



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:57 PM UTC

PDB ID : 6V4A / pdb_00006v4a
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 types of validation reports are described at

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

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

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

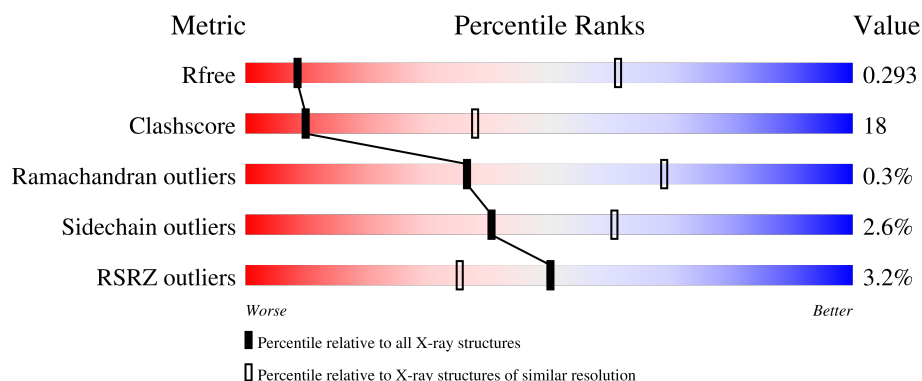
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)

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	642	 2% 61% 26% 5% 8%
1	B	642	 4% 60% 26% 5% 8%
1	C	642	 3% 61% 27% 5% 8%
1	D	642	 3% 62% 26% 5% 8%
1	E	642	 2% 62% 25% 5% 8%

2 Entry composition [i](#)

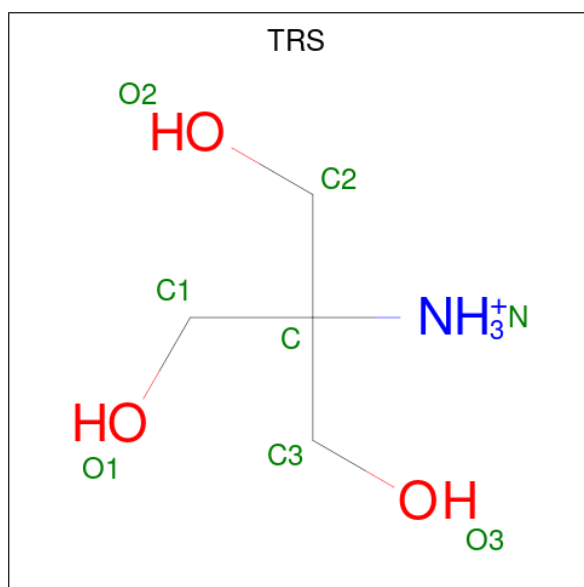
There are 3 unique types of molecules in this entry. The entry contains 23190 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: TRS) (formula: C₄H₁₂NO₃).



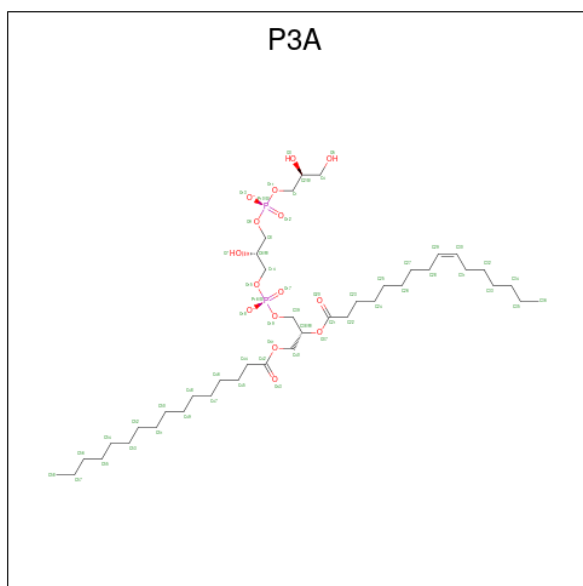
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		

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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 (CCD ID: P3A) (formula: $C_{41}H_{78}O_{15}P_2$).

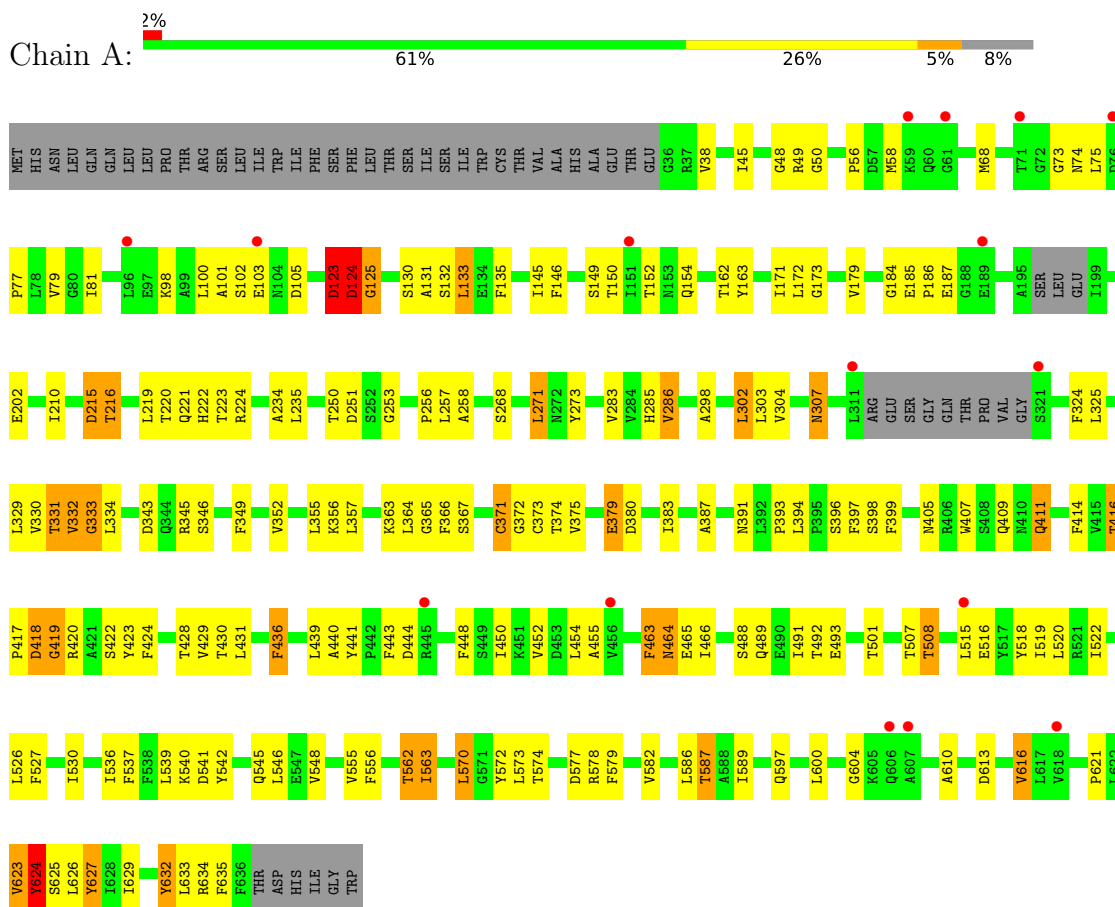


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			20	7	11	2		
3	A	1	Total	C	O	P	0	0
			21	8	11	2		
3	E	1	Total	C	O	P	0	0
			20	7	11	2		
3	C	1	Total	C	O	P	0	0
			20	7	11	2		
3	B	1	Total	C	O	P	0	0
			21	8	11	2		

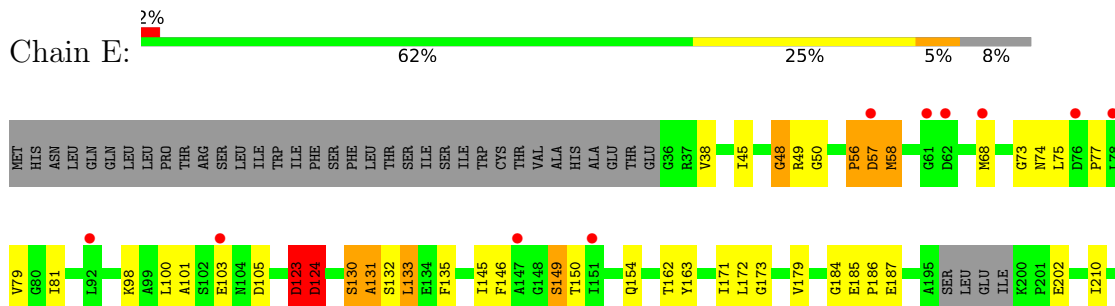
3 Residue-property plots

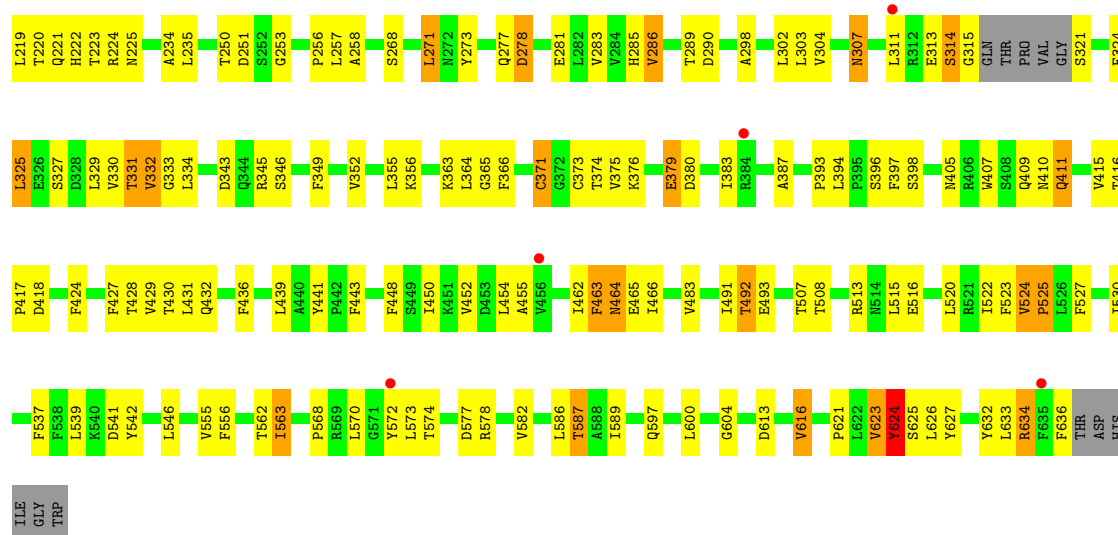
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

