:567:LEU:HB2	1:C:570:LEU:HD11	1.79	0.65
1:C:568:PRO:O	1:C:570:LEU:CG	2.37	0.64
1:E:597:GLN:NE2	1:E:613:ASP:OD1	2.30	0.64
1:E:79:VAL:CG1	1:E:131:ALA:HB1	2.27	0.64
1:D:145:ILE:HD13	1:D:172:LEU:HD21	1.79	0.64
1:C:145:ILE:HD13	1:C:172:LEU:HD21	1.80	0.64
1:E:145:ILE:HD13	1:E:172:LEU:HD21	1.79	0.64
1:B:540:LYS:NZ	1:B:610:ALA:HB1	2.12	0.64
1:B:407:TRP:HB2	1:B:428:THR:HB	1.78	0.63
1:D:77:PRO:O	1:D:124:ASP:N	2.31	0.63
1:A:536:ILE:HD11	1:A:548:VAL:CG1	2.27	0.63
1:A:145:ILE:HD13	1:A:172:LEU:HD21	1.81	0.63
1:C:573:LEU:HD13	1:C:578:ARG:CG	2.29	0.63
1:A:416:THR:HG22	1:A:420:ARG:H	1.64	0.62
1:A:518:TYR:HD1	1:A:522:ILE:HD12	1.65	0.62
1:C:416:THR:CG2	1:C:417:PRO:HD3	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:LEU:HD12	1:D:364:LEU:O	1.99	0.62
1:C:524:VAL:CG1	1:C:525:PRO:CD	2.77	0.62
1:A:45:ILE:CG1	1:A:75:LEU:CD1	2.78	0.62
1:B:623:VAL:HA	1:B:626:LEU:HG	1.80	0.62
1:C:496:PHE:CE2	1:B:424:PHE:CZ	2.88	0.61
1:E:513:ARG:O	1:E:515:LEU:CD1	2.48	0.61
1:A:489:GLN:CG	1:A:507:THR:HG23	2.31	0.61
1:B:105:ASP:OD1	1:B:106:LEU:N	2.34	0.61
1:E:56:PRO:C	1:E:57:ASP:OD1	2.37	0.61
1:B:489:GLN:CG	1:B:507:THR:HG23	2.31	0.61
1:C:489:GLN:CG	1:C:507:THR:HG23	2.31	0.60
1:A:416:THR:CG2	1:A:418:ASP:HB2	2.31	0.60
1:B:364:LEU:O	1:B:364:LEU:HD12	2.01	0.60
1:C:364:LEU:O	1:C:364:LEU:HD12	2.02	0.60
1:B:515:LEU:HD23	1:B:519:ILE:HB	1.84	0.60
1:B:567:LEU:HB2	1:B:570:LEU:HD11	1.84	0.60
1:D:489:GLN:CG	1:D:507:THR:HG23	2.31	0.60
1:A:416:THR:HG21	1:A:418:ASP:HB2	1.83	0.60
1:D:123:ASP:CB	1:D:124:ASP:OD1	2.45	0.60
1:A:355:LEU:HD23	1:A:397:PHE:CE2	2.36	0.60
1:B:436:PHE:HD2	1:B:438:PHE:CE2	2.20	0.60
1:A:441:TYR:HB3	1:A:574:THR:OG1	2.02	0.60
1:D:355:LEU:CD2	1:D:397:PHE:HE2	2.15	0.59
1:E:45:ILE:CG1	1:E:75:LEU:CD1	2.79	0.59
1:D:623:VAL:HA	1:D:626:LEU:HD21	1.83	0.59
1:B:45:ILE:CG1	1:B:75:LEU:CD1	2.80	0.59
1:B:208:LEU:HD23	1:B:209:GLU:N	2.17	0.59
1:B:53:TYR:HB2	1:B:145:ILE:CG1	2.32	0.59
1:E:570:LEU:HD22	1:E:572:TYR:CE1	2.38	0.59
1:B:522:ILE:HG22	1:B:563:ILE:CG2	2.30	0.59
1:E:355:LEU:CD2	1:E:397:PHE:HE2	2.15	0.59
1:A:570:LEU:HD22	1:A:572:TYR:CE1	2.37	0.58
1:E:513:ARG:O	1:E:515:LEU:HD12	2.02	0.58
1:C:492:THR:HG22	1:C:493:GLU:N	2.19	0.58
1:B:350:SER:HG	1:B:430:THR:HG22	1.65	0.58
1:D:213:ASP:O	1:D:217:ARG:CD	2.51	0.58
1:D:355:LEU:CD2	1:D:397:PHE:CE2	2.86	0.58
1:D:573:LEU:HD13	1:D:578:ARG:CG	2.29	0.58
1:A:124:ASP:HB3	1:A:150:THR:HG21	1.85	0.58
1:B:145:ILE:CD1	1:B:172:LEU:CD1	2.73	0.58
1:B:623:VAL:HA	1:B:626:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:LEU:HD21	1:B:519:ILE:HD13	1.86	0.58
1:B:623:VAL:HA	1:B:626:LEU:CG	2.34	0.58
1:E:77:PRO:O	1:E:124:ASP:N	2.37	0.58
1:E:573:LEU:HD13	1:E:578:ARG:CG	2.29	0.58
1:A:597:GLN:NE2	1:A:613:ASP:OD1	2.36	0.57
1:C:567:LEU:HD13	1:C:570:LEU:CD1	2.34	0.57
1:B:77:PRO:O	1:B:124:ASP:N	2.38	0.57
1:D:515:LEU:O	1:D:515:LEU:HG	2.03	0.57
1:E:355:LEU:CD2	1:E:397:PHE:CE2	2.87	0.57
1:D:521:ARG:O	1:D:522:ILE:HD13	2.05	0.57
1:D:570:LEU:HD22	1:D:572:TYR:CE1	2.39	0.57
1:E:623:VAL:HA	1:E:626:LEU:HD21	1.85	0.57
1:C:124:ASP:HB3	1:C:150:THR:HG21	1.86	0.57
1:E:124:ASP:HB3	1:E:150:THR:HG21	1.85	0.57
1:B:124:ASP:HB3	1:B:150:THR:HG21	1.86	0.57
1:A:77:PRO:O	1:A:124:ASP:N	2.38	0.57
1:B:208:LEU:HD23	1:B:209:GLU:O	2.05	0.57
1:E:334:LEU:HD22	1:E:507:THR:HG21	1.86	0.57
1:E:398:SER:HB2	1:D:410:ASN:ND2	2.20	0.57
1:C:77:PRO:O	1:C:124:ASP:N	2.37	0.56
1:E:277:GLN:HG3	1:E:278:ASP:H	1.71	0.56
1:A:391:ASN:HD21	1:E:376:LYS:HD2	1.70	0.56
1:D:492:THR:HG22	1:D:493:GLU:N	2.21	0.56
1:A:364:LEU:HD12	1:A:364:LEU:O	2.05	0.56
1:E:48:GLY:HA2	1:E:149:SER:HB3	1.88	0.56
1:C:513:ARG:O	1:C:515:LEU:CD1	2.54	0.56
1:D:124:ASP:HB3	1:D:150:THR:HG21	1.87	0.56
1:E:315:GLY:O	1:E:321:SER:N	2.39	0.56
1:B:145:ILE:HD13	1:B:172:LEU:HD21	1.88	0.56
1:E:364:LEU:O	1:E:364:LEU:HD12	2.06	0.55
1:A:515:LEU:HD23	1:A:519:ILE:HB	1.87	0.55
1:B:522:ILE:CD1	1:B:523:PHE:CD1	2.89	0.55
1:C:315:GLY:O	1:C:321:SER:N	2.40	0.55
1:C:560:ASN:O	1:C:563:ILE:HG13	2.06	0.55
1:D:496:PHE:CE2	1:C:424:PHE:CZ	2.94	0.55
1:D:623:VAL:HA	1:D:626:LEU:HG	1.88	0.55
1:E:441:TYR:HB3	1:E:574:THR:OG1	2.07	0.55
1:B:492:THR:HG22	1:B:493:GLU:N	2.21	0.55
1:B:626:LEU:C	1:B:626:LEU:HD12	2.27	0.55
1:D:441:TYR:HB3	1:D:574:THR:OG1	2.07	0.55
1:B:540:LYS:HZ3	1:B:610:ALA:HA	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASP:OD1	1:A:124:ASP:OD1	2.24	0.55
1:A:371:CYS:O	1:A:373:CYS:N	2.40	0.54
1:A:493:GLU:HG2	1:A:501:THR:HB	1.88	0.54
1:D:48:GLY:HA2	1:D:149:SER:CB	2.37	0.54
1:D:371:CYS:O	1:D:373:CYS:N	2.40	0.54
1:E:48:GLY:HA2	1:E:149:SER:CB	2.37	0.54
1:A:334:LEU:HD22	1:A:507:THR:HG21	1.89	0.54
1:A:518:TYR:CD1	1:A:522:ILE:HD12	2.42	0.54
1:D:623:VAL:HA	1:D:626:LEU:CG	2.37	0.54
1:C:441:TYR:HB3	1:C:574:THR:OG1	2.07	0.54
1:A:363:LYS:O	1:A:364:LEU:HG	2.07	0.54
1:A:574:THR:HG22	1:A:577:ASP:CG	2.28	0.54
1:B:371:CYS:O	1:B:373:CYS:N	2.39	0.54
1:E:454:LEU:HD21	1:E:463:PHE:CE1	2.43	0.54
1:C:371:CYS:O	1:C:373:CYS:N	2.40	0.54
1:D:315:GLY:O	1:D:321:SER:N	2.40	0.54
1:A:626:LEU:C	1:A:626:LEU:HD12	2.27	0.54
1:E:574:THR:HG22	1:E:577:ASP:CG	2.28	0.54
1:C:568:PRO:HG2	1:C:570:LEU:CD2	2.35	0.53
1:A:416:THR:HG23	1:A:419:GLY:H	1.73	0.53
1:A:250:THR:HG21	1:A:285:HIS:NE2	2.24	0.53
1:B:334:LEU:HD22	1:B:507:THR:HG21	1.91	0.53
1:C:518:TYR:HD1	1:C:522:ILE:HD12	1.72	0.53
1:E:371:CYS:O	1:E:373:CYS:N	2.40	0.53
1:B:75:LEU:HD23	1:B:77:PRO:CD	2.39	0.53
1:E:363:LYS:O	1:E:364:LEU:HG	2.08	0.53
1:B:454:LEU:HD21	1:B:463:PHE:CE1	2.44	0.53
1:D:48:GLY:HA2	1:D:149:SER:HB3	1.90	0.53
1:E:250:THR:HG21	1:E:285:HIS:NE2	2.23	0.53
1:E:524:VAL:CG2	1:E:525:PRO:CD	2.86	0.53
1:B:123:ASP:OD1	1:B:124:ASP:OD1	2.26	0.53
1:A:454:LEU:HD21	1:A:463:PHE:CE1	2.44	0.53
1:A:626:LEU:HD12	1:A:627:TYR:CA	2.38	0.53
1:A:48:GLY:HA2	1:A:149:SER:CB	2.39	0.53
1:D:218:TYR:CZ	1:C:158:LYS:HA	2.45	0.52
1:D:250:THR:HG21	1:D:285:HIS:NE2	2.23	0.52
1:C:363:LYS:O	1:C:364:LEU:HG	2.09	0.52
1:A:45:ILE:HB	1:A:75:LEU:HD12	1.90	0.52
1:D:524:VAL:CG2	1:D:525:PRO:CD	2.87	0.52
1:C:48:GLY:HA2	1:C:149:SER:CB	2.39	0.52
1:D:363:LYS:O	1:D:364:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLY:HA2	1:A:149:SER:HB3	1.91	0.52
1:B:145:ILE:HD11	1:B:172:LEU:CD1	2.25	0.52
1:C:574:THR:HG22	1:C:577:ASP:CG	2.29	0.52
1:B:48:GLY:HA2	1:B:149:SER:CB	2.39	0.52
1:D:574:THR:HG22	1:D:577:ASP:CG	2.29	0.52
1:D:334:LEU:HD22	1:D:507:THR:HG21	1.91	0.52
1:B:250:THR:HG21	1:B:285:HIS:NE2	2.25	0.52
1:C:454:LEU:HD21	1:C:463:PHE:CE1	2.45	0.52
1:C:123:ASP:OD1	1:C:124:ASP:OD1	2.27	0.52
1:D:454:LEU:HD21	1:D:463:PHE:CE1	2.44	0.52
1:B:48:GLY:HA2	1:B:149:SER:HB3	1.92	0.52
1:B:383:ILE:HD12	1:B:387:ALA:HB2	1.92	0.52
1:C:250:THR:HG21	1:C:285:HIS:NE2	2.24	0.51
1:C:202:GLU:H	1:C:307:ASN:ND2	2.08	0.51
1:C:334:LEU:HD22	1:C:507:THR:HG21	1.93	0.51
1:C:489:GLN:HG3	1:C:507:THR:HG23	1.92	0.51
1:A:416:THR:HG1	1:A:417:PRO:HD2	1.71	0.51
1:B:431:LEU:HD11	1:B:450:ILE:HG23	1.93	0.51
1:B:626:LEU:HD12	1:B:627:TYR:CA	2.40	0.51
1:E:257:LEU:HD13	1:E:273:TYR:CZ	2.46	0.51
1:E:626:LEU:HD12	1:E:627:TYR:CA	2.40	0.51
1:A:355:LEU:CD2	1:A:397:PHE:HE2	2.23	0.51
1:A:431:LEU:HD11	1:A:450:ILE:HG23	1.93	0.51
1:E:429:VAL:CG1	1:E:431:LEU:HG	2.41	0.51
1:C:48:GLY:HA2	1:C:149:SER:HB3	1.92	0.51
1:C:597:GLN:CG	1:C:612:ILE:HD11	2.41	0.51
1:A:355:LEU:CD2	1:A:397:PHE:CE2	2.94	0.50
1:C:383:ILE:HD12	1:C:387:ALA:HB2	1.91	0.50
1:D:202:GLU:H	1:D:307:ASN:ND2	2.09	0.50
1:A:429:VAL:CG1	1:A:431:LEU:HG	2.41	0.50
1:B:53:TYR:HB2	1:B:145:ILE:HG12	1.93	0.50
1:C:429:VAL:CG1	1:C:431:LEU:HG	2.42	0.50
1:A:492:THR:HG22	1:A:493:GLU:N	2.26	0.50
1:B:343:ASP:OD1	1:B:346:SER:N	2.45	0.50
1:C:513:ARG:O	1:C:515:LEU:HD12	2.11	0.50
1:D:458:THR:OG1	1:D:501:THR:HG23	2.11	0.50
1:A:536:ILE:CG2	1:A:545:GLN:HG2	2.40	0.50
1:D:77:PRO:O	1:D:124:ASP:HA	2.11	0.50
1:D:431:LEU:HD11	1:D:450:ILE:HG23	1.94	0.50
1:E:623:VAL:HA	1:E:626:LEU:HG	1.93	0.50
1:E:81:ILE:HG21	1:E:135:PHE:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:VAL:CG1	1:B:431:LEU:HG	2.42	0.50
1:C:244:LEU:HD22	1:C:262:ILE:HD11	1.92	0.50
1:D:626:LEU:HD12	1:D:627:TYR:CA	2.41	0.50
1:A:343:ASP:OD1	1:A:346:SER:N	2.45	0.50
1:B:45:ILE:HB	1:B:75:LEU:HD12	1.94	0.50
1:C:431:LEU:HD11	1:C:450:ILE:HG23	1.93	0.50
1:E:396:SER:HB2	1:E:455:ALA:HB3	1.94	0.50
1:A:536:ILE:HG23	1:A:545:GLN:CG	2.40	0.50
1:D:81:ILE:HG21	1:D:135:PHE:CD2	2.47	0.50
1:E:626:LEU:HD12	1:E:626:LEU:C	2.31	0.50
1:B:100:LEU:HB3	1:B:105:ASP:OD2	2.12	0.49
1:D:429:VAL:CG1	1:D:431:LEU:HG	2.42	0.49
1:D:626:LEU:C	1:D:626:LEU:HD12	2.31	0.49
1:E:79:VAL:HG12	1:E:131:ALA:CB	2.32	0.49
1:A:489:GLN:HG3	1:A:507:THR:HG23	1.93	0.49
1:C:343:ASP:OD1	1:C:346:SER:N	2.44	0.49
1:E:383:ILE:HD12	1:E:387:ALA:HB2	1.92	0.49
1:E:623:VAL:HA	1:E:626:LEU:CG	2.42	0.49
1:B:75:LEU:CD2	1:B:77:PRO:HG3	2.42	0.49
1:C:81:ILE:HG21	1:C:135:PHE:CD2	2.47	0.49
1:D:489:GLN:HG3	1:D:507:THR:HG23	1.93	0.49
1:D:604:GLY:HA2	1:D:606:GLN:HE21	1.78	0.49
1:E:45:ILE:HB	1:E:75:LEU:HD12	1.93	0.49
1:B:257:LEU:HD13	1:B:273:TYR:CZ	2.47	0.49
1:B:98:LYS:HB3	1:B:100:LEU:HG	1.94	0.49
1:D:257:LEU:HD13	1:D:273:TYR:CZ	2.48	0.49
1:A:489:GLN:HG2	1:A:507:THR:HG23	1.95	0.49
1:B:81:ILE:HG21	1:B:135:PHE:CD2	2.47	0.49
1:D:383:ILE:HD12	1:D:387:ALA:HB2	1.93	0.49
1:D:391:ASN:HD21	1:C:376:LYS:HD2	1.78	0.49
1:E:431:LEU:HD11	1:E:450:ILE:HG23	1.94	0.49
1:A:257:LEU:HD13	1:A:273:TYR:CZ	2.48	0.49
1:D:250:THR:HA	1:D:256:PRO:HA	1.95	0.49
1:B:540:LYS:HZ2	1:B:610:ALA:CB	2.20	0.49
1:B:604:GLY:HA2	1:B:606:GLN:HE21	1.78	0.49
1:C:47:ASP:OD1	1:C:47:ASP:O	2.31	0.49
1:E:123:ASP:OD1	1:E:124:ASP:OD1	2.31	0.49
1:E:562:THR:O	1:E:563:ILE:C	2.50	0.49
1:B:250:THR:HA	1:B:256:PRO:HA	1.95	0.49
1:C:250:THR:HA	1:C:256:PRO:HA	1.95	0.49
1:A:81:ILE:HG21	1:A:135:PHE:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ILE:HD12	1:A:387:ALA:HB2	1.95	0.48
1:B:489:GLN:HG3	1:B:507:THR:HG23	1.94	0.48
1:B:562:THR:O	1:B:563:ILE:C	2.50	0.48
1:E:235:LEU:HD11	1:E:268:SER:HB3	1.95	0.48
1:E:277:GLN:HG3	1:E:278:ASP:N	2.27	0.48
1:E:492:THR:HG22	1:E:493:GLU:N	2.28	0.48
1:E:632:TYR:O	1:E:636:PHE:HB2	2.13	0.48
1:A:250:THR:HA	1:A:256:PRO:HA	1.95	0.48
1:B:235:LEU:HD11	1:B:268:SER:HB3	1.96	0.48
1:B:363:LYS:O	1:B:364:LEU:HG	2.13	0.48
1:E:250:THR:HA	1:E:256:PRO:HA	1.95	0.48
1:B:210:ILE:HD13	1:B:286:VAL:HG21	1.95	0.48
1:E:432:GLN:HE22	1:D:338:GLN:HB3	1.78	0.48
1:D:445:ARG:HD3	1:D:512:LYS:NZ	2.28	0.48
1:B:105:ASP:O	1:B:109:GLU:HG2	2.13	0.48
1:D:218:TYR:CE1	1:C:158:LYS:HA	2.49	0.48
1:A:562:THR:O	1:A:563:ILE:C	2.51	0.48
1:A:202:GLU:H	1:A:307:ASN:ND2	2.08	0.48
1:B:332:VAL:HG13	1:B:463:PHE:CD1	2.49	0.48
1:E:366:PHE:CZ	1:E:371:CYS:HB3	2.49	0.48
1:C:604:GLY:HA2	1:C:606:GLN:HE21	1.79	0.47
1:D:235:LEU:HD11	1:D:268:SER:HB3	1.96	0.47
1:D:586:LEU:HD21	1:D:624:TYR:HE1	1.79	0.47
1:A:332:VAL:HG13	1:A:463:PHE:CD1	2.49	0.47
1:A:586:LEU:HD21	1:A:624:TYR:HE1	1.79	0.47
1:B:489:GLN:HG2	1:B:507:THR:HG23	1.94	0.47
1:B:518:TYR:O	1:B:522:ILE:CG1	2.55	0.47
1:C:586:LEU:HD21	1:C:624:TYR:HE1	1.79	0.47
1:C:98:LYS:HB3	1:C:100:LEU:HG	1.95	0.47
1:E:522:ILE:HG12	1:E:563:ILE:HG22	1.95	0.47
1:A:98:LYS:HB3	1:A:100:LEU:HG	1.96	0.47
1:C:366:PHE:CZ	1:C:371:CYS:HB3	2.49	0.47
1:E:405:ASN:HB2	1:D:407:TRP:CE3	2.49	0.47
1:B:45:ILE:HG12	1:B:75:LEU:CD1	2.45	0.47
1:C:235:LEU:HD11	1:C:268:SER:HB3	1.96	0.47
1:C:332:VAL:HG13	1:C:463:PHE:CD1	2.50	0.47
1:C:562:THR:O	1:C:563:ILE:C	2.51	0.47
1:D:98:LYS:HB3	1:D:100:LEU:HG	1.95	0.47
1:B:277:GLN:HG3	1:B:278:ASP:H	1.80	0.47
1:A:623:VAL:HA	1:A:626:LEU:CD2	2.44	0.47
1:B:235:LEU:HB3	1:B:303:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:PHE:CD2	1:B:438:PHE:CE2	3.02	0.47
1:C:257:LEU:HD13	1:C:273:TYR:CZ	2.49	0.47
1:C:74:ASN:HD22	1:C:154:GLN:HE21	1.63	0.47
1:D:74:ASN:HD22	1:D:154:GLN:HE21	1.63	0.47
1:E:235:LEU:HB3	1:E:303:LEU:HB2	1.97	0.47
1:B:515:LEU:CD2	1:B:519:ILE:HB	2.44	0.47
1:B:567:LEU:HD13	1:B:570:LEU:CD1	2.45	0.47
1:B:74:ASN:HD22	1:B:154:GLN:HE21	1.63	0.47
1:C:496:PHE:HE2	1:B:424:PHE:CZ	2.31	0.47
1:C:235:LEU:HB3	1:C:303:LEU:HB2	1.97	0.47
1:A:45:ILE:HG12	1:A:75:LEU:CD1	2.45	0.46
1:A:536:ILE:HG22	1:A:545:GLN:HG3	1.96	0.46
1:A:600:LEU:O	1:A:604:GLY:O	2.33	0.46
1:B:540:LYS:NZ	1:B:610:ALA:CB	2.77	0.46
1:B:537:PHE:CE2	1:B:616:VAL:HG11	2.49	0.46
1:E:98:LYS:HB3	1:E:100:LEU:HG	1.96	0.46
1:B:540:LYS:HZ3	1:B:610:ALA:CA	2.27	0.46
1:D:332:VAL:HG13	1:D:463:PHE:CD1	2.50	0.46
1:A:235:LEU:HB3	1:A:303:LEU:HB2	1.97	0.46
1:A:235:LEU:HD11	1:A:268:SER:HB3	1.97	0.46
1:A:537:PHE:CE2	1:A:616:VAL:HG11	2.51	0.46
1:B:277:GLN:HG3	1:B:278:ASP:N	2.30	0.46
1:B:574:THR:HG23	1:B:577:ASP:OD2	2.16	0.46
1:C:518:TYR:CD1	1:C:522:ILE:HD12	2.49	0.46
1:C:68:MET:HB3	1:C:131:ALA:HB3	1.97	0.46
1:D:343:ASP:OD1	1:D:346:SER:N	2.44	0.46
1:E:586:LEU:HD21	1:E:624:TYR:HE1	1.80	0.46
1:A:366:PHE:CZ	1:A:371:CYS:HB3	2.51	0.46
1:C:489:GLN:HG2	1:C:507:THR:HG23	1.97	0.46
1:D:600:LEU:O	1:D:604:GLY:O	2.33	0.46
1:E:75:LEU:HD23	1:E:77:PRO:CD	2.45	0.46
1:A:407:TRP:CE3	1:B:405:ASN:HB2	2.51	0.46
1:D:396:SER:HB2	1:D:455:ALA:HB3	1.97	0.46
1:A:162:THR:HG22	1:A:163:TYR:N	2.31	0.46
1:A:414:PHE:HB2	1:A:422:SER:HB2	1.98	0.46
1:B:53:TYR:HB2	1:B:145:ILE:HG13	1.98	0.46
1:C:391:ASN:HD21	1:B:376:LYS:HD2	1.81	0.46
1:B:600:LEU:O	1:B:604:GLY:O	2.33	0.46
1:C:600:LEU:O	1:C:604:GLY:O	2.33	0.46
1:D:537:PHE:CE2	1:D:616:VAL:HG11	2.51	0.46
1:C:537:PHE:CE2	1:C:616:VAL:HG11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:CYS:SG	1:D:372:GLY:N	2.87	0.46
1:D:562:THR:O	1:D:563:ILE:C	2.51	0.46
1:E:343:ASP:OD1	1:E:346:SER:N	2.45	0.46
1:E:443:PHE:CD1	1:E:515:LEU:CD2	2.97	0.46
1:B:586:LEU:HD21	1:B:624:TYR:HE1	1.79	0.46
1:E:74:ASN:HD22	1:E:154:GLN:HE21	1.64	0.46
1:E:332:VAL:HG13	1:E:463:PHE:CD1	2.50	0.45
1:B:133:LEU:HD23	1:B:133:LEU:C	2.37	0.45
1:D:489:GLN:HG2	1:D:507:THR:HG23	1.96	0.45
1:D:441:TYR:HD2	1:D:574:THR:HG21	1.81	0.45
1:D:133:LEU:C	1:D:133:LEU:HD23	2.37	0.45
1:D:259:PHE:HB2	1:C:104:ASN:H	1.81	0.45
1:D:235:LEU:HB3	1:D:303:LEU:HB2	1.97	0.45
1:E:600:LEU:O	1:E:604:GLY:O	2.33	0.45
1:D:123:ASP:O	1:D:130:SER:O	2.34	0.45
1:D:162:THR:HG22	1:D:163:TYR:N	2.31	0.45
1:D:355:LEU:O	1:D:424:PHE:HA	2.16	0.45
1:D:75:LEU:O	1:D:77:PRO:HD3	2.17	0.45
1:E:68:MET:HB3	1:E:131:ALA:HB3	1.97	0.45
1:E:133:LEU:HD23	1:E:133:LEU:C	2.37	0.45
1:C:162:THR:HG22	1:C:163:TYR:N	2.31	0.45
1:D:68:MET:HB3	1:D:131:ALA:HB3	1.98	0.45
1:E:45:ILE:HG12	1:E:75:LEU:CD1	2.46	0.45
1:B:162:THR:HG22	1:B:163:TYR:N	2.31	0.45
1:B:383:ILE:HD12	1:B:387:ALA:CB	2.47	0.45
1:B:522:ILE:O	1:B:526:LEU:HB2	2.17	0.45
1:B:597:GLN:HE21	1:B:612:ILE:HG23	1.81	0.45
1:D:210:ILE:HD13	1:D:286:VAL:HG21	1.99	0.45
1:E:162:THR:HG22	1:E:163:TYR:N	2.31	0.45
1:A:210:ILE:HD13	1:A:286:VAL:HG21	1.99	0.45
1:E:202:GLU:H	1:E:307:ASN:ND2	2.09	0.45
1:A:221:GLN:HB3	1:A:325:LEU:HD22	1.98	0.45
1:C:355:LEU:O	1:C:424:PHE:HA	2.17	0.45
1:D:464:ASN:OD1	1:D:465:GLU:HG2	2.16	0.45
1:A:133:LEU:C	1:A:133:LEU:HD23	2.37	0.45
1:A:102:SER:CB	1:B:259:PHE:CD1	3.00	0.45
1:B:582:VAL:HG21	1:B:627:TYR:CZ	2.52	0.45
1:D:259:PHE:CD1	1:C:102:SER:CB	3.00	0.45
1:A:623:VAL:HA	1:A:626:LEU:HD21	1.98	0.45
1:A:75:LEU:HD23	1:A:77:PRO:CD	2.47	0.45
1:A:518:TYR:OH	1:B:569:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASP:OD1	1:B:289:THR:HG22	2.17	0.44
1:C:133:LEU:HD23	1:C:133:LEU:C	2.37	0.44
1:C:396:SER:HB2	1:C:455:ALA:HB3	1.99	0.44
1:D:173:GLY:HA3	1:D:179:VAL:HG21	2.00	0.44
1:C:259:PHE:CD1	1:B:102:SER:CB	2.99	0.44
1:B:68:MET:HB3	1:B:131:ALA:HB3	1.98	0.44
1:C:210:ILE:HD13	1:C:286:VAL:HG21	1.98	0.44
1:A:68:MET:HB3	1:A:131:ALA:HB3	1.99	0.44
1:D:221:GLN:HB3	1:D:325:LEU:HD22	1.98	0.44
1:D:366:PHE:CZ	1:D:371:CYS:HB3	2.53	0.44
1:A:79:VAL:HG11	1:A:131:ALA:HB1	1.94	0.44
1:B:47:ASP:O	1:B:47:ASP:OD1	2.34	0.44
1:E:210:ILE:HD13	1:E:286:VAL:HG21	1.97	0.44
1:E:231:THR:OG1	1:E:306:ILE:O	2.35	0.44
1:A:231:THR:OG1	1:A:306:ILE:O	2.36	0.44
1:A:396:SER:HB2	1:A:455:ALA:HB3	1.98	0.44
1:A:515:LEU:CD2	1:A:519:ILE:HB	2.47	0.44
1:B:231:THR:OG1	1:B:306:ILE:O	2.35	0.44
1:B:366:PHE:CZ	1:B:371:CYS:HB3	2.52	0.44
1:C:371:CYS:SG	1:C:372:GLY:N	2.88	0.44
1:C:632:TYR:O	1:C:636:PHE:HB2	2.18	0.44
1:E:537:PHE:CE2	1:E:616:VAL:HG11	2.51	0.44
1:B:125:GLY:N	1:B:130:SER:OG	2.50	0.44
1:B:355:LEU:O	1:B:424:PHE:HA	2.17	0.44
1:A:173:GLY:HA3	1:A:179:VAL:HG21	2.00	0.44
1:B:515:LEU:HD21	1:B:519:ILE:CD1	2.48	0.44
1:E:355:LEU:O	1:E:424:PHE:HA	2.17	0.44
1:E:582:VAL:HG21	1:E:627:TYR:CZ	2.53	0.44
1:A:582:VAL:HG21	1:A:627:TYR:CZ	2.52	0.43
1:C:569:ARG:HD3	1:B:517:TYR:CE2	2.53	0.43
1:D:582:VAL:HG21	1:D:627:TYR:CZ	2.53	0.43
1:A:439:LEU:HD12	1:A:574:THR:HA	1.99	0.43
1:A:536:ILE:HG22	1:A:545:GLN:CG	2.47	0.43
1:B:208:LEU:HD23	1:B:209:GLU:C	2.39	0.43
1:B:145:ILE:HD13	1:B:172:LEU:CD2	2.48	0.43
1:B:75:LEU:HD23	1:B:77:PRO:HD3	2.00	0.43
1:C:496:PHE:CZ	1:B:424:PHE:CE1	3.07	0.43
1:B:58:MET:HA	1:B:58:MET:CE	2.48	0.43
1:C:383:ILE:HD12	1:C:387:ALA:CB	2.48	0.43
1:C:173:GLY:HA3	1:C:179:VAL:HG21	2.00	0.43
1:E:221:GLN:HB3	1:E:325:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:ILE:CD1	1:E:491:ILE:HD11	2.49	0.43
1:A:440:ALA:O	1:A:443:PHE:HB2	2.17	0.43
1:A:493:GLU:CG	1:A:501:THR:HB	2.49	0.43
1:C:210:ILE:HD12	1:C:302:LEU:HB2	2.01	0.43
1:C:496:PHE:CE2	1:B:424:PHE:CE1	3.07	0.43
1:C:439:LEU:HD12	1:C:574:THR:HA	2.01	0.43
1:B:79:VAL:HG11	1:B:131:ALA:HB1	1.96	0.43
1:B:436:PHE:CD2	1:B:438:PHE:HE2	2.36	0.43