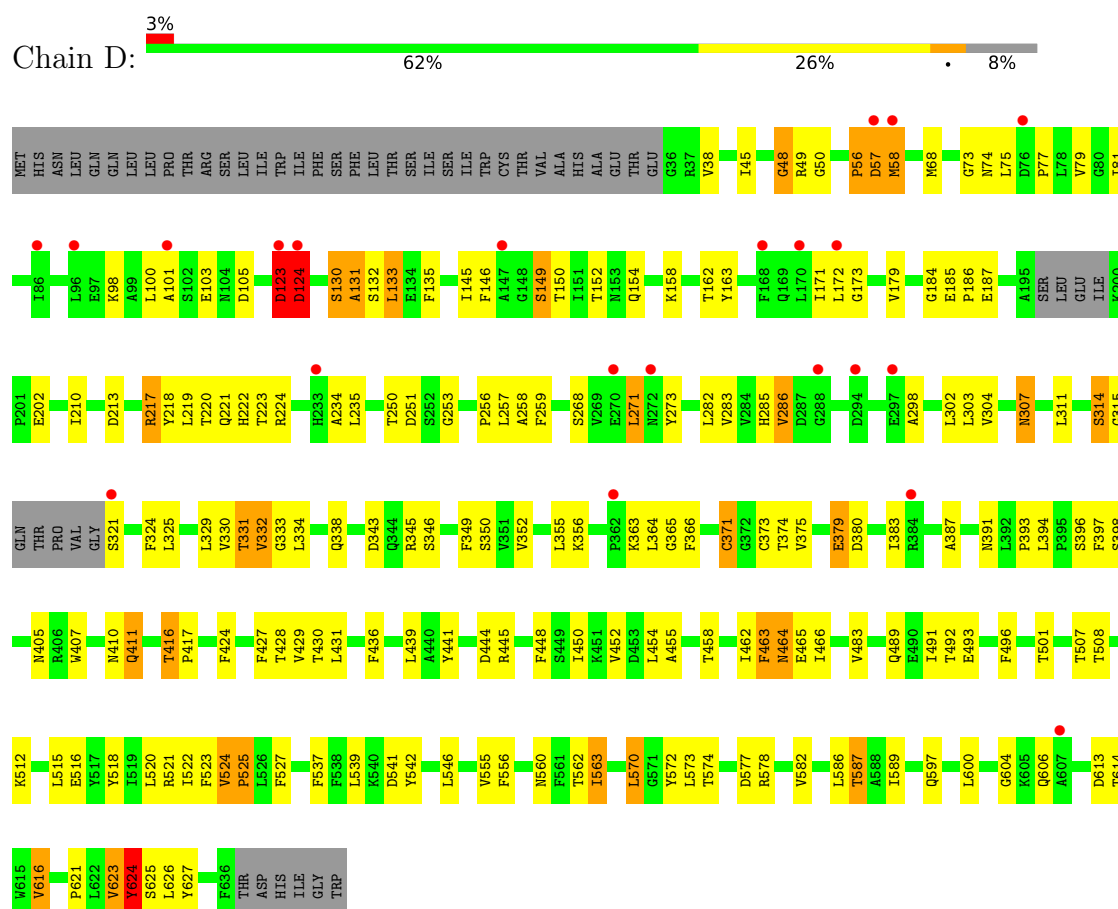


- Molecule 1: Neur_chan_LBD domain-containing protein



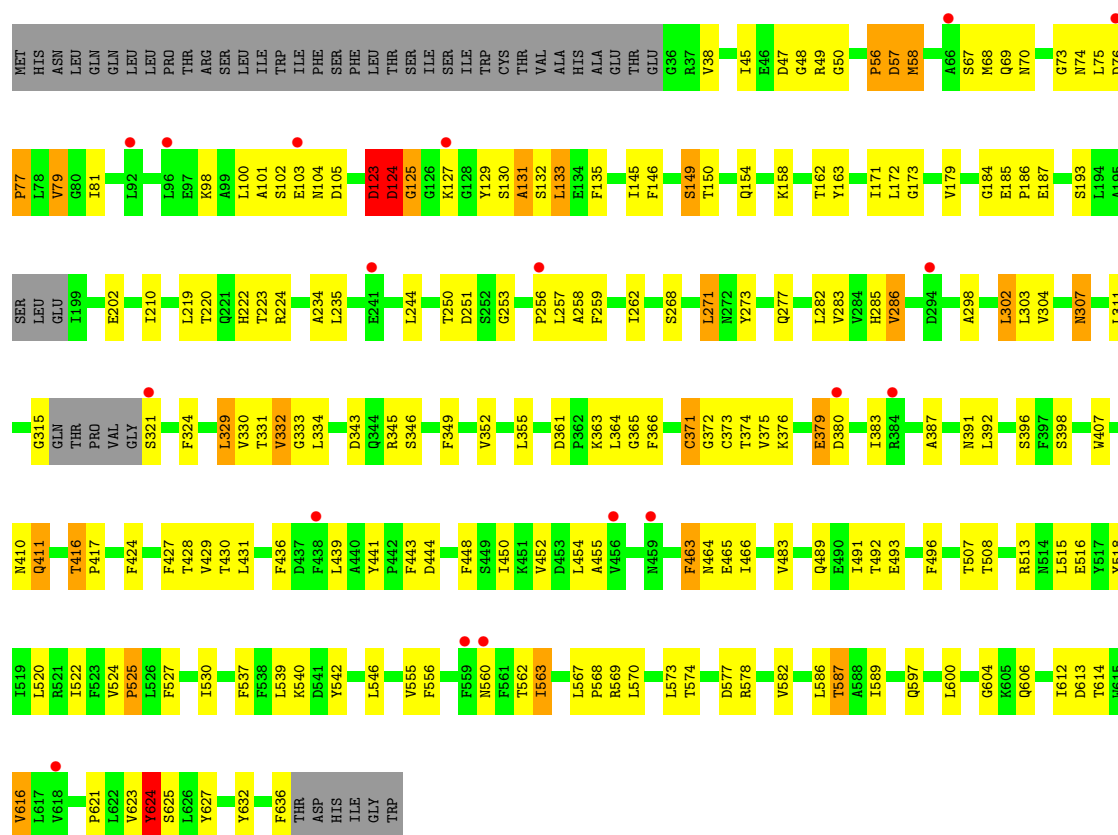


• Molecule 1: Neur_chan_LBD domain-containing protein

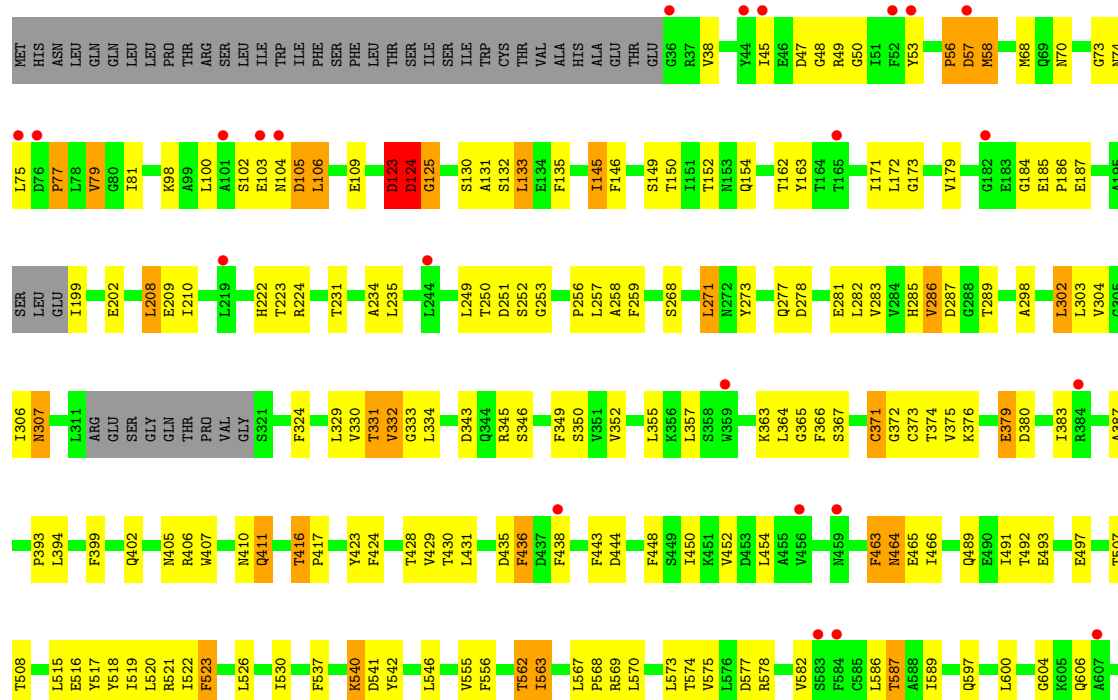


• Molecule 1: Neur_chan_LBD domain-containing protein





• Molecule 1: Neur_chan_LBD domain-containing protein



A610	Q611	I612	D613	T614	W615	V616	P621	L622	V623	Y624	S625	L626	Y627	F636	THR	ASP	HIS	ILE	GLY	TRP
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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) 73.3 (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 (3.77%)	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 , 86.6	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: P3A, TRS

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	1.05	5/4702 (0.1%)	1.35	49/6402 (0.8%)
1	B	1.05	6/4702 (0.1%)	1.39	55/6402 (0.9%)
1	C	1.06	7/4732 (0.1%)	1.37	50/6441 (0.8%)
1	D	1.07	6/4724 (0.1%)	1.38	53/6430 (0.8%)
1	E	1.07	7/4707 (0.1%)	1.42	64/6409 (1.0%)
All	All	1.06	31/23567 (0.1%)	1.38	271/32084 (0.8%)

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 (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	525	PRO	N-CD	15.79	1.69	1.47
1	D	525	PRO	N-CD	15.41	1.69	1.47
1	A	418	ASP	CA-C	12.39	1.69	1.52
1	C	77	PRO	N-CD	-11.62	1.31	1.47
1	C	57	ASP	CA-C	8.65	1.64	1.52
1	B	57	ASP	CA-C	8.64	1.64	1.52
1	E	57	ASP	CA-C	8.54	1.64	1.52
1	E	187	GLU	CA-C	8.50	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	57	ASP	CA-C	8.44	1.64	1.52
1	D	187	GLU	CA-C	8.36	1.62	1.52
1	C	187	GLU	CA-C	8.19	1.62	1.52
1	A	187	GLU	CA-C	8.18	1.62	1.52
1	D	124	ASP	C-O	7.75	1.33	1.24
1	C	525	PRO	N-CD	7.74	1.58	1.47
1	B	187	GLU	CA-C	7.61	1.61	1.52
1	B	77	PRO	N-CD	-6.93	1.38	1.47
1	E	123	ASP	C-O	-6.56	1.15	1.23
1	B	105	ASP	CA-C	6.52	1.61	1.52
1	E	418	ASP	CA-C	6.26	1.61	1.52
1	E	131	ALA	CA-C	-6.16	1.43	1.53
1	A	436	PHE	N-CA	-5.82	1.39	1.46
1	C	307	ASN	CA-C	5.63	1.59	1.52
1	D	307	ASN	CA-C	5.62	1.59	1.52
1	A	540	LYS	C-O	-5.53	1.17	1.23
1	B	540	LYS	C-O	-5.50	1.17	1.23
1	B	307	ASN	CA-C	5.40	1.59	1.52
1	A	307	ASN	CA-C	5.32	1.59	1.52
1	D	131	ALA	CA-C	-5.23	1.45	1.53
1	E	307	ASN	CA-C	5.20	1.59	1.52
1	C	131	ALA	CA-C	-5.04	1.45	1.53
1	C	76	ASP	CA-C	5.00	1.58	1.52

All (271) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	623	VAL	N-CA-C	-17.28	93.27	110.72
1	A	625	SER	N-CA-C	14.57	127.16	111.28
1	C	540	LYS	N-CA-C	14.33	130.35	112.86
1	E	623	VAL	N-CA-C	-14.17	93.38	111.09
1	D	623	VAL	N-CA-C	-14.04	93.53	111.09
1	B	104	ASN	N-CA-C	13.95	129.40	112.38
1	D	625	SER	N-CA-C	13.78	126.30	111.28
1	E	625	SER	N-CA-C	13.64	126.15	111.28
1	A	623	VAL	N-CA-C	-13.62	94.06	111.09
1	B	625	SER	N-CA-C	13.43	125.44	111.07
1	B	623	VAL	N-CA-C	-13.43	94.31	111.09
1	E	124	ASP	N-CA-C	12.93	138.34	110.80
1	E	314	SER	N-CA-C	12.51	128.91	109.52
1	D	124	ASP	N-CA-C	11.70	135.72	110.80
1	E	123	ASP	N-CA-C	11.44	125.99	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	625	SER	N-CA-C	11.31	123.60	111.28
1	B	106	LEU	N-CA-CB	10.66	125.46	110.01
1	C	123	ASP	N-CA-C	10.28	125.73	110.52
1	B	123	ASP	N-CA-C	10.16	125.56	110.52
1	D	123	ASP	N-CA-C	10.10	124.19	110.55
1	B	307	ASN	N-CA-C	10.01	126.73	113.72
1	C	307	ASN	N-CA-C	9.96	126.67	113.72
1	A	516	GLU	N-CA-C	-9.94	99.46	111.69
1	A	123	ASP	N-CA-C	9.73	124.92	110.52
1	D	307	ASN	N-CA-C	9.66	126.28	113.72
1	E	464	ASN	N-CA-C	9.62	125.71	113.88
1	A	307	ASN	N-CA-C	9.59	126.19	113.72
1	B	541	ASP	N-CA-C	-9.56	88.79	107.62
1	B	106	LEU	N-CA-C	-9.37	101.04	111.07
1	E	307	ASN	N-CA-C	9.35	125.88	113.72
1	D	624	TYR	N-CA-CB	9.30	123.96	109.82
1	B	624	TYR	N-CA-CB	9.02	123.08	109.91
1	D	525	PRO	N-CA-CB	8.95	112.65	103.25
1	E	525	PRO	N-CA-CB	8.79	112.48	103.25
1	E	624	TYR	N-CA-CB	8.69	123.03	109.82
1	C	539	LEU	N-CA-C	8.69	121.54	111.11
1	E	634	ARG	N-CA-C	-8.57	101.91	111.07
1	E	525	PRO	CA-N-CD	-8.53	100.06	112.00
1	C	77	PRO	N-CA-CB	-8.53	93.22	102.85
1	C	298	ALA	N-CA-C	-8.52	94.11	108.26
1	B	187	GLU	N-CA-C	8.48	124.24	113.55
1	B	58	MET	N-CA-C	-8.48	97.97	110.52
1	D	525	PRO	CA-N-CD	-8.46	100.16	112.00
1	A	418	ASP	CA-C-O	8.45	132.59	120.51
1	E	463	PHE	N-CA-C	-8.45	95.44	109.46
1	E	58	MET	N-CA-C	-8.43	98.05	110.52
1	E	298	ALA	N-CA-C	-8.43	94.27	108.26
1	D	58	MET	N-CA-C	-8.43	98.05	110.52
1	D	298	ALA	N-CA-C	-8.41	94.30	108.26
1	C	187	GLU	N-CA-C	8.38	124.10	113.55
1	B	298	ALA	N-CA-C	-8.37	94.37	108.26
1	C	58	MET	N-CA-C	-8.32	98.21	110.52
1	D	464	ASN	N-CA-C	8.31	124.10	113.88
1	E	524	VAL	CB-CA-C	-8.24	105.62	114.35
1	D	187	GLU	N-CA-C	8.22	123.91	113.55
1	E	464	ASN	CB-CA-C	-8.12	95.87	109.03
1	A	298	ALA	N-CA-C	-8.12	94.31	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	GLU	N-CA-C	8.11	123.76	113.55
1	B	497	GLU	CA-CB-CG	8.10	130.31	114.10
1	E	187	GLU	N-CA-C	8.04	123.68	113.55
1	B	56	PRO	N-CA-C	8.01	123.63	111.14
1	D	524	VAL	CB-CA-C	-7.97	105.90	114.35
1	C	56	PRO	N-CA-C	7.95	123.54	111.14
1	D	56	PRO	N-CA-C	7.94	123.53	111.14
1	E	56	PRO	N-CA-C	7.86	123.40	111.14
1	B	516	GLU	N-CA-C	-7.69	102.23	111.69
1	B	463	PHE	N-CA-C	-7.67	96.73	109.46
1	A	624	TYR	N-CA-CB	7.62	121.40	109.82
1	D	463	PHE	N-CA-C	-7.56	96.91	109.46
1	D	508	THR	N-CA-C	7.54	121.02	108.73
1	E	508	THR	N-CA-C	7.51	120.98	108.73
1	C	516	GLU	N-CA-C	-7.50	102.46	111.69
1	B	435	ASP	N-CA-C	7.50	120.28	109.71
1	A	463	PHE	N-CA-C	-7.50	97.02	109.46
1	B	464	ASN	N-CA-C	7.49	122.98	113.55
1	C	508	THR	N-CA-C	7.48	120.92	108.73
1	A	508	THR	N-CA-C	7.30	120.42	108.52
1	B	508	THR	N-CA-C	7.26	120.35	108.52
1	B	616	VAL	N-CA-C	7.26	117.98	110.36
1	C	77	PRO	CA-N-CD	7.23	122.12	112.00
1	A	616	VAL	N-CA-C	7.21	117.93	110.36
1	E	616	VAL	N-CA-C	7.19	117.91	110.36
1	D	520	LEU	N-CA-C	7.18	120.14	111.82
1	D	258	ALA	N-CA-C	7.16	119.05	108.60
1	E	541	ASP	N-CA-C	-7.15	93.53	107.62
1	C	616	VAL	N-CA-C	7.15	117.87	110.36
1	E	520	LEU	N-CA-C	7.14	120.10	111.82
1	C	520	LEU	N-CA-C	7.13	120.10	111.82
1	C	258	ALA	N-CA-C	7.13	119.01	108.60
1	E	417	PRO	N-CA-C	-7.07	103.36	113.47
1	D	523	PHE	N-CA-C	7.05	120.00	111.40
1	D	541	ASP	N-CA-C	-7.04	93.75	107.62
1	E	258	ALA	N-CA-C	7.03	118.86	108.60
1	D	616	VAL	N-CA-C	7.02	117.73	110.36
1	E	103	GLU	N-CA-C	6.99	119.55	111.02
1	C	324	PHE	N-CA-C	6.97	121.39	113.02
1	A	215	ASP	N-CA-C	6.96	122.13	112.45
1	A	464	ASN	N-CA-C	6.93	122.28	113.55
1	B	258	ALA	N-CA-C	6.93	118.72	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	VAL	N-CA-C	6.92	117.73	106.72
1	C	452	VAL	N-CA-C	6.90	117.69	106.72
1	C	103	GLU	N-CA-C	6.87	119.40	111.02
1	E	568	PRO	CB-CA-C	-6.86	101.96	110.95
1	D	217	ARG	CB-CG-CD	6.82	126.98	111.30
1	A	258	ALA	N-CA-C	6.80	118.53	108.60
1	E	452	VAL	N-CA-C	6.80	117.53	106.72
1	D	452	VAL	N-CA-C	6.73	117.42	106.72
1	B	324	PHE	N-CA-C	6.71	121.08	113.02
1	D	103	GLU	N-CA-C	6.69	119.19	111.02
1	C	463	PHE	N-CA-C	-6.68	98.36	109.46
1	A	452	VAL	N-CA-C	6.66	117.31	106.72
1	D	324	PHE	N-CA-C	6.59	120.93	113.02
1	A	324	PHE	N-CA-C	6.58	120.91	113.02
1	B	464	ASN	CB-CA-C	-6.55	99.19	109.34
1	D	314	SER	N-CA-C	6.53	119.00	109.07
1	D	464	ASN	CB-CA-C	-6.49	98.52	109.03
1	A	103	GLU	N-CA-C	6.45	118.89	111.02
1	B	103	GLU	N-CA-C	6.45	118.88	111.02
1	E	324	PHE	N-CA-C	6.44	120.74	113.02
1	A	541	ASP	N-CA-C	-6.41	94.99	107.62
1	B	444	ASP	N-CA-C	6.32	120.18	110.20
1	D	444	ASP	N-CA-C	6.28	120.13	110.20
1	B	435	ASP	CB-CA-C	-6.28	102.78	112.07
1	A	419	GLY	N-CA-C	-6.28	98.31	113.18
1	C	624	TYR	N-CA-CB	6.21	119.26	109.82
1	A	539	LEU	N-CA-C	6.18	117.68	111.07
1	E	539	LEU	N-CA-C	6.15	117.65	111.07
1	B	105	ASP	N-CA-C	6.12	120.59	113.18
1	E	124	ASP	CB-CA-C	-6.12	98.24	110.42
1	E	325	LEU	N-CA-C	-6.11	97.75	108.20
1	A	632	TYR	N-CA-C	-6.10	103.58	111.02
1	D	539	LEU	N-CA-C	6.10	117.60	111.07
1	B	332	VAL	CB-CA-C	-6.09	102.87	111.21
1	A	633	LEU	N-CA-C	6.08	118.40	111.11
1	B	105	ASP	CB-CA-C	-6.07	97.88	109.95
1	E	314	SER	N-CA-CB	-6.06	101.00	111.55
1	D	516	GLU	N-CA-C	-6.06	104.23	111.69
1	E	415	VAL	N-CA-C	6.05	117.40	108.45
1	D	416	THR	CB-CA-C	-6.01	100.94	109.96
1	B	132	SER	N-CA-C	6.00	118.49	108.96
1	E	416	THR	CB-CA-C	-5.99	99.85	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	587	THR	N-CA-C	-5.98	104.76	111.28
1	C	132	SER	N-CA-C	5.97	118.46	108.96
1	A	132	SER	N-CA-C	5.97	118.45	108.96
1	A	371	CYS	CA-CB-SG	-5.97	100.67	114.40
1	C	587	THR	N-CA-C	-5.96	104.78	111.28
1	A	587	THR	N-CA-C	-5.96	104.79	111.28
1	B	587	THR	N-CA-C	-5.96	104.79	111.28
1	D	587	THR	N-CA-C	-5.95	104.79	111.28
1	B	371	CYS	CA-CB-SG	-5.95	100.72	114.40
1	A	464	ASN	CB-CA-C	-5.92	100.16	109.34
1	E	332	VAL	CB-CA-C	-5.91	103.11	111.21
1	B	380	ASP	N-CA-C	5.90	117.40	110.97
1	E	523	PHE	N-CA-C	5.89	118.58	111.40
1	E	563	ILE	N-CA-C	-5.88	101.43	109.37
1	C	311	LEU	N-CA-C	5.85	118.89	111.69
1	D	132	SER	N-CA-C	5.85	118.26	108.96
1	A	216	THR	N-CA-CB	5.83	118.44	110.57
1	E	48	GLY	N-CA-C	5.83	123.11	115.36
1	C	124	ASP	N-CA-C	5.83	123.22	110.80
1	C	371	CYS	CA-CB-SG	-5.82	101.02	114.40
1	B	145	ILE	CA-CB-CG2	5.82	120.39	110.50
1	C	380	ASP	N-CA-C	5.82	117.31	110.97
1	A	332	VAL	CB-CA-C	-5.80	103.26	111.21
1	E	289	THR	N-CA-C	5.80	120.48	113.41
1	C	332	VAL	CB-CA-C	-5.79	103.27	111.21
1	E	327	SER	N-CA-CB	-5.76	101.42	110.69
1	A	380	ASP	N-CA-C	5.75	117.24	110.97
1	E	333	GLY	N-CA-C	-5.75	101.40	111.46
1	D	124	ASP	CB-CA-C	-5.72	99.03	110.42
1	D	371	CYS	CA-CB-SG	-5.69	101.31	114.40
1	E	380	ASP	N-CA-C	5.69	117.17	110.97
1	E	278	ASP	N-CA-C	5.69	117.16	111.07
1	D	333	GLY	N-CA-C	-5.69	101.51	111.46
1	C	76	ASP	C-N-CD	-5.69	101.69	125.00
1	C	333	GLY	N-CA-C	-5.68	101.52	111.46
1	B	124	ASP	N-CA-C	5.68	122.90	110.80
1	E	371	CYS	CA-CB-SG	-5.68	101.34	114.40
1	D	332	VAL	CB-CA-C	-5.67	103.44	111.21
1	A	444	ASP	N-CA-C	5.66	119.15	110.20
1	B	523	PHE	N-CA-CB	5.66	118.51	110.13
1	A	345	ARG	CB-CA-C	-5.64	102.27	110.96
1	D	311	LEU	N-CA-C	5.64	118.63	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	GLY	N-CA-C	-5.63	101.61	111.46
1	E	311	LEU	N-CA-C	5.62	118.61	111.69
1	A	562	THR	N-CA-C	5.61	117.84	111.11
1	E	418	ASP	CA-C-O	5.61	128.53	120.51
1	D	380	ASP	N-CA-C	5.60	117.08	110.97
1	E	132	SER	N-CA-C	5.58	117.83	108.96
1	C	416	THR	CB-CA-C	-5.57	101.60	109.96
1	A	542	TYR	N-CA-C	5.57	117.43	111.36
1	A	563	ILE	N-CA-C	-5.57	101.85	109.37
1	B	542	TYR	N-CA-C	5.56	117.42	111.36
1	C	345	ARG	CB-CA-C	-5.55	102.42	110.96
1	E	345	ARG	CB-CA-C	-5.54	102.43	110.96
1	D	345	ARG	CB-CA-C	-5.53	102.20	110.88
1	B	345	ARG	CB-CA-C	-5.53	102.45	110.96
1	B	563	ILE	N-CA-C	-5.53	101.91	109.37
1	B	520	LEU	N-CA-C	5.52	119.19	112.23
1	A	124	ASP	N-CA-C	5.50	122.51	110.80
1	C	331	THR	N-CA-C	5.46	117.61	107.99
1	A	411	GLN	N-CA-C	-5.46	95.70	107.49
1	B	521	ARG	N-CA-C	5.44	120.03	113.17
1	A	627	TYR	N-CA-CB	5.43	117.89	110.01
1	B	79	VAL	N-CA-C	5.42	116.39	108.53
1	B	411	GLN	N-CA-C	-5.42	96.34	107.67
1	C	542	TYR	N-CA-C	5.39	117.24	111.36
1	E	411	GLN	N-CA-C	-5.39	95.85	107.49
1	B	614	THR	N-CA-C	-5.38	105.49	111.36
1	D	542	TYR	N-CA-C	5.38	117.22	111.36
1	A	627	TYR	N-CA-C	-5.37	105.32	111.07
1	A	333	GLY	N-CA-C	-5.37	102.07	111.46
1	A	520	LEU	N-CA-C	5.37	118.99	112.23
1	C	79	VAL	N-CA-C	5.35	116.29	108.53
1	C	411	GLN	N-CA-C	-5.35	96.48	107.67
1	E	563	ILE	N-CA-CB	5.33	117.28	110.13
1	C	563	ILE	N-CA-CB	5.32	117.25	110.13
1	D	527	PHE	N-CA-C	-5.31	105.39	111.07
1	C	282	LEU	N-CA-C	5.30	118.13	109.59
1	C	427	PHE	N-CA-C	5.30	117.25	109.24
1	B	57	ASP	CA-C-O	5.28	128.06	120.51
1	B	332	VAL	N-CA-CB	5.27	117.84	110.56
1	C	392	LEU	N-CA-C	-5.27	103.50	110.40
1	E	313	GLU	N-CA-C	5.27	115.24	108.34
1	B	331	THR	N-CA-C	5.26	117.25	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	48	GLY	N-CA-C	5.26	122.36	115.36
1	C	563	ILE	N-CA-C	-5.26	102.27	109.37
1	E	464	ASN	CA-C-O	5.25	125.17	119.24
1	E	542	TYR	N-CA-C	5.24	117.07	111.36
1	C	57	ASP	CA-C-O	5.24	128.00	120.51
1	D	614	THR	N-CA-C	-5.24	105.65	111.36
1	C	149	SER	N-CA-C	5.23	118.75	109.96
1	B	416	THR	CB-CA-C	-5.23	102.11	109.96
1	E	332	VAL	N-CA-CB	5.22	117.77	110.56
1	E	516	GLU	N-CA-C	-5.21	105.28	111.69
1	E	331	THR	N-CA-C	5.21	117.16	107.99
1	A	332	VAL	N-CA-CB	5.21	117.75	110.56
1	C	332	VAL	N-CA-CB	5.21	117.75	110.56
1	A	331	THR	N-CA-C	5.21	117.15	107.99
1	D	563	ILE	N-CA-CB	5.20	117.09	110.13
1	D	57	ASP	CA-C-O	5.18	127.92	120.51
1	E	492	THR	N-CA-C	-5.18	101.42	109.14
1	C	614	THR	N-CA-C	-5.18	105.72	111.36
1	A	56	PRO	N-CA-C	5.17	119.60	111.38
1	E	527	PHE	N-CA-C	-5.17	105.54	111.07
1	D	331	THR	N-CA-C	5.17	117.09	107.99
1	E	130	SER	CA-C-N	-5.16	114.91	123.37
1	E	130	SER	C-N-CA	-5.16	114.91	123.37
1	A	367	SER	CA-C-N	-5.15	116.45	121.65
1	A	367	SER	C-N-CA	-5.15	116.45	121.65
1	B	562	THR	N-CA-C	5.15	117.29	111.11
1	C	527	PHE	N-CA-C	-5.14	105.57	111.07
1	E	57	ASP	CA-C-O	5.14	127.86	120.51
1	D	411	GLN	N-CA-C	-5.14	96.39	107.49
1	B	367	SER	CA-C-N	-5.13	116.47	121.65
1	B	367	SER	C-N-CA	-5.13	116.47	121.65
1	C	193	SER	N-CA-C	5.11	115.08	107.88
1	C	525	PRO	N-CA-CB	5.09	108.67	103.23
1	D	427	PHE	N-CA-C	5.08	116.92	109.24
1	E	427	PHE	N-CA-C	5.08	116.91	109.24
1	D	282	LEU	N-CA-C	5.08	118.02	109.95
1	B	575	VAL	N-CA-CB	5.07	116.15	110.62
1	A	527	PHE	N-CA-C	-5.06	105.66	111.07
1	D	149	SER	N-CA-C	5.05	118.45	109.96
1	C	444	ASP	N-CA-C	5.04	118.42	109.96
1	E	149	SER	N-CA-C	5.03	118.41	109.96
1	B	208	LEU	N-CA-C	5.02	116.82	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	VAL	N-CA-C	5.02	116.50	108.87
1	A	416	THR	CB-CA-C	-5.01	102.44	109.96
1	D	130	SER	CA-C-N	-5.01	115.15	123.37
1	D	130	SER	C-N-CA	-5.01	115.15	123.37

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	167	0
1	B	4598	0	4490	202	0
1	C	4628	0	4517	159	0
1	D	4620	0	4506	156	0
1	E	4604	0	4484	148	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	802	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 18.