1:D:259:PHE:CE1	1:C:102:SER:CB	3.02	0.43
1:D:626:LEU:CD1	1:D:627:TYR:N	2.75	0.43
1:E:77:PRO:O	1:E:124:ASP:HA	2.18	0.43
1:C:73:GLY:HA2	1:C:365:GLY:HA3	2.01	0.43
1:C:582:VAL:HG21	1:C:627:TYR:CZ	2.54	0.43
1:C:58:MET:CE	1:C:58:MET:HA	2.49	0.43
1:E:173:GLY:HA3	1:E:179:VAL:HG21	2.00	0.43
1:E:450:ILE:O	1:E:507:THR:HG22	2.18	0.43
1:E:464:ASN:C	1:E:464:ASN:OD1	2.53	0.43
1:E:58:MET:CE	1:E:58:MET:HA	2.48	0.43
1:A:74:ASN:HD22	1:A:154:GLN:HE21	1.64	0.43
1:A:38:VAL:HB	1:A:185:GLU:O	2.19	0.43
1:C:38:VAL:HB	1:C:185:GLU:O	2.19	0.43
1:C:466:ILE:CD1	1:C:491:ILE:HD11	2.49	0.43
1:C:492:THR:CG2	1:C:493:GLU:N	2.82	0.43
1:C:68:MET:O	1:C:130:SER:HB3	2.19	0.43
1:D:68:MET:O	1:D:130:SER:HB3	2.19	0.43
1:D:383:ILE:HD12	1:D:387:ALA:CB	2.49	0.43
1:E:73:GLY:HA2	1:E:365:GLY:HA3	2.01	0.43
1:E:441:TYR:HD2	1:E:574:THR:HG21	1.84	0.43
1:A:171:ILE:HG21	1:A:184:GLY:HA3	2.01	0.42
1:A:68:MET:O	1:A:130:SER:HB3	2.19	0.42
1:C:349:PHE:CZ	1:C:448:PHE:HB3	2.54	0.42
1:D:171:ILE:HG21	1:D:184:GLY:HA3	2.01	0.42
1:D:73:GLY:HA2	1:D:365:GLY:HA3	2.01	0.42
1:D:58:MET:HA	1:D:58:MET:CE	2.49	0.42
1:E:219:LEU:HG	1:E:220:THR:N	2.34	0.42
1:E:68:MET:O	1:E:130:SER:HB3	2.19	0.42
1:A:349:PHE:CZ	1:A:448:PHE:HB3	2.55	0.42
1:D:223:THR:HG22	1:D:224:ARG:N	2.34	0.42
1:D:466:ILE:CD1	1:D:491:ILE:HD11	2.49	0.42
1:E:383:ILE:HD12	1:E:387:ALA:CB	2.49	0.42
1:B:38:VAL:O	1:B:186:PRO:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ILE:HD12	1:B:302:LEU:HB2	2.02	0.42
1:B:371:CYS:SG	1:B:372:GLY:N	2.87	0.42
1:B:466:ILE:CD1	1:B:491:ILE:HD11	2.49	0.42
1:C:223:THR:HG22	1:C:224:ARG:N	2.34	0.42
1:D:271:LEU:HD13	1:D:271:LEU:C	2.40	0.42
1:E:271:LEU:C	1:E:271:LEU:HD13	2.40	0.42
1:E:633:LEU:HD12	1:E:633:LEU:C	2.39	0.42
1:A:271:LEU:HD13	1:A:271:LEU:C	2.40	0.42
1:A:610:ALA:O	1:A:613:ASP:HB2	2.19	0.42
1:B:68:MET:O	1:B:130:SER:HB3	2.19	0.42
1:B:623:VAL:CA	1:B:626:LEU:HG	2.48	0.42
1:C:38:VAL:O	1:C:186:PRO:HA	2.19	0.42
1:D:222:HIS:HA	1:D:283:VAL:HG22	2.01	0.42
1:E:439:LEU:HD12	1:E:574:THR:HA	2.00	0.42
1:B:145:ILE:HD13	1:B:145:ILE:HG21	1.87	0.42
1:B:173:GLY:HA3	1:B:179:VAL:HG21	2.00	0.42
1:B:349:PHE:CZ	1:B:448:PHE:HB3	2.55	0.42
1:B:586:LEU:HA	1:B:589:ILE:CG1	2.50	0.42
1:D:38:VAL:O	1:D:186:PRO:HA	2.19	0.42
1:D:586:LEU:HA	1:D:589:ILE:HB	2.02	0.42
1:D:586:LEU:HD12	1:D:587:THR:N	2.35	0.42
1:E:429:VAL:CG1	1:E:430:THR:N	2.83	0.42
1:E:524:VAL:HG23	1:E:525:PRO:N	2.34	0.42
1:A:586:LEU:HD12	1:A:587:THR:N	2.35	0.42
1:C:125:GLY:N	1:C:130:SER:OG	2.50	0.42
1:C:271:LEU:HD13	1:C:271:LEU:C	2.40	0.42
1:D:429:VAL:CG1	1:D:430:THR:N	2.83	0.42
1:E:462:ILE:HG22	1:E:463:PHE:O	2.19	0.42
1:B:171:ILE:HG21	1:B:184:GLY:HA3	2.02	0.42
1:B:271:LEU:C	1:B:271:LEU:HD13	2.40	0.42
1:B:492:THR:HG22	1:B:493:GLU:H	1.84	0.42
1:B:586:LEU:HA	1:B:589:ILE:HB	2.02	0.42
1:E:349:PHE:CZ	1:E:448:PHE:HB3	2.55	0.42
1:A:405:ASN:HB2	1:E:407:TRP:CE3	2.55	0.42
1:E:626:LEU:CD1	1:E:627:TYR:N	2.74	0.42
1:A:250:THR:HG22	1:A:283:VAL:O	2.20	0.42
1:A:383:ILE:HD12	1:A:387:ALA:CB	2.49	0.42
1:A:379:GLU:HA	1:A:411:GLN:O	2.20	0.42
1:B:50:GLY:HA3	1:B:146:PHE:CE1	2.55	0.42
1:B:75:LEU:HD22	1:B:77:PRO:HG3	2.01	0.42
1:D:45:ILE:HG23	1:D:49:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLY:HA3	1:E:146:PHE:CE1	2.55	0.42
1:A:466:ILE:HD11	1:A:491:ILE:HG13	2.01	0.42
1:A:629:ILE:O	1:A:632:TYR:HB3	2.19	0.42
1:B:123:ASP:O	1:B:130:SER:O	2.38	0.42
1:B:38:VAL:HB	1:B:185:GLU:O	2.19	0.42
1:C:429:VAL:CG1	1:C:430:THR:N	2.83	0.42
1:C:586:LEU:HD12	1:C:587:THR:N	2.35	0.42
1:D:405:ASN:HB2	1:C:407:TRP:CE3	2.55	0.42
1:D:439:LEU:HD12	1:D:574:THR:HA	2.01	0.42
1:E:222:HIS:HA	1:E:283:VAL:HG22	2.02	0.42
1:A:38:VAL:O	1:A:186:PRO:HA	2.19	0.42
1:A:223:THR:HG22	1:A:224:ARG:N	2.35	0.42
1:B:222:HIS:HA	1:B:283:VAL:HG22	2.02	0.42
1:B:443:PHE:N	1:B:443:PHE:CD2	2.87	0.42
1:D:515:LEU:HD12	1:D:518:TYR:CB	2.43	0.42
1:E:38:VAL:HB	1:E:185:GLU:O	2.19	0.42
1:A:586:LEU:HA	1:A:589:ILE:CG1	2.50	0.41
1:A:73:GLY:HA2	1:A:365:GLY:HA3	2.02	0.41
1:B:223:THR:HG22	1:B:224:ARG:N	2.35	0.41
1:B:57:ASP:O	1:B:57:ASP:OD1	2.38	0.41
1:B:586:LEU:HD12	1:B:587:THR:N	2.35	0.41
1:C:171:ILE:HG21	1:C:184:GLY:HA3	2.01	0.41
1:C:219:LEU:HG	1:C:220:THR:N	2.34	0.41
1:C:57:ASP:O	1:C:57:ASP:OD1	2.38	0.41
1:D:38:VAL:HB	1:D:185:GLU:O	2.19	0.41
1:D:586:LEU:HA	1:D:589:ILE:CG1	2.50	0.41
1:E:314:SER:O	1:E:315:GLY:C	2.58	0.41
1:A:398:SER:HB2	1:E:410:ASN:ND2	2.35	0.41
1:E:586:LEU:HA	1:E:589:ILE:HB	2.02	0.41
1:A:123:ASP:O	1:A:130:SER:O	2.38	0.41
1:A:333:GLY:O	1:A:355:LEU:HD12	2.20	0.41
1:A:355:LEU:O	1:A:424:PHE:HA	2.19	0.41
1:A:429:VAL:CG1	1:A:430:THR:N	2.82	0.41
1:D:50:GLY:HA3	1:D:146:PHE:CE1	2.55	0.41
1:A:210:ILE:HD12	1:A:302:LEU:HB2	2.02	0.41
1:B:73:GLY:HA2	1:B:365:GLY:HA3	2.03	0.41
1:C:123:ASP:O	1:C:130:SER:O	2.38	0.41
1:C:443:PHE:CD1	1:C:515:LEU:CD2	2.99	0.41
1:D:464:ASN:C	1:D:464:ASN:OD1	2.58	0.41
1:E:379:GLU:HA	1:E:411:GLN:O	2.20	0.41
1:E:586:LEU:HD12	1:E:587:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLY:N	1:A:130:SER:OG	2.50	0.41
1:C:441:TYR:HD2	1:C:574:THR:HG21	1.86	0.41
1:D:524:VAL:HG23	1:D:525:PRO:N	2.35	0.41
1:E:38:VAL:O	1:E:186:PRO:HA	2.19	0.41
1:A:222:HIS:HA	1:A:283:VAL:HG22	2.02	0.41
1:A:488:SER:O	1:A:508:THR:N	2.53	0.41
1:A:515:LEU:HG	1:A:518:TYR:HB2	2.01	0.41
1:B:379:GLU:HA	1:B:411:GLN:O	2.20	0.41
1:B:522:ILE:HD12	1:B:523:PHE:N	2.35	0.41
1:C:45:ILE:HG23	1:C:49:ARG:O	2.20	0.41
1:C:586:LEU:HA	1:C:589:ILE:HB	2.01	0.41
1:C:586:LEU:HA	1:C:589:ILE:CG1	2.50	0.41
1:D:250:THR:HG22	1:D:283:VAL:O	2.21	0.41
1:D:573:LEU:HD12	1:D:573:LEU:C	2.41	0.41
1:E:371:CYS:SG	1:E:372:GLY:N	2.87	0.41
1:E:45:ILE:HG23	1:E:49:ARG:O	2.20	0.41
1:A:50:GLY:HA3	1:A:146:PHE:CE1	2.55	0.41
1:B:357:LEU:N	1:B:423:TYR:O	2.37	0.41
1:B:515:LEU:CD2	1:B:519:ILE:HD13	2.50	0.41
1:C:222:HIS:HA	1:C:283:VAL:HG22	2.02	0.41
1:C:50:GLY:HA3	1:C:146:PHE:CE1	2.55	0.41
1:C:67:SER:OG	1:C:69:GLN:NE2	2.53	0.41
1:E:250:THR:HG22	1:E:283:VAL:O	2.20	0.41
1:E:75:LEU:CD2	1:E:77:PRO:HG3	2.51	0.41
1:B:45:ILE:HG23	1:B:49:ARG:O	2.20	0.41
1:C:145:ILE:CD1	1:C:172:LEU:HD21	2.49	0.41
1:E:225:ASN:OD1	1:E:281:GLU:HG2	2.21	0.41
1:E:524:VAL:CG2	1:E:525:PRO:HD3	2.46	0.41
1:A:371:CYS:SG	1:A:372:GLY:N	2.88	0.41
1:A:393:PRO:O	1:A:394:LEU:HD12	2.21	0.41
1:A:586:LEU:HA	1:A:589:ILE:HB	2.02	0.41
1:B:70:ASN:ND2	1:B:75:LEU:O	2.51	0.41
1:C:530:ILE:HG12	1:C:624:TYR:CZ	2.56	0.41
1:D:349:PHE:CZ	1:D:448:PHE:HB3	2.55	0.41
1:A:145:ILE:CD1	1:A:172:LEU:HD21	2.50	0.41
1:A:409:GLN:OE1	1:B:399:PHE:N	2.52	0.41
1:A:416:THR:HG23	1:A:418:ASP:HB2	2.02	0.41
1:A:357:LEU:N	1:A:423:TYR:O	2.37	0.41
1:E:223:THR:HG22	1:E:224:ARG:N	2.35	0.41
1:E:530:ILE:HG12	1:E:624:TYR:CZ	2.56	0.41
1:A:150:THR:CG2	1:A:152:THR:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:LEU:CD1	1:A:627:TYR:N	2.73	0.41
1:B:145:ILE:CD1	1:B:172:LEU:HD21	2.50	0.41
1:B:250:THR:HG22	1:B:283:VAL:O	2.21	0.41
1:B:530:ILE:HG12	1:B:624:TYR:CZ	2.56	0.41
1:C:79:VAL:HG11	1:C:131:ALA:HB1	1.96	0.41
1:C:379:GLU:HA	1:C:411:GLN:O	2.21	0.41
1:C:597:GLN:HG2	1:C:612:ILE:HD11	2.02	0.41
1:D:150:THR:CG2	1:D:152:THR:HG23	2.51	0.41
1:D:379:GLU:HA	1:D:411:GLN:O	2.21	0.41
1:E:586:LEU:HA	1:E:589:ILE:CG1	2.50	0.41
1:B:68:MET:SD	1:B:77:PRO:HB3	2.62	0.41
1:E:431:LEU:HD13	1:E:450:ILE:HG12	2.03	0.41
1:A:530:ILE:HG12	1:A:624:TYR:CZ	2.56	0.40
1:B:150:THR:CG2	1:B:152:THR:HG23	2.51	0.40
1:D:219:LEU:HG	1:D:220:THR:N	2.36	0.40
1:D:462:ILE:HG22	1:D:463:PHE:O	2.21	0.40
1:E:277:GLN:CG	1:E:278:ASP:H	2.33	0.40
1:A:219:LEU:HG	1:A:220:THR:N	2.36	0.40
1:A:68:MET:SD	1:A:77:PRO:HB3	2.62	0.40
1:D:496:PHE:CZ	1:C:424:PHE:CE1	3.09	0.40
1:D:57:ASP:O	1:D:57:ASP:OD1	2.38	0.40
1:E:171:ILE:HG21	1:E:184:GLY:HA3	2.02	0.40
1:B:393:PRO:O	1:B:394:LEU:HD12	2.21	0.40
1:B:429:VAL:CG1	1:B:430:THR:N	2.83	0.40
1:C:431:LEU:HD13	1:C:450:ILE:HG12	2.04	0.40
1:C:68:MET:SD	1:C:77:PRO:HB3	2.61	0.40
1:D:492:THR:HG22	1:D:493:GLU:H	1.85	0.40
1:E:393:PRO:O	1:E:394:LEU:HD12	2.21	0.40
1:A:526:LEU:CD2	1:A:579:PHE:CE2	3.04	0.40
1:A:45:ILE:HG23	1:A:49:ARG:O	2.21	0.40
1:D:393:PRO:O	1:D:394:LEU:HD12	2.21	0.40
1:A:399:PHE:N	1:E:409:GLN:OE1	2.52	0.40
1:E:68:MET:SD	1:E:77:PRO:HB3	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/642 (91%)	547 (94%)	34 (6%)	2 (0%)	43	79
1	B	583/642 (91%)	545 (94%)	36 (6%)	2 (0%)	43	79
1	C	587/642 (91%)	550 (94%)	35 (6%)	2 (0%)	43	79
1	D	586/642 (91%)	548 (94%)	37 (6%)	1 (0%)	49	83
1	E	586/642 (91%)	540 (92%)	45 (8%)	1 (0%)	49	83
All	All	2925/3210 (91%)	2730 (93%)	187 (6%)	8 (0%)	43	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	124	ASP
1	D	124	ASP
1	A	125	GLY
1	C	125	GLY
1	B	125	GLY
1	A	124	ASP
1	C	124	ASP
1	B	124	ASP

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	496/557 (89%)	491 (99%)	5 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	496/557 (89%)	492 (99%)	4 (1%)	83	92
1	C	499/557 (90%)	495 (99%)	4 (1%)	83	92
1	D	498/557 (89%)	494 (99%)	4 (1%)	83	92
1	E	495/557 (89%)	491 (99%)	4 (1%)	83	92
All	All	2484/2785 (89%)	2463 (99%)	21 (1%)	83	92

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	LEU
1	A	436	PHE
1	A	572	TYR
1	A	615	TRP
1	A	624	TYR
1	E	329	LEU
1	E	436	PHE
1	E	572	TYR
1	E	624	TYR
1	D	329	LEU
1	D	436	PHE
1	D	572	TYR
1	D	624	TYR
1	C	329	LEU
1	C	436	PHE
1	C	572	TYR
1	C	624	TYR
1	B	329	LEU
1	B	436	PHE
1	B	572	TYR
1	B	624	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	154	GLN
1	A	277	GLN
1	A	307	ASN
1	A	310	ASN
1	A	391	ASN

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Mol	Chain	Res	Type
1	A	552	ASN
1	E	69	GLN
1	E	154	GLN
1	E	307	ASN
1	E	410	ASN
1	E	432	GLN
1	E	552	ASN
1	D	69	GLN
1	D	154	GLN
1	D	307	ASN
1	D	310	ASN
1	D	391	ASN
1	D	410	ASN
1	D	552	ASN
1	D	606	GLN
1	C	69	GLN
1	C	154	GLN
1	C	307	ASN
1	C	310	ASN
1	C	391	ASN
1	C	552	ASN
1	C	606	GLN
1	B	69	GLN
1	B	154	GLN
1	B	307	ASN
1	B	310	ASN
1	B	552	ASN
1	B	606	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 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
3	P3A	A	703	-	20,20,57	0.60	0	22,27,67	0.54	0
2	TRS	C	701	-	7,7,7	0.35	0	9,9,9	0.34	0
3	P3A	A	702	-	18,18,57	1.00	1 (5%)	21,25,67	0.94	1 (4%)
2	TRS	E	701	-	7,7,7	0.38	0	9,9,9	0.41	0
2	TRS	D	701	-	7,7,7	0.35	0	9,9,9	0.25	0
2	TRS	A	701	-	7,7,7	0.32	0	9,9,9	0.20	0
2	TRS	B	701	-	7,7,7	0.31	0	9,9,9	0.47	0
3	P3A	C	702	-	19,19,57	0.58	0	21,26,67	0.52	0
3	P3A	B	702	-	20,20,57	0.58	0	22,27,67	0.52	0
3	P3A	E	702	-	19,19,57	0.59	0	21,26,67	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P3A	A	703	-	-	8/24/24/65	-
2	TRS	C	701	-	-	0/9/9/9	-
3	P3A	A	702	-	-	9/20/20/65	-
2	TRS	E	701	-	-	3/9/9/9	-
2	TRS	D	701	-	-	1/9/9/9	-
2	TRS	A	701	-	-	0/9/9/9	-
2	TRS	B	701	-	-	3/9/9/9	-
3	P3A	C	702	-	-	11/23/23/65	-
3	P3A	B	702	-	-	14/24/24/65	-
3	P3A	E	702	-	-	9/23/23/65	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	P3A	P16-O17	3.54	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	P3A	O18-P16-O19	2.98	119.02	107.64