All (802) 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:N	1:E:525:PRO:CD	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:HD23	1:A:515:LEU:O	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:HD23	1:B:515:LEU:O	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:C:464:ASN:OD1	1:C:465:GLU:N	1.92	1.02
1:B:145:ILE:CD1	1:B:172:LEU:HD11	1.88	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:D:416:THR:HG22	1:D:417:PRO:HD2	1.05	1.02
1:B:416:THR:HG23	1:B:417:PRO:CD	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:56:PRO:O	1:D:57:ASP:OD1	1.91	0.89
1:B:518:TYR:O	1:B:522:ILE:HG13	1.73	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:D:573:LEU:HD13	1:D:578:ARG:HG3	1.56	0.85
1:B:416:THR:HG23	1:B:417:PRO:HD3	1.58	0.85
1:A:79:VAL:CG1	1:A:131:ALA:HB1	2.07	0.85
1:E:626:LEU:HD12	1:E:627:TYR:N	1.91	0.84
1:D:626:LEU:HD12	1:D:627:TYR:N	1.93	0.84
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:540:LYS:HZ2	1:B:610:ALA:HB1	1.45	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:45:ILE:HG13	1:B:75:LEU:HD11	1.62	0.81
1:B:330:VAL:O	1:B:463:PHE:HA	1.80	0.81
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:OD1	1:E:290:ASP:O	2.04	0.75
1:E:45:ILE:CG1	1:E:75:LEU:HD11	2.17	0.74
1:C:416:THR:HG23	1:C:417:PRO:HD2	1.47	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:HD12	1:C:573:LEU:O	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ARG:NH2	1:A:635:PHE:CZ	2.58	0.72
1:E:202:GLU:H	1:E:307:ASN:HD22	1.38	0.72
1:D:202:GLU:H	1:D:307:ASN:HD22	1.38	0.71
1:B:573:LEU:HD13	1:B:578:ARG:CG	2.19	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:HD12	1:A:573:LEU:O	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:E:633:LEU:HD12	1:E:634:ARG:N	2.06	0.70
1:C:443:PHE:CD1	1:C:515:LEU:HD21	2.26	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:C:597:GLN:NE2	1:C:613:ASP:OD1	2.25	0.69
1:B:234:ALA:HB3	1:B:271:LEU:HD12	1.74	0.69
1:D:522:ILE:HD12	1:D:563:ILE:CG2	2.22	0.69
1:B:597:GLN:NE2	1:B:613:ASP:OD1	2.25	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
1:A:374:THR:HG23	1:A:375:VAL:HG23	1.77	0.67
1:E:450:ILE:HB	1:E:507:THR:CG2	2.22	0.67
1:B:202:GLU:H	1:B:307:ASN:HD22	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:56:PRO:C	1:E:57:ASP:OD1	2.37	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:58:MET:HA	1:B:58:MET:HE2	1.77	0.65
1:D:355:LEU:HD23	1:D:397:PHE:CE2	2.31	0.65
1:B:567:LEU:HD13	1:B:570:LEU:HD12	1.76	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:E:58:MET:HA	1:E:58:MET:HE2	1.78	0.65
1:E:355:LEU:HD23	1:E:397:PHE:CE2	2.32	0.65
1:E:374:THR:HG23	1:E:375:VAL:HG23	1.77	0.65
1:D:524:VAL:HG23	1:D:525:PRO:HD3	1.78	0.65
1:C:567:LEU:HB2	1:C:570:LEU:HD11	1.79	0.65
1:B:568:PRO:HG2	1:B:570:LEU:CD2	2.25	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:58:MET:HE2	1:D:58:MET:HA	1.78	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:C:58:MET:HE2	1:C:58:MET:HA	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:513:ARG:O	1:E:515:LEU:CD1	2.48	0.61
1:C:496:PHE:CE2	1:B:424:PHE:CZ	2.88	0.61
1:A:489:GLN:CG	1:A:507:THR:HG23	2.31	0.61
1:A:58:MET:HE2	1:A:58:MET:HA	1.82	0.61
1:B:105:ASP:OD1	1:B:106:LEU:N	2.34	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:B:350:SER:HG	1:B:430:THR:HG22	1.62	0.60
1:C:416:THR:HG22	1:C:417:PRO:N	2.04	0.60
1:A:416:THR:CG2	1:A:418:ASP:HB2	2.31	0.60
1:C:364:LEU:HD12	1:C:364:LEU:O	2.02	0.60
1:B:364:LEU:O	1:B:364:LEU:HD12	2.01	0.60
1:B:515:LEU:HD23	1:B:519:ILE:HB	1.84	0.60
1:D:489:GLN:CG	1:D:507:THR:HG23	2.31	0.60
1:B:567:LEU:HB2	1:B:570:LEU:HD11	1.84	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:B:626:LEU:HD12	1:B:626:LEU:C	2.27	0.60
1:A:441:TYR:HB3	1:A:574:THR:OG1	2.02	0.60
1:E:45:ILE:CG1	1:E:75:LEU:CD1	2.79	0.59
1:D:355:LEU:CD2	1:D:397:PHE:HE2	2.15	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:E:570:LEU:HD22	1:E:572:TYR:CE1	2.38	0.59
1:B:53:TYR:HB2	1:B:145:ILE:CG1	2.32	0.59
1:E:355:LEU:CD2	1:E:397:PHE:HE2	2.15	0.59
1:B:522:ILE:HG22	1:B:563:ILE:CG2	2.30	0.59
1:A:570:LEU:HD22	1:A:572:TYR:CE1	2.37	0.58
1:A:574:THR:HG22	1:A:577:ASP:CG	2.28	0.58
1:E:513:ARG:O	1:E:515:LEU:HD12	2.02	0.58
1:A:626:LEU:HD12	1:A:626:LEU:C	2.27	0.58
1:E:574:THR:HG22	1:E:577:ASP:CG	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:THR:HG22	1:C:493:GLU:N	2.19	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
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: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: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:E:355:LEU:CD2	1:E:397:PHE:CE2	2.87	0.57
1:D:515:LEU:O	1:D:515:LEU:HG	2.03	0.57
1:B:77:PRO:O	1:B:124:ASP:N	2.38	0.57
1:D:574:THR:HG22	1:D:577:ASP:CG	2.29	0.57
1:E:623:VAL:HA	1:E:626:LEU:HD21	1.85	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: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:E:334:LEU:HD22	1:E:507:THR:HG21	1.86	0.57
1:C:574:THR:HG22	1:C:577:ASP:CG	2.29	0.57
1:B:208:LEU:HD23	1:B:209:GLU:O	2.05	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:A:391:ASN:HD21	1:E:376:LYS:HD2	1.70	0.56
1:E:277:GLN:HG3	1:E:278:ASP:H	1.71	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:D:124:ASP:HB3	1:D:150:THR:HG21	1.87	0.56
1:C:513:ARG:O	1:C:515:LEU:CD1	2.54	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:HD12	1:E:364:LEU:O	2.06	0.55
1:A:515:LEU:HD23	1:A:519:ILE:HB	1.87	0.55
1:C:315:GLY:O	1:C:321:SER:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:ASN:O	1:C:563:ILE:HG13	2.06	0.55
1:B:522:ILE:CD1	1:B:523:PHE:CD1	2.89	0.55
1:E:441:TYR:HB3	1:E:574:THR:OG1	2.07	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:D:441:TYR:HB3	1:D:574:THR:OG1	2.07	0.55
1:B:492:THR:HG22	1:B:493:GLU:N	2.21	0.55
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:E:48:GLY:HA2	1:E:149:SER:CB	2.37	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: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:E:626:LEU:HD12	1:E:626:LEU:C	2.31	0.54
1:D:623:VAL:HA	1:D:626:LEU:CG	2.37	0.54
1:D:626:LEU:HD12	1:D:626:LEU:C	2.31	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:E:454:LEU:HD21	1:E:463:PHE:CE1	2.43	0.54
1:B:371:CYS:O	1:B:373:CYS:N	2.39	0.54
1:D:315:GLY:O	1:D:321:SER:N	2.40	0.54
1:C:371:CYS:O	1:C:373:CYS:N	2.40	0.54
1:B:540:LYS:HZ3	1:B:610:ALA:HA	1.73	0.54
1:E:562:THR:O	1:E:563:ILE:C	2.50	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:B:562:THR:O	1:B:563:ILE:C	2.50	0.53
1:A:250:THR:HG21	1:A:285:HIS:NE2	2.24	0.53
1:E:371:CYS:O	1:E:373:CYS:N	2.40	0.53
1:C:518:TYR:HD1	1:C:522:ILE:HD12	1.72	0.53
1:B:334:LEU:HD22	1:B:507:THR:HG21	1.91	0.53
1:E:363:LYS:O	1:E:364:LEU:HG	2.08	0.53
1:B:75:LEU:HD23	1:B:77:PRO:CD	2.39	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:D:48:GLY:HA2	1:D:149:SER:HB3	1.90	0.53
1:B:454:LEU:HD21	1:B:463:PHE:CE1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:562:THR:O	1:A:563:ILE:C	2.51	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:E:464:ASN:OD1	1:E:464:ASN:C	2.53	0.52
1:D:524:VAL:CG2	1:D:525:PRO:CD	2.87	0.52
1:D:363:LYS:O	1:D:364:LEU:HG	2.10	0.52
1:C:48:GLY:HA2	1:C:149:SER:CB	2.39	0.52
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:B:48:GLY:HA2	1:B:149:SER:CB	2.39	0.52
1:D:334:LEU:HD22	1:D:507:THR:HG21	1.91	0.52
1:C:454:LEU:HD21	1:C:463:PHE:CE1	2.45	0.52
1:C:562:THR:O	1:C:563:ILE:C	2.51	0.52
1:B:250:THR:HG21	1:B:285:HIS:NE2	2.25	0.52
1:D:454:LEU:HD21	1:D:463:PHE:CE1	2.44	0.52
1:C:123:ASP:OD1	1:C:124:ASP:OD1	2.27	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: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:B:626:LEU:HD12	1:B: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:D:202:GLU:H	1:D:307:ASN:ND2	2.09	0.50
1:D:562:THR:O	1:D:563:ILE:C	2.51	0.50
1:C:383:ILE:HD12	1:C:387:ALA:HB2	1.91	0.50
1:A:429:VAL:CG1	1:A:431:LEU:HG	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:458:THR:OG1	1:D:501:THR:HG23	2.11	0.50
1:C:513:ARG:O	1:C:515:LEU:HD12	2.11	0.50
1:B:133:LEU:HD23	1:B:133:LEU:C	2.37	0.50
1:B:343:ASP:OD1	1:B:346:SER:N	2.45	0.50
1:A:536:ILE:CG2	1:A:545:GLN:HG2	2.40	0.50
1:E:81:ILE:HG21	1:E:135:PHE:CD2	2.47	0.50
1:E:623:VAL:HA	1:E:626:LEU:HG	1.93	0.50
1:D:77:PRO:O	1:D:124:ASP:HA	2.11	0.50
1:D:133:LEU:C	1:D:133:LEU:HD23	2.37	0.50
1:D:431:LEU:HD11	1:D:450:ILE:HG23	1.94	0.50
1:E:133:LEU:C	1:E:133:LEU:HD23	2.37	0.50
1:D:626:LEU:HD12	1:D:627:TYR:CA	2.41	0.50
1:C:244:LEU:HD22	1:C:262:ILE:HD11	1.92	0.50
1:B:429:VAL:CG1	1:B:431:LEU:HG	2.42	0.50
1:A:343:ASP:OD1	1:A:346:SER:N	2.45	0.50
1:E:396:SER:HB2	1:E:455:ALA:HB3	1.94	0.50
1:C:431:LEU:HD11	1:C:450:ILE:HG23	1.93	0.50
1:B:45:ILE:HB	1:B:75:LEU:HD12	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:B:540:LYS:HZ2	1:B:610:ALA:CB	2.19	0.50
1:E:79:VAL:HG12	1:E:131:ALA:CB	2.32	0.49
1:D:429:VAL:CG1	1:D:431:LEU:HG	2.42	0.49
1:B:100:LEU:HB3	1:B:105:ASP:OD2	2.12	0.49
1:A:489:GLN:HG3	1:A:507:THR:HG23	1.93	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:C:343:ASP:OD1	1:C:346:SER:N	2.44	0.49
1:B:75:LEU:CD2	1:B:77:PRO:HG3	2.42	0.49
1:A:133:LEU:C	1:A:133:LEU:HD23	2.37	0.49
1:E:45:ILE:HB	1:E:75:LEU:HD12	1.93	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:C:81:ILE:HG21	1:C:135:PHE:CD2	2.47	0.49
1:C:133:LEU:C	1:C:133:LEU:HD23	2.37	0.49
1:B:257:LEU:HD13	1:B:273:TYR:CZ	2.47	0.49
1:D:257:LEU:HD13	1:D:273:TYR:CZ	2.48	0.49
1:B:98:LYS:HB3	1:B:100:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLN:HG2	1:A:507:THR:HG23	1.95	0.49
1:E:431:LEU:HD11	1:E:450:ILE:HG23	1.94	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:B:81:ILE:HG21	1:B:135:PHE:CD2	2.47	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:E:123:ASP:OD1	1:E:124:ASP:OD1	2.31	0.49
1:C:47:ASP:OD1	1:C:47:ASP:O	2.31	0.49
1:B:604:GLY:HA2	1:B:606:GLN:HE21	1.78	0.49
1:C:250:THR:HA	1:C:256:PRO:HA	1.95	0.49
1:B:250:THR:HA	1:B:256:PRO:HA	1.95	0.49
1:A:81:ILE:HG21	1:A:135:PHE:CD2	2.48	0.48
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: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:E:250:THR:HA	1:E:256:PRO:HA	1.95	0.48
1:B:208:LEU:HD23	1:B:209:GLU:C	2.39	0.48
1:B:363:LYS:O	1:B:364:LEU:HG	2.13	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:210:ILE:HD13	1:B:286:VAL:HG21	1.95	0.48
1:D:218:TYR:CE1	1:C:158:LYS:HA	2.49	0.48
1:B:105:ASP:O	1:B:109:GLU:HG2	2.13	0.48
1:A:202:GLU:H	1:A:307:ASN:ND2	2.08	0.48
1:E:366:PHE:CZ	1:E:371:CYS:HB3	2.49	0.48
1:B:332:VAL:HG13	1:B:463:PHE:CD1	2.49	0.48
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:C:604:GLY:HA2	1:C:606:GLN:HE21	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:E:522:ILE:HG12	1:E:563:ILE:HG22	1.95	0.47
1:C:98:LYS:HB3	1:C:100:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:LEU:HD21	1:C:624:TYR:HE1	1.79	0.47
1:A:98:LYS:HB3	1:A:100:LEU:HG	1.96	0.47
1:E:405:ASN:HB2	1:D:407:TRP:CE3	2.49	0.47
1:E:633:LEU:HD12	1:E:633:LEU:C	2.39	0.47
1:C:366:PHE:CZ	1:C:371:CYS:HB3	2.49	0.47
1:E:271:LEU:C	1:E:271:LEU:HD13	2.40	0.47
1:D:98:LYS:HB3	1:D:100:LEU:HG	1.95	0.47
1:D:271:LEU:C	1:D:271:LEU:HD13	2.40	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:B:45:ILE:HG12	1:B:75:LEU:CD1	2.45	0.47
1:A:271:LEU:HD13	1:A:271:LEU:C	2.40	0.47
1:A:623:VAL:HA	1:A:626:LEU:CD2	2.44	0.47
1:C:257:LEU:HD13	1:C:273:TYR:CZ	2.49	0.47
1:B:235:LEU:HB3	1:B:303:LEU:HB2	1.97	0.47
1:B:277:GLN:HG3	1:B:278:ASP:H	1.80	0.47
1:B:436:PHE:CD2	1:B:438:PHE:CE2	3.02	0.47
1:E:235:LEU:HB3	1:E:303:LEU:HB2	1.97	0.47
1:D:74:ASN:HD22	1:D:154:GLN:HE21	1.63	0.47
1:C:74:ASN:HD22	1:C:154:GLN:HE21	1.63	0.47
1:C:271:LEU:HD13	1:C:271:LEU:C	2.40	0.47
1:B:74:ASN:HD22	1:B:154:GLN:HE21	1.63	0.47
1:B:271:LEU:C	1:B:271:LEU:HD13	2.40	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:C:235:LEU:HB3	1:C:303:LEU:HB2	1.97	0.47