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	P3A	O15-C14-C6-C8
3	B	702	P3A	C39-O19-P16-O17
3	B	702	P3A	C39-O19-P16-O18
3	B	702	P3A	C39-O19-P16-O15
3	B	702	P3A	C14-O15-P16-O18
3	B	702	P3A	C8-O9-P10-O12
3	B	702	P3A	C8-O9-P10-O13
3	B	702	P3A	C1-O11-P10-O12
3	B	702	P3A	C1-O11-P10-O13
3	A	702	P3A	C14-O15-P16-O19
3	A	702	P3A	C8-O9-P10-O13
3	A	702	P3A	C1-C2-C4-O5
2	D	701	TRS	N-C-C3-O3
2	B	701	TRS	C1-C-C3-O3
2	B	701	TRS	C2-C-C3-O3
2	B	701	TRS	N-C-C3-O3
3	C	702	P3A	C39-O19-P16-O18
3	C	702	P3A	C1-O11-P10-O9
3	C	702	P3A	O11-C1-C2-O3
3	E	702	P3A	C1-O11-P10-O13
3	A	703	P3A	O15-C14-C6-O7
3	C	702	P3A	O11-C1-C2-C4
3	E	702	P3A	O11-C1-C2-C4
3	E	702	P3A	O11-C1-C2-O3
3	A	702	P3A	O15-C14-C6-O7
3	C	702	P3A	O7-C6-C8-O9
3	A	703	P3A	C14-O15-P16-O19
3	A	703	P3A	C8-O9-P10-O11
3	B	702	P3A	C14-O15-P16-O19
3	B	702	P3A	C8-O9-P10-O11
3	B	702	P3A	C1-O11-P10-O9

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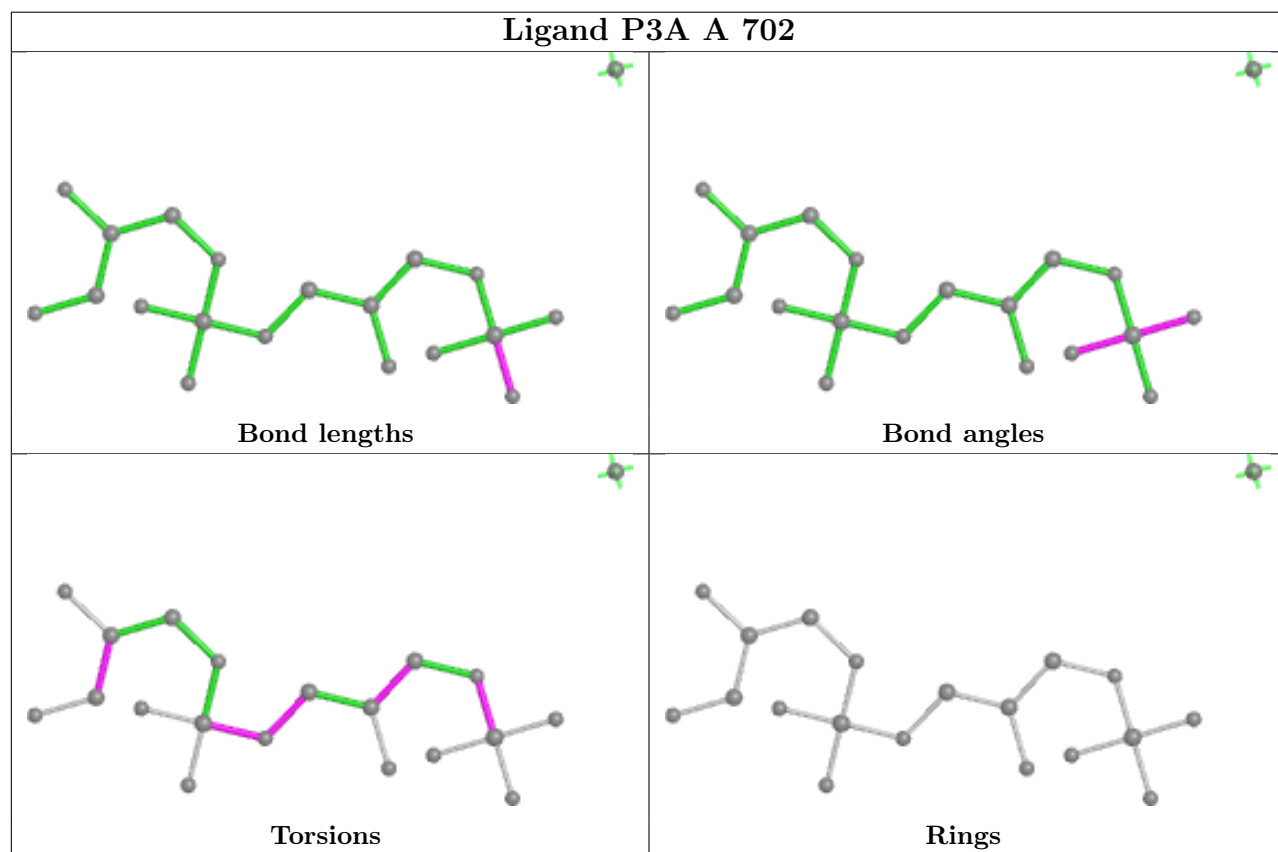
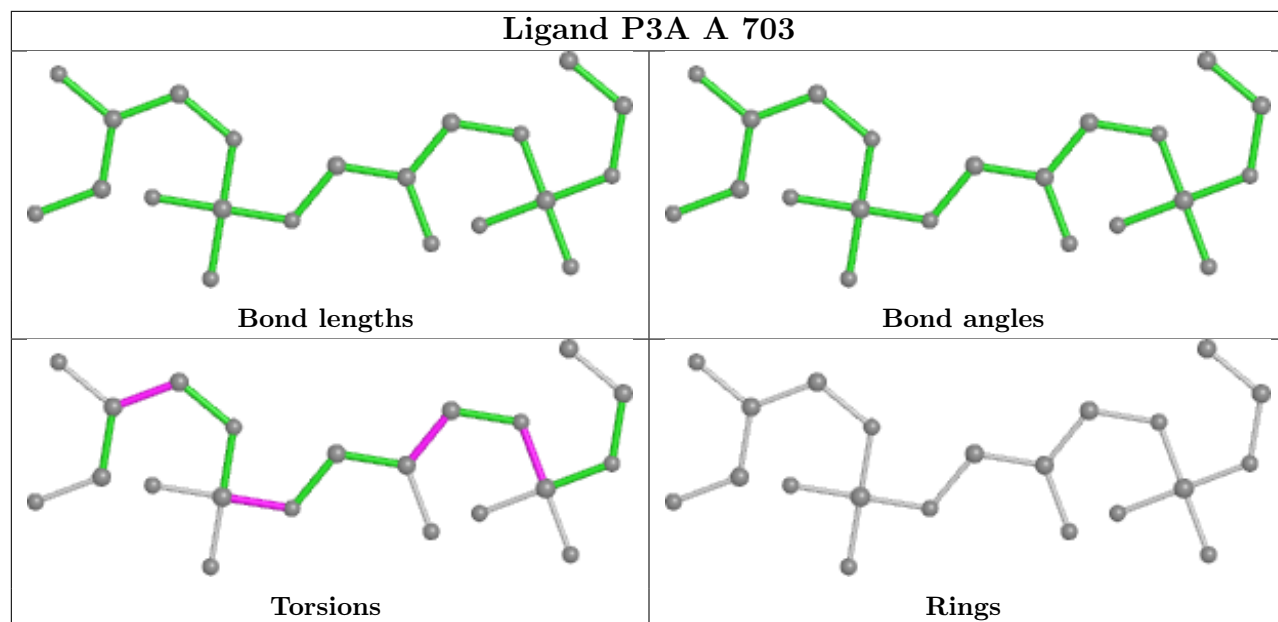
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Mol	Chain	Res	Type	Atoms
3	E	702	P3A	C14-O15-P16-O19
3	E	702	P3A	C1-O11-P10-O9
3	A	702	P3A	O15-C14-C6-C8
3	C	702	P3A	C14-C6-C8-O9
3	A	702	P3A	O3-C2-C4-O5
2	E	701	TRS	C1-C-C3-O3
3	E	702	P3A	C39-O19-P16-O17
3	A	703	P3A	O11-C1-C2-C4
3	B	702	P3A	O11-C1-C2-C4
2	E	701	TRS	N-C-C3-O3
3	A	703	P3A	C14-O15-P16-O17
3	A	703	P3A	C8-O9-P10-O12
3	B	702	P3A	C14-O15-P16-O17
3	C	702	P3A	C1-O11-P10-O13
3	A	702	P3A	C8-O9-P10-O11
3	C	702	P3A	C14-O15-P16-O19
3	E	702	P3A	O7-C6-C8-O9
3	E	702	P3A	C14-C6-C8-O9
2	E	701	TRS	C2-C-C3-O3
3	B	702	P3A	O11-C1-C2-O3
3	C	702	P3A	C6-C8-O9-P10
3	A	702	P3A	C6-C8-O9-P10
3	A	702	P3A	C8-O9-P10-O12
3	C	702	P3A	C14-O15-P16-O17
3	C	702	P3A	C8-O9-P10-O12
3	E	702	P3A	C14-O15-P16-O17
3	A	703	P3A	O11-C1-C2-O3