1:C:496:PHE:HE2	1:B:424:PHE:CZ	2.31	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:E:98:LYS:HB3	1:E:100:LEU:HG	1.96	0.46
1:B:537:PHE:CE2	1:B:616:VAL:HG11	2.49	0.46
1:B:540:LYS:NZ	1:B:610:ALA:CB	2.77	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:E:314:SER:O	1:E:315:GLY:C	2.58	0.46
1:B:277:GLN:HG3	1:B:278:ASP:N	2.30	0.46
1:E:586:LEU:HD21	1:E:624:TYR:HE1	1.80	0.46
1:D:343:ASP:OD1	1:D:346:SER:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:MET:HB3	1:C:131:ALA:HB3	1.97	0.46
1:C:518:TYR:CD1	1:C:522:ILE:HD12	2.49	0.46
1:B:574:THR:HG23	1:B:577:ASP:OD2	2.16	0.46
1:A:366:PHE:CZ	1:A:371:CYS:HB3	2.51	0.46
1:E:75:LEU:HD23	1:E:77:PRO:CD	2.45	0.46
1:D:464:ASN:OD1	1:D:464:ASN:C	2.58	0.46
1:D:600:LEU:O	1:D:604:GLY:O	2.33	0.46
1:C:489:GLN:HG2	1:C:507:THR:HG23	1.97	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:D:573:LEU:HD12	1:D:573:LEU:C	2.41	0.46
1:A:414:PHE:HB2	1:A:422:SER:HB2	1.98	0.46
1:D:537:PHE:CE2	1:D:616:VAL:HG11	2.51	0.46
1:C:391:ASN:HD21	1:B:376:LYS:HD2	1.81	0.46
1:C:600:LEU:O	1:C:604:GLY:O	2.33	0.46
1:B:53:TYR:HB2	1:B:145:ILE:HG13	1.98	0.46
1:B:600:LEU:O	1:B:604:GLY:O	2.33	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:C:537:PHE:CE2	1:C:616:VAL:HG11	2.51	0.46
1:E:74:ASN:HD22	1:E:154:GLN:HE21	1.64	0.46
1:B:586:LEU:HD21	1:B:624:TYR:HE1	1.79	0.46
1:E:332:VAL:HG13	1:E:463:PHE:CD1	2.50	0.45
1:B:540:LYS:HZ3	1:B:610:ALA:CA	2.28	0.45
1:D:441:TYR:HD2	1:D:574:THR:HG21	1.81	0.45
1:D:489:GLN:HG2	1:D:507:THR:HG23	1.96	0.45
1:E:600:LEU:O	1:E:604:GLY:O	2.33	0.45
1:D:235:LEU:HB3	1:D:303:LEU:HB2	1.97	0.45
1:D:259:PHE:HB2	1:C:104:ASN:H	1.81	0.45
1:E:68:MET:HB3	1:E:131:ALA:HB3	1.97	0.45
1:D:75:LEU:O	1:D:77:PRO:HD3	2.17	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:C:464:ASN:OD1	1:C:464:ASN:C	2.58	0.45
1:E:45:ILE:HG12	1:E:75:LEU:CD1	2.46	0.45
1:D:68:MET:HB3	1:D:131:ALA:HB3	1.98	0.45
1:C:162:THR:HG22	1:C:163:TYR:N	2.31	0.45
1:E:162:THR:HG22	1:E:163:TYR:N	2.31	0.45
1:D:210:ILE:HD13	1:D:286:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:464:ASN:OD1	1:D:465:GLU:HG2	2.16	0.45
1:C:355:LEU:O	1:C:424:PHE:HA	2.17	0.45
1:A:102:SER:CB	1:B:259:PHE:CD1	3.00	0.45
1:D:259:PHE:CD1	1:C:102:SER:CB	3.00	0.45
1:C:555:VAL:O	1:C:556:PHE:C	2.60	0.45
1:B:582:VAL:HG21	1:B:627:TYR:CZ	2.52	0.45
1:A:75:LEU:HD23	1:A:77:PRO:CD	2.47	0.45
1:A:623:VAL:HA	1:A:626:LEU:HD21	1.98	0.45
1:A:518:TYR:OH	1:B:569:ARG:NH1	2.50	0.44
1:D:555:VAL:O	1:D:556:PHE:C	2.60	0.44
1:C:396:SER:HB2	1:C:455:ALA:HB3	1.99	0.44
1:B:287:ASP:OD1	1:B:289:THR:HG22	2.17	0.44
1:D:173:GLY:HA3	1:D:179:VAL:HG21	2.00	0.44
1:C:210:ILE:HD13	1:C:286:VAL:HG21	1.98	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: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:E:210:ILE:HD13	1:E:286:VAL:HG21	1.97	0.44
1:B:47:ASP:OD1	1:B:47:ASP:O	2.34	0.44
1:B:586:LEU:C	1:B:586:LEU:HD12	2.43	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:E:537:PHE:CE2	1:E:616:VAL:HG11	2.51	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: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: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:E:355:LEU:O	1:E:424:PHE:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:555:VAL:O	1:E:556:PHE:C	2.60	0.44
1:E:582:VAL:HG21	1:E:627:TYR:CZ	2.53	0.44
1:C:251:ASP:OD1	1:C:253:GLY:C	2.61	0.44
1:B:515:LEU:HD21	1:B:519:ILE:CD1	2.48	0.44
1:A:582:VAL:HG21	1:A:627:TYR:CZ	2.52	0.43
1:A:586:LEU:HD12	1:A:586:LEU:C	2.43	0.43
1:D:251:ASP:OD1	1:D:253:GLY:C	2.61	0.43
1:D:582:VAL:HG21	1:D:627:TYR:CZ	2.53	0.43
1:C:569:ARG:HD3	1:B:517:TYR:CE2	2.53	0.43
1:B:105:ASP:OD1	1:B:105:ASP:C	2.61	0.43
1:B:573:LEU:HD12	1:B:573:LEU:C	2.43	0.43
1:A:439:LEU:HD12	1:A:574:THR:HA	1.99	0.43
1:A:464:ASN:OD1	1:A:464:ASN:C	2.61	0.43
1:A:536:ILE:HG22	1:A:545:GLN:CG	2.47	0.43
1:C:586:LEU:HD12	1:C:586:LEU:C	2.43	0.43
1:A:555:VAL:O	1:A:556:PHE:C	2.60	0.43
1:B:75:LEU:HD23	1:B:77:PRO:HD3	2.00	0.43
1:B:145:ILE:HD13	1:B:172:LEU:CD2	2.48	0.43
1:B:555:VAL:O	1:B:556:PHE:C	2.60	0.43
1:A:251:ASP:OD1	1:A:253:GLY:C	2.61	0.43
1:C:383:ILE:HD12	1:C:387:ALA:CB	2.48	0.43
1:C:496:PHE:CZ	1:B:424:PHE:CE1	3.07	0.43
1:E:221:GLN:HB3	1:E:325:LEU:HD22	1.99	0.43
1:E:466:ILE:CD1	1:E:491:ILE:HD11	2.49	0.43
1:E:573:LEU:HD12	1:E:573:LEU:C	2.41	0.43
1:C:173:GLY:HA3	1:C:179:VAL:HG21	2.00	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:D:586:LEU:C	1:D:586:LEU:HD12	2.43	0.43
1:C:210:ILE:HD12	1:C:302:LEU:HB2	2.01	0.43
1:C:439:LEU:HD12	1:C:574:THR:HA	2.01	0.43
1:C:496:PHE:CE2	1:B:424:PHE:CE1	3.07	0.43
1:E:77:PRO:O	1:E:124:ASP:HA	2.18	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:B:79:VAL:HG11	1:B:131:ALA:HB1	1.96	0.43
1:B:251:ASP:OD1	1:B:253:GLY:C	2.61	0.43
1:B:436:PHE:CD2	1:B:438:PHE:HE2	2.36	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:C:73:GLY:HA2	1:C:365:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:VAL:HG21	1:C:627:TYR:CZ	2.54	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: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:E:586:LEU:C	1:E:586:LEU:HD12	2.43	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:C:38:VAL:HB	1:C:185:GLU:O	2.19	0.43
1:C:68:MET:O	1:C:130:SER:HB3	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:A:68:MET:O	1:A:130:SER:HB3	2.19	0.42
1:A:171:ILE:HG21	1:A:184:GLY:HA3	2.01	0.42
1:E:68:MET:O	1:E:130:SER:HB3	2.19	0.42
1:E:219:LEU:HG	1:E:220:THR:N	2.34	0.42
1:E:251:ASP:OD1	1:E:253:GLY:C	2.61	0.42
1:D:73:GLY:HA2	1:D:365:GLY:HA3	2.01	0.42
1:D:171:ILE:HG21	1:D:184:GLY:HA3	2.01	0.42
1:C:349:PHE:CZ	1:C:448:PHE:HB3	2.54	0.42
1:A:349:PHE:CZ	1:A:448:PHE:HB3	2.55	0.42
1:E:383:ILE:HD12	1:E:387:ALA:CB	2.49	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:C:223:THR:HG22	1:C:224:ARG:N	2.34	0.42
1:B:38:VAL:O	1:B:186:PRO:HA	2.19	0.42
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:A:610:ALA:O	1:A:613:ASP:HB2	2.19	0.42
1:E:439:LEU:HD12	1:E:574:THR:HA	2.00	0.42
1:D:222:HIS:HA	1:D:283:VAL:HG22	2.01	0.42
1:C:38:VAL:O	1:C:186:PRO:HA	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: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:D:38:VAL:O	1:D:186:PRO:HA	2.19	0.42
1:D:586:LEU:HD12	1:D:587:THR:N	2.35	0.42
1:D:586:LEU:HA	1:D:589:ILE:HB	2.02	0.42
1:B:145:ILE:HD13	1:B:145:ILE:HG21	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:586:LEU:HD12	1:A:587:THR:N	2.35	0.42
1:E:462:ILE:HG22	1:E:463:PHE:O	2.19	0.42
1:D:429:VAL:CG1	1:D:430:THR:N	2.83	0.42
1:C:125:GLY:N	1:C:130:SER:OG	2.50	0.42
1:C:546:LEU:C	1:C:546:LEU:HD23	2.44	0.42
1:A:405:ASN:HB2	1:E:407:TRP:CE3	2.55	0.42
1:E:349:PHE:CZ	1:E:448:PHE:HB3	2.55	0.42
1:E:626:LEU:CD1	1:E:627:TYR:N	2.74	0.42
1:B:171:ILE:HG21	1:B:184:GLY:HA3	2.02	0.42
1:B:492:THR:HG22	1:B:493:GLU:H	1.84	0.42
1:B:546:LEU:C	1:B:546:LEU:HD23	2.45	0.42
1:B:586:LEU:HA	1:B:589:ILE:HB	2.02	0.42
1:A:250:THR:HG22	1:A:283:VAL:O	2.20	0.42
1:A:379:GLU:HA	1:A:411:GLN:O	2.20	0.42
1:A:383:ILE:HD12	1:A:387:ALA:CB	2.49	0.42
1:E:50:GLY:HA3	1:E:146:PHE:CE1	2.55	0.42
1:D:45:ILE:HG23	1:D:49:ARG:O	2.19	0.42
1:D:314:SER:O	1:D:315:GLY:C	2.63	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: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:E:222:HIS:HA	1:E:283:VAL:HG22	2.02	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: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:B:38:VAL:HB	1:B:185:GLU:O	2.19	0.42
1:B:123:ASP:O	1:B:130:SER:O	2.38	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:E:38:VAL:HB	1:E:185:GLU:O	2.19	0.42
1:D:515:LEU:HD12	1:D:518:TYR:CB	2.43	0.42
1:B:56:PRO:C	1:B:57:ASP:OD1	2.63	0.42
1:B:222:HIS:HA	1:B:283:VAL:HG22	2.02	0.42
1:B:443:PHE:CD2	1:B:443:PHE:N	2.87	0.42
1:B:464:ASN:OD1	1:B:464:ASN:C	2.58	0.42
1:A:73:GLY:HA2	1:A:365:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:SER:HB2	1:E:410:ASN:ND2	2.35	0.41
1:A:546:LEU:C	1:A:546:LEU:HD23	2.44	0.41
1:A:586:LEU:HA	1:A:589:ILE:CG1	2.50	0.41
1:E:586:LEU:HA	1:E:589:ILE:HB	2.02	0.41
1:D:38:VAL:HB	1:D:185:GLU:O	2.19	0.41
1:D:546:LEU:HD23	1:D:546:LEU:C	2.45	0.41
1:D:586:LEU:HA	1:D:589:ILE:CG1	2.50	0.41
1:C:57:ASP:OD1	1:C:57:ASP:O	2.38	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:B:57:ASP:OD1	1:B:57:ASP:O	2.38	0.41
1:B:223:THR:HG22	1:B:224:ARG:N	2.35	0.41
1:B:586:LEU:HD12	1:B:587:THR:N	2.35	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:E:546:LEU:C	1:E:546:LEU:HD23	2.45	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:A:573:LEU:HD12	1:A:573:LEU:C	2.44	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
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:B:73:GLY:HA2	1:B:365:GLY:HA3	2.03	0.41
1:A:125:GLY:N	1:A:130:SER:OG	2.50	0.41
1:E:38:VAL:O	1:E:186:PRO:HA	2.19	0.41
1:C:441:TYR:HD2	1:C:574:THR:HG21	1.86	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:E:45:ILE:HG23	1:E:49:ARG:O	2.20	0.41
1:D:250:THR:HG22	1:D:283:VAL:O	2.21	0.41
1:C:45:ILE:HG23	1:C:49:ARG:O	2.20	0.41
1:C:573:LEU:HD12	1:C:573:LEU:C	2.42	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: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:A:50:GLY:HA3	1:A:146:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:LEU:CD2	1:E:77:PRO:HG3	2.51	0.41
1:E:250:THR:HG22	1:E:283:VAL:O	2.20	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:C:222:HIS:HA	1:C:283:VAL:HG22	2.02	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:A:626:LEU:C	1:A:626:LEU:CD1	2.93	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:C:145:ILE:CD1	1:C:172:LEU:HD21	2.49	0.41
1:B:45:ILE:HG23	1:B:49:ARG:O	2.20	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:409:GLN:CD	1:B:402:GLN:OE1	2.63	0.41
1:A:586:LEU:HA	1:A:589:ILE:HB	2.02	0.41
1:D:349:PHE:CZ	1:D:448:PHE:HB3	2.55	0.41
1:C:530:ILE:HG12	1:C:624:TYR:CZ	2.56	0.41
1:B:70:ASN:ND2	1:B:75:LEU:O	2.51	0.41
1:A:123:ASP:CG	1:A:124:ASP:OD1	2.63	0.41
1:A:145:ILE:CD1	1:A:172:LEU:HD21	2.50	0.41
1:A:150:THR:CG2	1:A:152:THR:HG23	2.51	0.41
1:A:357:LEU:N	1:A:423:TYR:O	2.37	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:626:LEU:CD1	1:A:627:TYR:N	2.73	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:E:586:LEU:HA	1:E:589:ILE:CG1	2.50	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:C:79:VAL:HG11	1:C:131:ALA:HB1	1.96	0.41
1:C:127:LYS:C	1:C:129:TYR:N	2.79	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:B:123:ASP:CG	1:B:124:ASP:OD1	2.64	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:E:431:LEU:HD13	1:E:450:ILE:HG12	2.03	0.41
1:B:68:MET:SD	1:B:77:PRO:HB3	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ILE:HG12	1:A:624:TYR:CZ	2.56	0.40
1:E:277:GLN:CG	1:E:278:ASP:H	2.33	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:C:361:ASP:C	1:C:363:LYS:N	2.79	0.40
1:B:150:THR:CG2	1:B:152:THR:HG23	2.51	0.40
1:A:68:MET:SD	1:A:77:PRO:HB3	2.62	0.40
1:A:219:LEU:HG	1:A:220:THR:N	2.36	0.40
1:E:171:ILE:HG21	1:E:184:GLY:HA3	2.02	0.40
1:D:57:ASP:OD1	1:D:57:ASP:O	2.38	0.40
1:D:496:PHE:CZ	1:C:424:PHE:CE1	3.09	0.40
1:C:123:ASP:CG	1:C:124:ASP:OD1	2.64	0.40
1:E:393:PRO:O	1:E:394:LEU:HD12	2.21	0.40
1:D:492:THR:HG22	1:D:493:GLU:H	1.85	0.40
1:C:68:MET:SD	1:C:77:PRO:HB3	2.61	0.40
1:C:431:LEU:HD13	1:C:450:ILE:HG12	2.04	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:A:526:LEU:CD2	1:A:579:PHE:CE2	3.04	0.40
1:D:524:VAL:HG23	1:D:525:PRO:N	2.35	0.40
1:A:45:ILE:HG23	1:A:49:ARG:O	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
1:D:393:PRO:O	1:D:394:LEU:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	583/642 (91%)	547 (94%)	34 (6%)	2 (0%)	36 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	583/642 (91%)	545 (94%)	36 (6%)	2 (0%)	36	69
1	C	587/642 (91%)	550 (94%)	35 (6%)	2 (0%)	36	69
1	D	586/642 (91%)	548 (94%)	37 (6%)	1 (0%)	43	74
1	E	586/642 (91%)	540 (92%)	45 (8%)	1 (0%)	43	74
All	All	2925/3210 (91%)	2730 (93%)	187 (6%)	8 (0%)	36	69