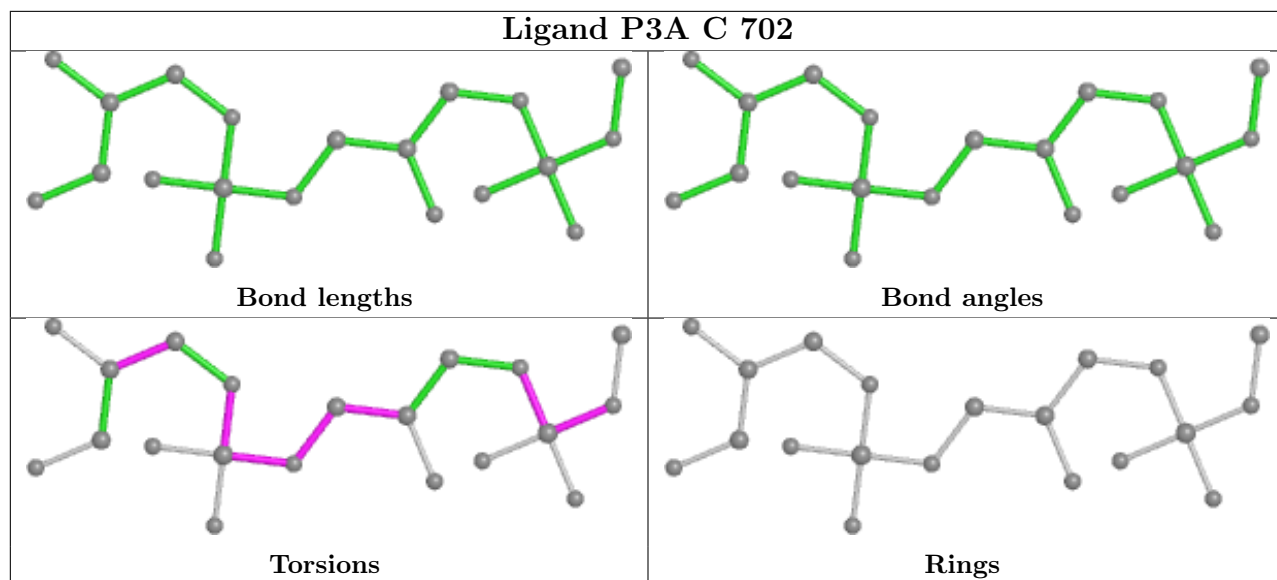
There are no ring outliers.

No monomer is involved in short contacts.

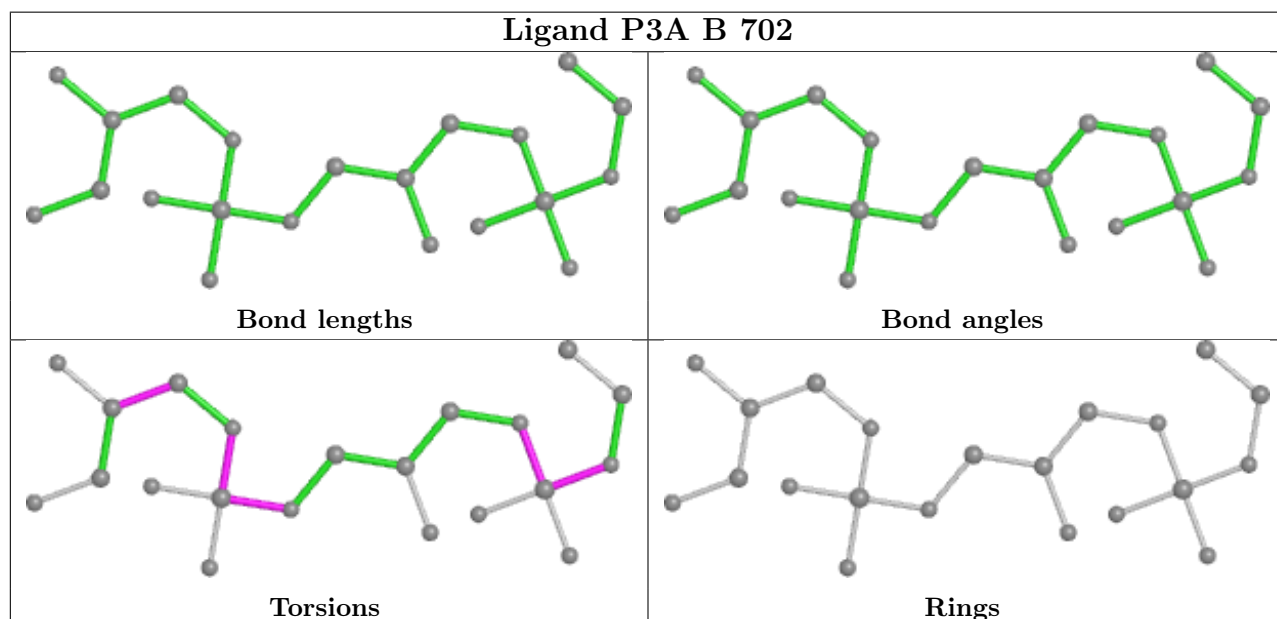
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



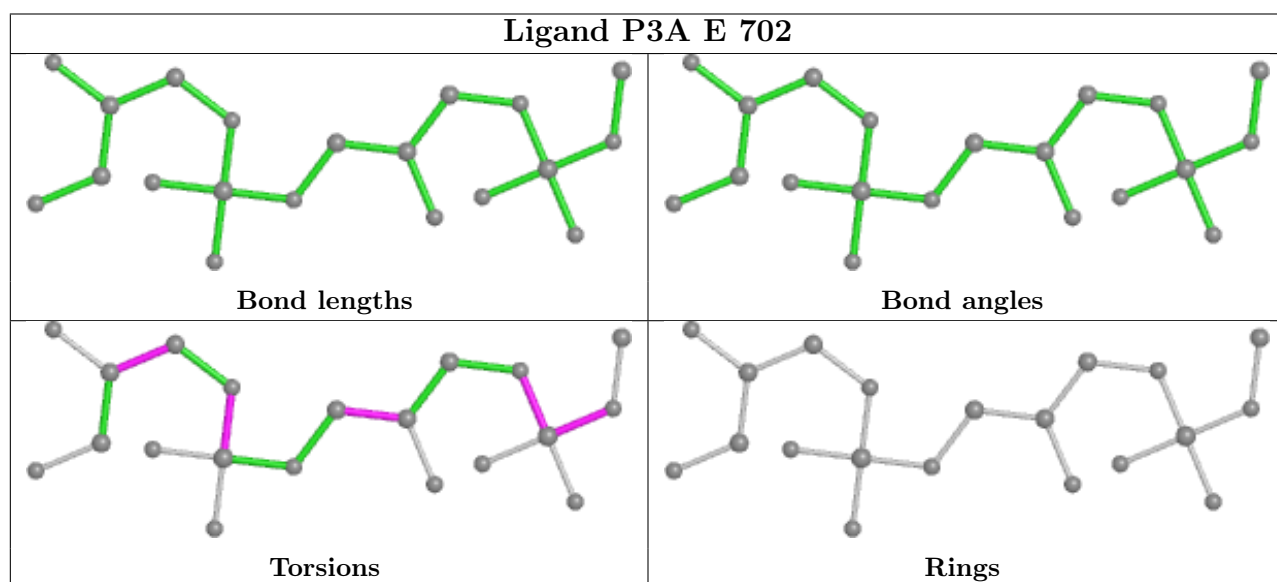
Ligand P3A C 702



Ligand P3A B 702



Ligand P3A E 702



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	589/642 (91%)	-0.36	15 (2%) 57 46	53, 143, 265, 338	0
1	B	589/642 (91%)	-0.36	12 (2%) 65 55	50, 149, 274, 340	0
1	C	593/642 (92%)	-0.38	7 (1%) 79 70	42, 136, 250, 312	0
1	D	592/642 (92%)	-0.32	15 (2%) 57 46	56, 144, 248, 291	0
1	E	592/642 (92%)	-0.39	9 (1%) 73 64	54, 143, 255, 294	0
All	All	2955/3210 (92%)	-0.36	58 (1%) 65 55	42, 144, 257, 340	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	312	ARG	4.9
1	D	140	ASP	4.4
1	A	61	GLY	4.1
1	E	294	ASP	3.9
1	C	80	GLY	3.8
1	E	268	SER	3.7
1	A	267	GLU	3.6
1	A	36	GLY	3.6
1	C	291	GLY	3.5
1	A	140	ASP	3.4
1	D	292	GLN	3.3
1	A	266	GLY	3.2
1	E	80	GLY	3.1
1	A	189	GLU	3.0
1	B	127	LYS	2.9
1	E	61	GLY	2.9
1	B	240	GLY	2.9
1	A	187	GLU	2.8
1	B	294	ASP	2.8
1	B	138	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	57	ASP	2.8
1	B	50	GLY	2.8
1	D	291	GLY	2.7
1	A	268	SER	2.7
1	D	57	ASP	2.6
1	C	140	ASP	2.6
1	A	606	GLN	2.6
1	B	91	SER	2.6
1	A	60	GLN	2.6
1	A	129	TYR	2.6
1	D	370	GLN	2.5
1	D	173	GLY	2.4
1	A	445	ARG	2.4
1	C	127	LYS	2.4
1	A	80	GLY	2.4
1	D	148	GLY	2.3
1	A	294	ASP	2.3
1	B	184	GLY	2.3
1	B	57	ASP	2.3
1	B	97	GLU	2.3
1	D	312	ARG	2.3
1	B	36	GLY	2.3
1	C	76	ASP	2.3
1	E	296	GLY	2.2
1	D	134	GLU	2.2
1	E	297	GLU	2.2
1	D	607	ALA	2.1
1	D	50	GLY	2.1
1	B	61	GLY	2.1
1	D	288	GLY	2.1
1	D	101	ALA	2.1
1	E	140	ASP	2.1
1	D	215	ASP	2.1
1	E	295	SER	2.1
1	E	309	PRO	2.0
1	B	239	ILE	2.0
1	D	80	GLY	2.0
1	A	607	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

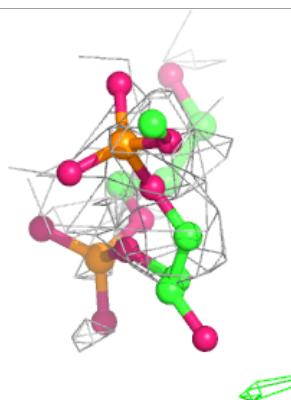
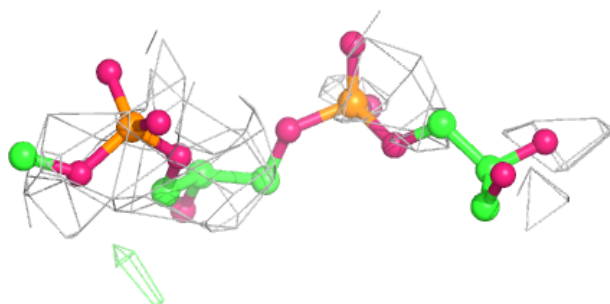
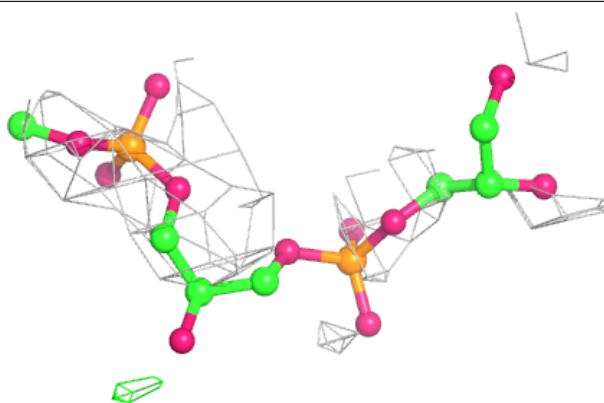
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	P3A	E	702	20/58	0.66	0.47	190,241,260,262	0
3	P3A	A	702	20/58	0.77	0.40	25,229,253,254	0
2	TRS	A	701	8/8	0.78	0.23	156,168,173,175	0
2	TRS	E	701	8/8	0.78	0.24	129,151,166,175	0
3	P3A	A	703	21/58	0.79	0.34	168,227,236,236	0
3	P3A	C	702	20/58	0.80	0.32	141,215,271,276	0
2	TRS	D	701	8/8	0.82	0.21	134,160,165,168	0
2	TRS	B	701	8/8	0.82	0.20	148,156,177,190	0
3	P3A	B	702	21/58	0.85	0.29	134,209,242,249	0
2	TRS	C	701	8/8	0.88	0.21	120,144,159,170	0

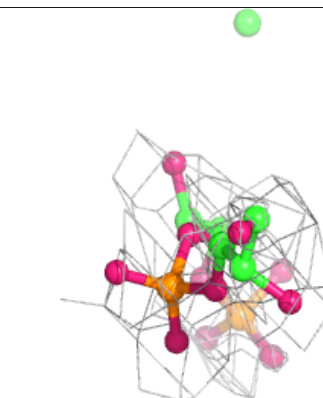
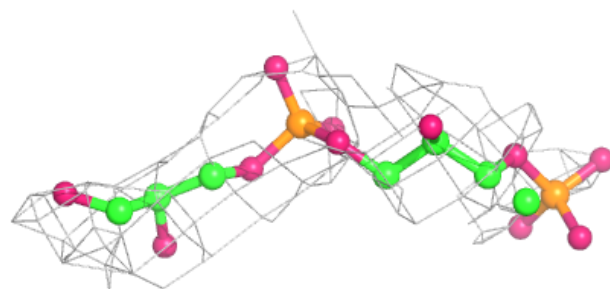
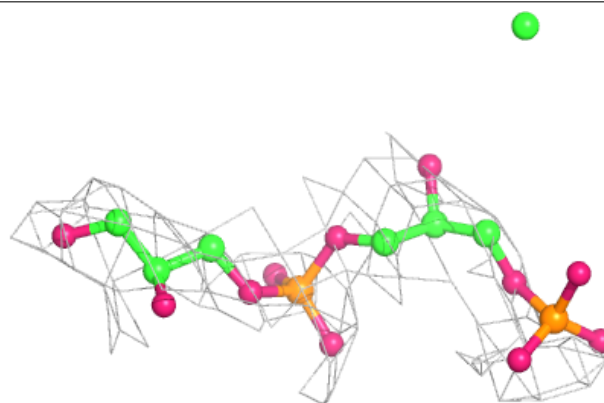
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P3A E 702:

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

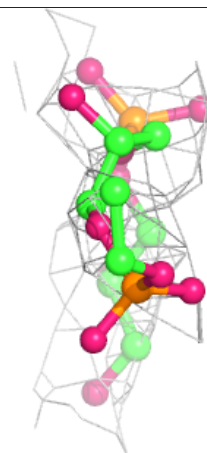
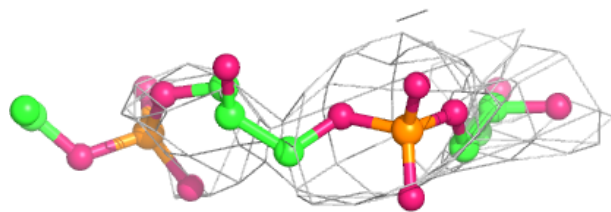
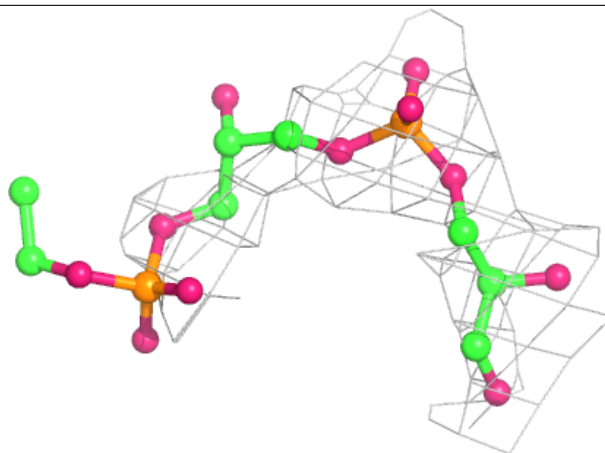
**Electron density around P3A A 702:**

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



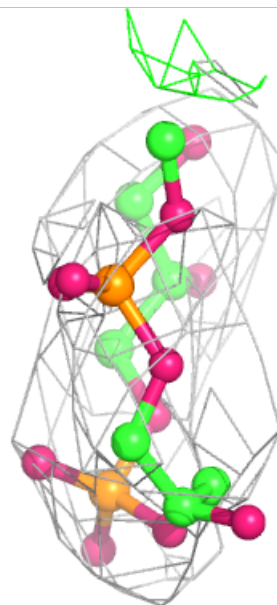
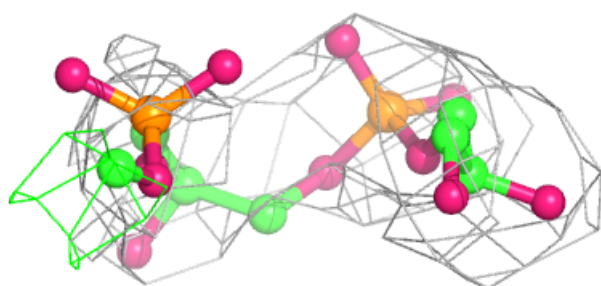
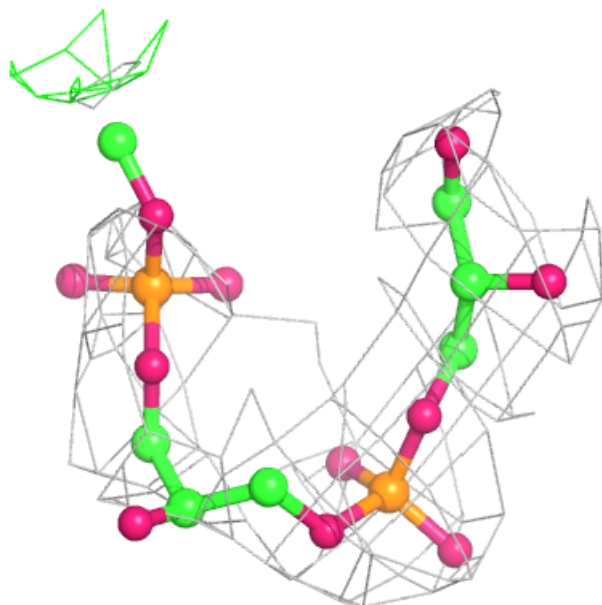
Electron density around P3A A 703:

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



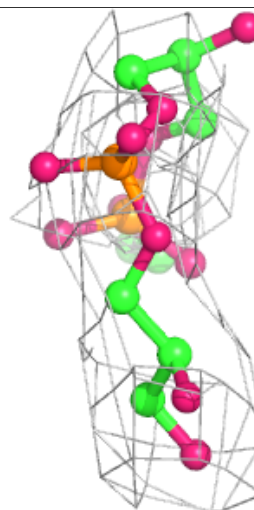
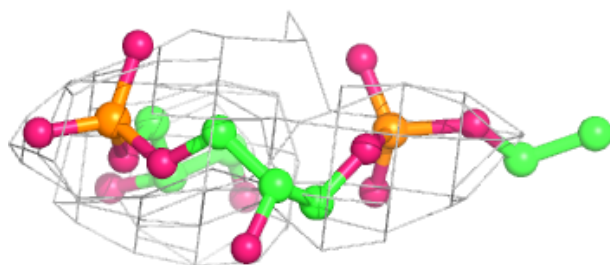
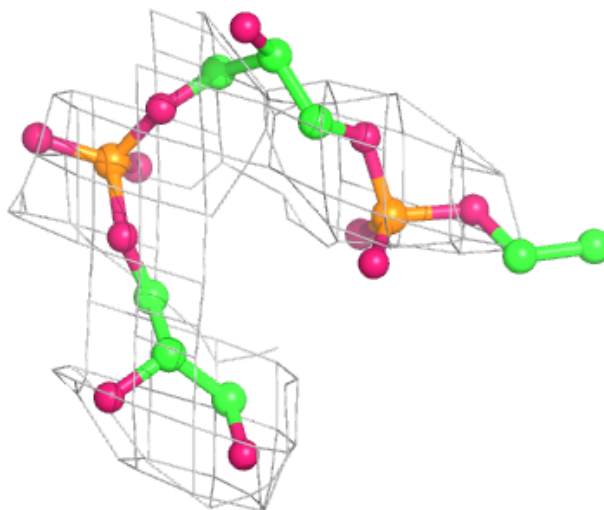
Electron density around P3A C 702:

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



Electron density around P3A B 702:

$2mF_o-DF_c$ (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.