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%)	483 (97%)	13 (3%)	40	61
1	B	496/557 (89%)	484 (98%)	12 (2%)	43	63
1	C	499/557 (90%)	487 (98%)	12 (2%)	43	63
1	D	498/557 (89%)	483 (97%)	15 (3%)	36	57
1	E	495/557 (89%)	482 (97%)	13 (3%)	40	61
All	All	2484/2785 (89%)	2419 (97%)	65 (3%)	40	61

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	LEU
1	A	271	LEU
1	A	286	VAL
1	A	302	LEU
1	A	304	VAL
1	A	329	LEU
1	A	331	THR
1	A	352	VAL
1	A	356	LYS
1	A	379	GLU
1	A	436	PHE
1	A	570	LEU
1	A	624	TYR
1	E	133	LEU
1	E	271	LEU
1	E	286	VAL
1	E	302	LEU
1	E	304	VAL
1	E	329	LEU
1	E	331	THR
1	E	352	VAL
1	E	356	LYS
1	E	379	GLU
1	E	436	PHE
1	E	483	VAL
1	E	624	TYR
1	D	133	LEU
1	D	158	LYS
1	D	271	LEU
1	D	286	VAL
1	D	302	LEU
1	D	304	VAL
1	D	329	LEU
1	D	331	THR
1	D	352	VAL
1	D	356	LYS
1	D	379	GLU
1	D	436	PHE
1	D	483	VAL
1	D	570	LEU
1	D	624	TYR
1	C	133	LEU
1	C	271	LEU

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Mol	Chain	Res	Type
1	C	277	GLN
1	C	286	VAL
1	C	302	LEU
1	C	304	VAL
1	C	329	LEU
1	C	352	VAL
1	C	379	GLU
1	C	436	PHE
1	C	483	VAL
1	C	624	TYR
1	B	133	LEU
1	B	199	ILE
1	B	271	LEU
1	B	286	VAL
1	B	302	LEU
1	B	304	VAL
1	B	329	LEU
1	B	331	THR
1	B	352	VAL
1	B	379	GLU
1	B	436	PHE
1	B	624	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	154	GLN
1	A	160	GLN
1	A	206	GLN
1	A	277	GLN
1	A	307	ASN
1	A	391	ASN
1	A	432	GLN
1	A	470	GLN
1	A	489	GLN
1	A	545	GLN
1	E	69	GLN
1	E	154	GLN
1	E	206	GLN
1	E	307	ASN
1	E	410	ASN

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Mol	Chain	Res	Type
1	E	432	GLN
1	E	470	GLN
1	E	545	GLN
1	E	560	ASN
1	D	69	GLN
1	D	154	GLN
1	D	206	GLN
1	D	307	ASN
1	D	391	ASN
1	D	432	GLN
1	D	470	GLN
1	D	545	GLN
1	D	606	GLN
1	C	69	GLN
1	C	154	GLN
1	C	307	ASN
1	C	391	ASN
1	C	432	GLN
1	C	459	ASN
1	C	470	GLN
1	C	545	GLN
1	C	606	GLN
1	B	69	GLN
1	B	154	GLN
1	B	307	ASN
1	B	405	ASN
1	B	432	GLN
1	B	545	GLN
1	B	597	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.61	0	22,27,67	0.55	0
3	P3A	C	702	-	19,19,57	0.62	0	21,26,67	0.54	0
3	P3A	B	702	-	20,20,57	0.59	0	22,27,67	0.53	0
2	TRS	D	701	-	7,7,7	0.35	0	9,9,9	0.28	0
2	TRS	A	701	-	7,7,7	0.33	0	9,9,9	0.20	0
2	TRS	E	701	-	7,7,7	0.41	0	9,9,9	0.49	0
3	P3A	A	702	-	18,18,57	1.03	1 (5%)	20,25,67	0.91	1 (5%)
2	TRS	C	701	-	7,7,7	0.36	0	9,9,9	0.39	0
2	TRS	B	701	-	7,7,7	0.33	0	9,9,9	0.53	0
3	P3A	E	702	-	19,19,57	0.62	0	21,26,67	0.57	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	-
3	P3A	C	702	-	-	10/23/23/65	-
3	P3A	B	702	-	-	14/24/24/65	-
2	TRS	D	701	-	-	2/9/9/9	-
2	TRS	A	701	-	-	1/9/9/9	-
2	TRS	E	701	-	-	4/9/9/9	-
3	P3A	A	702	-	-	8/20/20/65	-
2	TRS	C	701	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	B	701	-	-	3/9/9/9	-
3	P3A	E	702	-	-	8/23/23/65	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	P3A	P16-O17	3.69	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	2.99	119.02	107.80

There are no chirality outliers.

All (58) torsion outliers are listed below:

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

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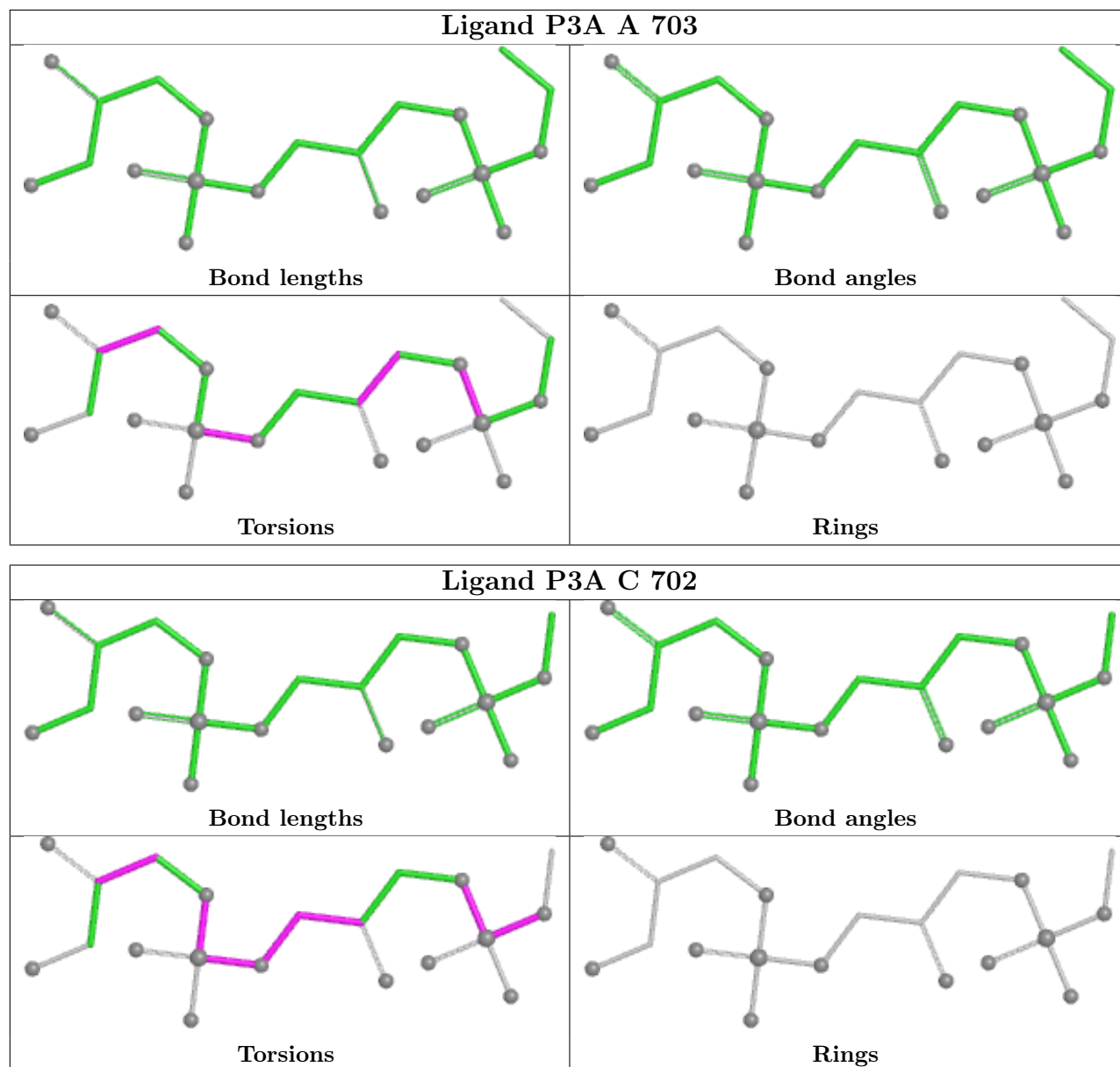
Mol	Chain	Res	Type	Atoms
3	B	702	P3A	C8-O9-P10-O11
3	B	702	P3A	C1-O11-P10-O9
3	B	702	P3A	C1-O11-P10-O12
3	B	702	P3A	C1-O11-P10-O13
3	A	703	P3A	O15-C14-C6-O7
3	E	702	P3A	O11-C1-C2-C4
3	C	702	P3A	O11-C1-C2-C4
3	E	702	P3A	O11-C1-C2-O3
3	A	702	P3A	O15-C14-C6-O7
3	C	702	P3A	O7-C6-C8-O9
3	A	702	P3A	O15-C14-C6-C8
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
2	E	701	TRS	N-C-C3-O3
3	A	703	P3A	O11-C1-C2-C4
3	B	702	P3A	O11-C1-C2-C4
2	E	701	TRS	C2-C-C3-O3
3	A	702	P3A	C8-O9-P10-O11
3	A	703	P3A	C14-O15-P16-O17
3	A	703	P3A	C8-O9-P10-O12
3	C	702	P3A	C14-O15-P16-O17
3	C	702	P3A	C8-O9-P10-O12
3	B	702	P3A	C14-O15-P16-O17
3	E	702	P3A	O7-C6-C8-O9
3	B	702	P3A	O11-C1-C2-O3
3	E	702	P3A	C14-C6-C8-O9
2	A	701	TRS	C3-C-C1-O1
2	E	701	TRS	C3-C-C1-O1
2	D	701	TRS	C2-C-C3-O3
3	A	702	P3A	C6-C8-O9-P10
3	C	702	P3A	C6-C8-O9-P10
3	A	703	P3A	O11-C1-C2-O3

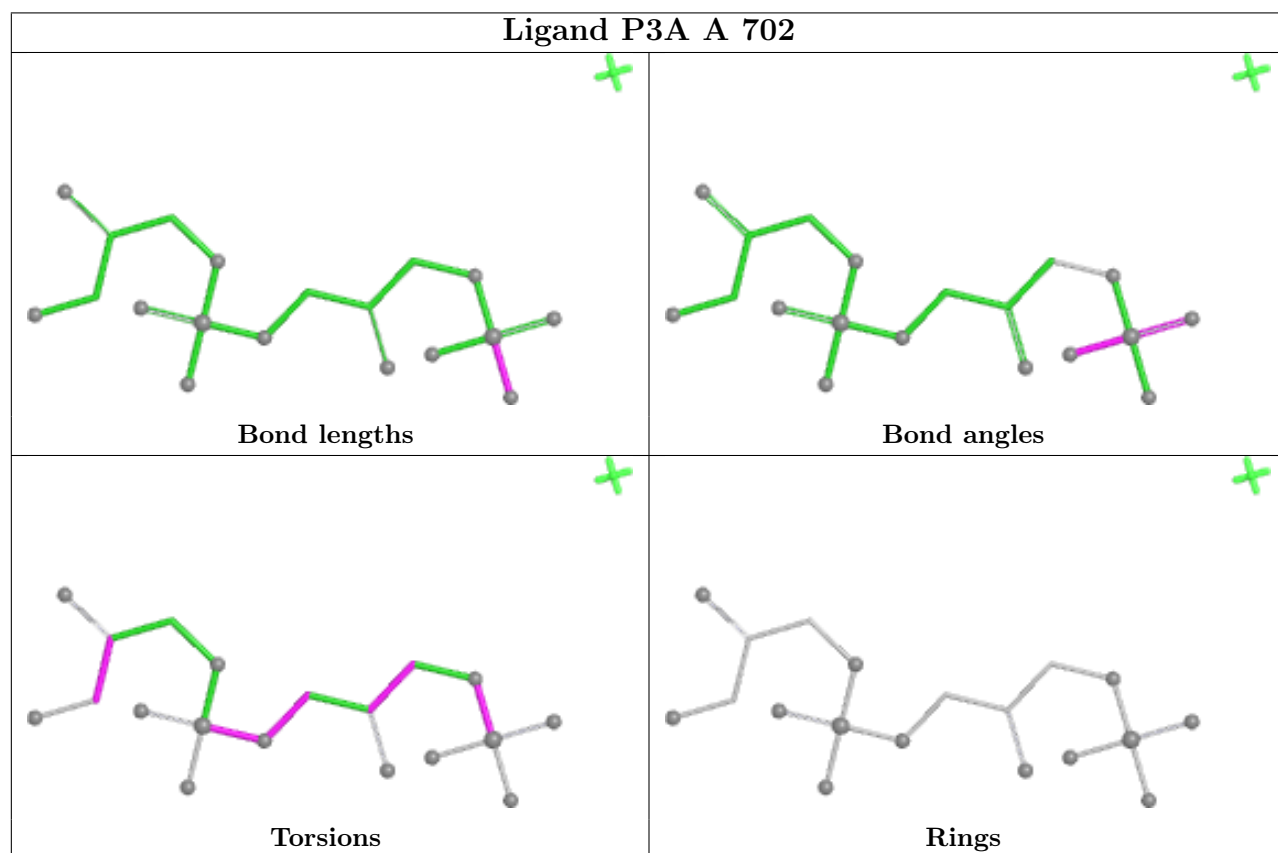
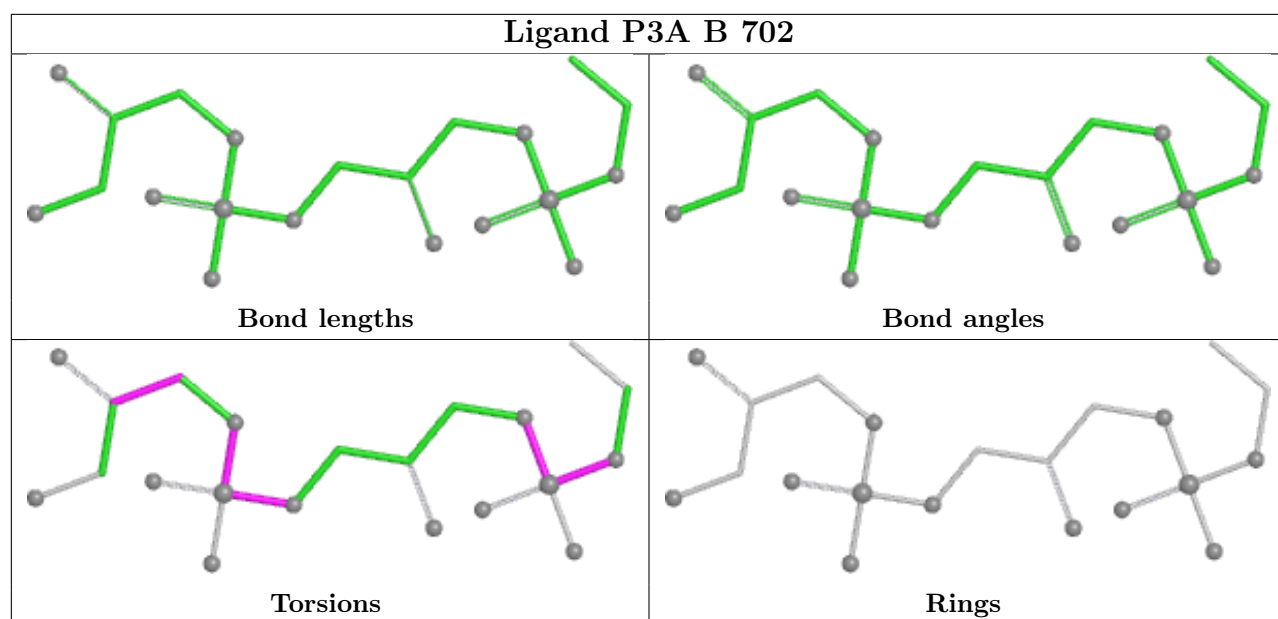
There are no ring outliers.

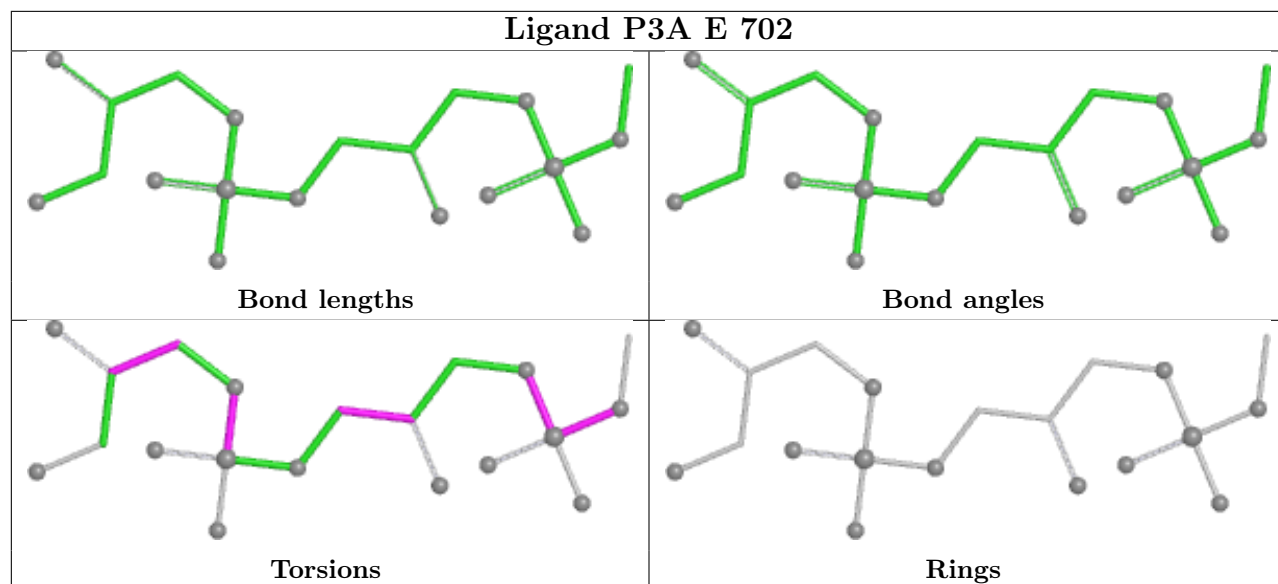
No monomer is involved in short contacts.

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.







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%)	0.21	16 (2%)	56 38	53, 143, 265, 338	0
1	B	589/642 (91%)	0.26	23 (3%)	43 31	50, 149, 274, 340	0
1	C	593/642 (92%)	0.21	18 (3%)	52 36	42, 136, 250, 312	0
1	D	592/642 (92%)	0.24	22 (3%)	45 32	56, 144, 248, 291	0
1	E	592/642 (92%)	0.13	15 (2%)	58 40	54, 143, 255, 294	0
All	All	2955/3210 (92%)	0.21	94 (3%)	50 35	42, 144, 257, 340	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	76	ASP	5.9
1	D	288	GLY	4.4
1	D	384	ARG	4.4
1	B	76	ASP	4.3
1	D	76	ASP	3.9
1	B	53	TYR	3.7
1	D	147	ALA	3.6
1	B	384	ARG	3.4
1	C	66	ALA	3.4
1	E	61	GLY	3.4
1	E	572	TYR	3.4
1	E	62	ASP	3.3
1	A	607	ALA	3.2
1	C	459	ASN	3.2
1	B	101	ALA	3.2
1	B	103	GLU	3.2
1	A	515	LEU	3.2
1	E	103	GLU	3.2
1	A	445	ARG	3.1
1	C	560	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	189	GLU	3.1
1	C	294	ASP	3.1
1	A	76	ASP	3.0
1	B	44	TYR	2.9
1	D	607	ALA	2.9
1	C	103	GLU	2.9
1	D	123	ASP	2.9
1	E	76	ASP	2.8
1	A	103	GLU	2.8
1	D	86	ILE	2.8
1	B	583	SER	2.8
1	B	359	TRP	2.8
1	D	124	ASP	2.7
1	C	559	PHE	2.7
1	C	456	VAL	2.7
1	A	606	GLN	2.7
1	B	438	PHE	2.7
1	A	321	SER	2.6
1	D	168	PHE	2.6
1	D	270	GLU	2.6
1	D	294	ASP	2.5
1	C	127	LYS	2.5
1	A	456	VAL	2.5
1	E	68	MET	2.5
1	E	151	ILE	2.5
1	C	96	LEU	2.5
1	D	58	MET	2.5
1	E	147	ALA	2.5
1	A	96	LEU	2.5
1	D	233	HIS	2.4
1	E	311	LEU	2.4
1	D	57	ASP	2.4
1	D	96	LEU	2.4
1	C	380	ASP	2.4
1	B	165	THR	2.4
1	E	92	LEU	2.4
1	C	92	LEU	2.4
1	A	311	LEU	2.3
1	D	321	SER	2.3
1	E	456	VAL	2.3
1	E	635	PHE	2.3
1	A	61	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	151	ILE	2.3
1	C	321	SER	2.3
1	C	384	ARG	2.3
1	D	272	ASN	2.2
1	A	59	LYS	2.2
1	A	618	VAL	2.2
1	B	244	LEU	2.2
1	B	45	ILE	2.2
1	D	297	GLU	2.2
1	D	101	ALA	2.2
1	D	170	LEU	2.2
1	C	241	GLU	2.2
1	B	104	ASN	2.2
1	B	459	ASN	2.2
1	D	362	PRO	2.1
1	C	618	VAL	2.1
1	B	456	VAL	2.1
1	C	256	PRO	2.1
1	B	182	GLY	2.1
1	B	57	ASP	2.1
1	A	71	THR	2.1
1	E	384	ARG	2.1
1	B	584	PHE	2.1
1	B	36	GLY	2.1
1	B	607	ALA	2.1
1	D	172	LEU	2.1
1	E	57	ASP	2.0
1	C	438	PHE	2.0
1	B	52	PHE	2.0
1	E	78	LEU	2.0
1	B	219	LEU	2.0
1	B	75	LEU	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

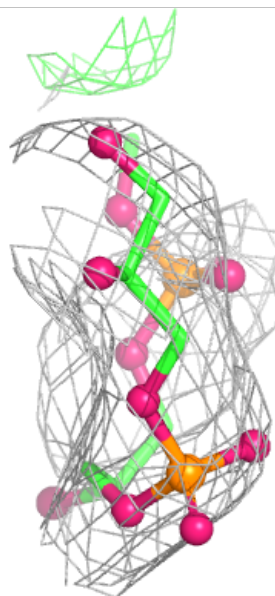
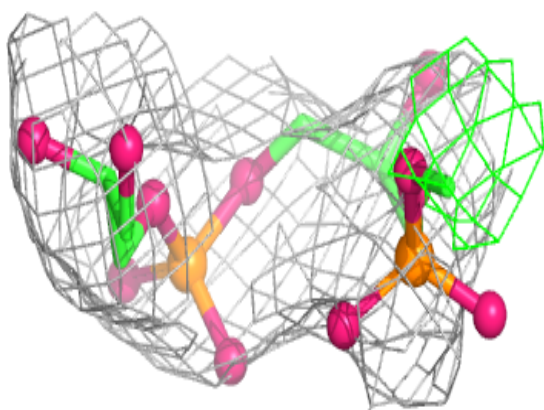
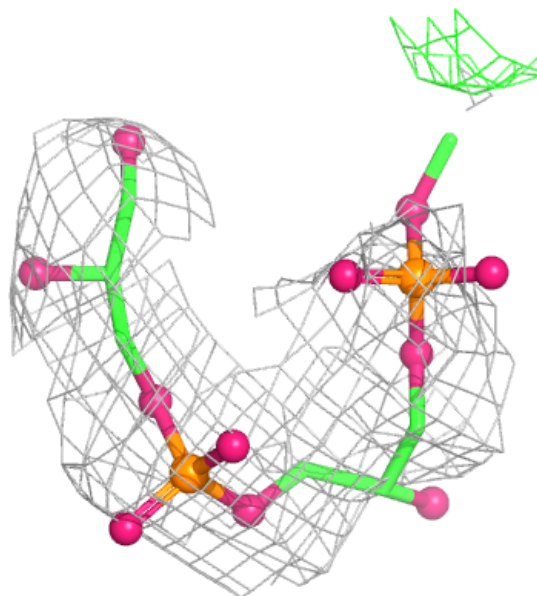
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TRS	E	701	8/8	0.76	0.11	129,151,166,175	0
3	P3A	C	702	20/58	0.76	0.17	141,215,271,276	0
3	P3A	A	703	21/58	0.77	0.19	168,227,236,236	0
2	TRS	D	701	8/8	0.79	0.14	134,160,165,168	0
3	P3A	E	702	20/58	0.81	0.20	190,241,260,262	0
3	P3A	A	702	20/58	0.84	0.17	25,229,253,254	0
2	TRS	A	701	8/8	0.87	0.10	156,168,173,175	0
3	P3A	B	702	21/58	0.88	0.15	134,209,242,249	0
2	TRS	B	701	8/8	0.92	0.12	148,156,177,190	0
2	TRS	C	701	8/8	0.92	0.11	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.

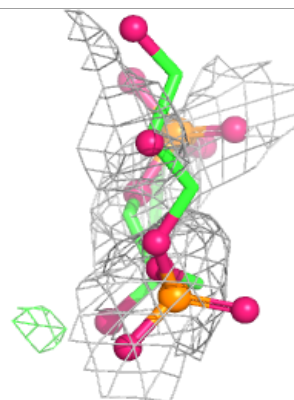
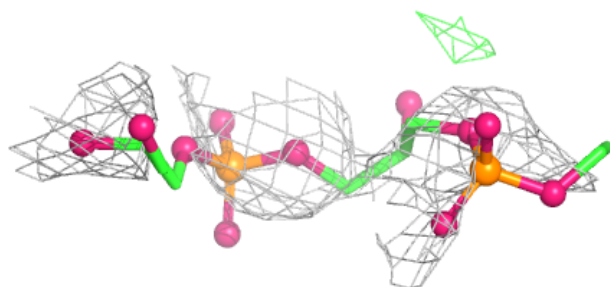
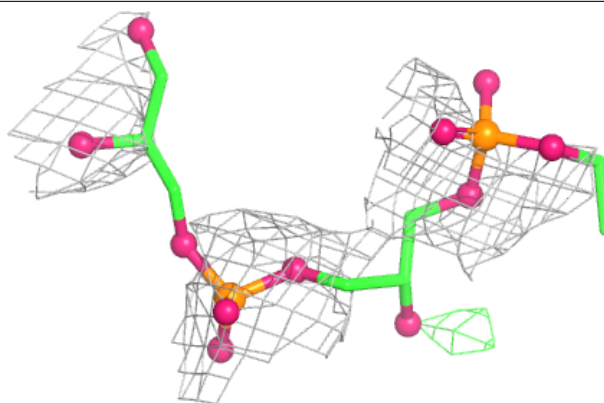
Electron density around P3A C 702:

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

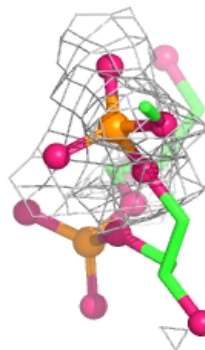
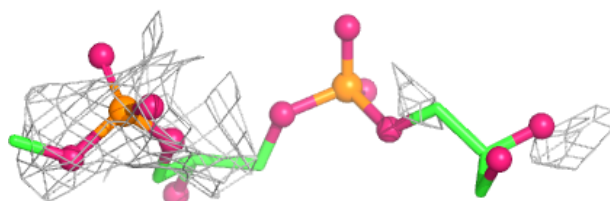
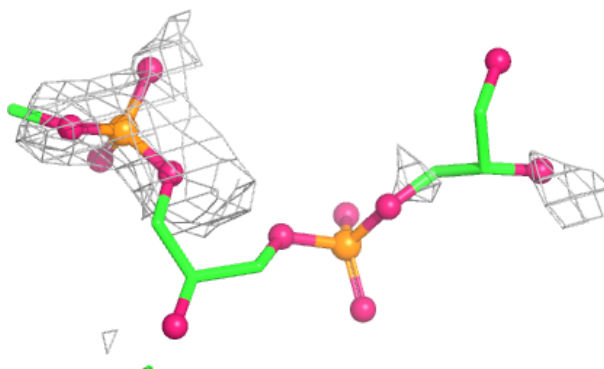


Electron density around P3A A 703:

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

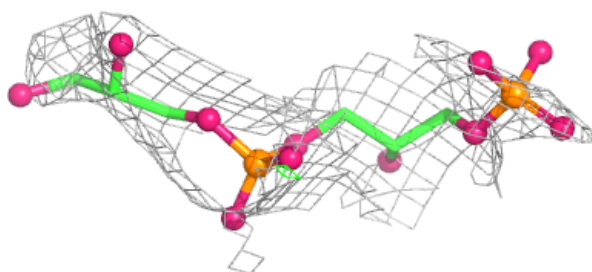
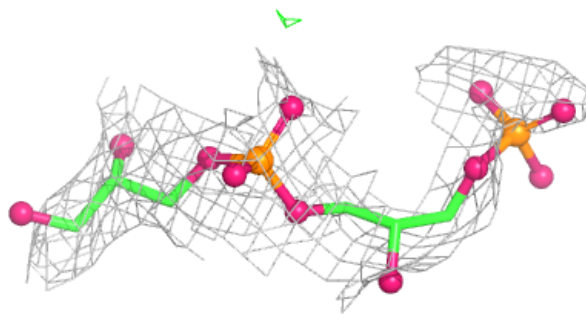
**Electron density around P3A E 702:**

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



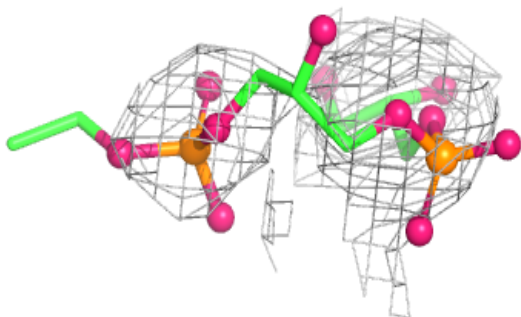
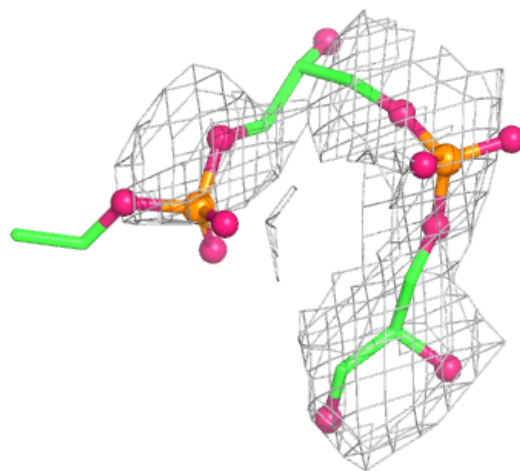
Electron density around P3A A 702:

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



Electron density around P3A 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.