



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:20 PM UTC

PDB ID : 4GDN / pdb_00004gdn
Title : Structure of FmtA-like protein
Authors : Cougnoux, A.; Gibold, L.; Delmas, J.; Robin, F.; Dalmaso, G.; Bonnet, R.
Deposited on : 2012-08-01
Resolution : 3.20 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

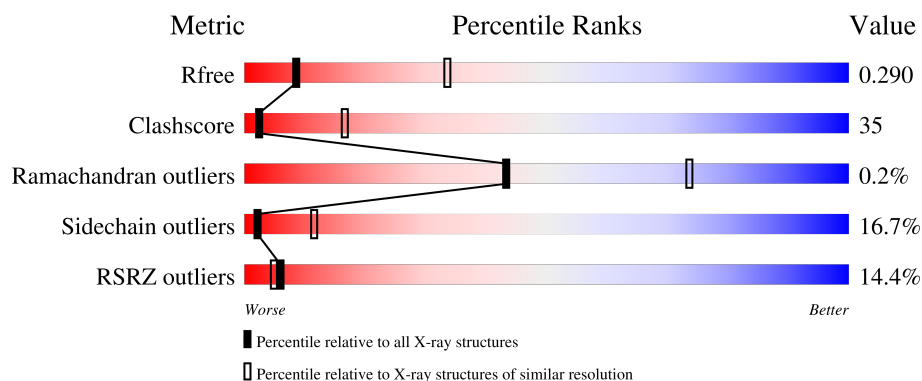
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	342	12% 46% 38% 12% ..
1	B	342	17% 46% 37% 13% ..
1	C	342	14% 51% 32% 12% ..
1	D	342	13% 49% 37% 10% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10649 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.

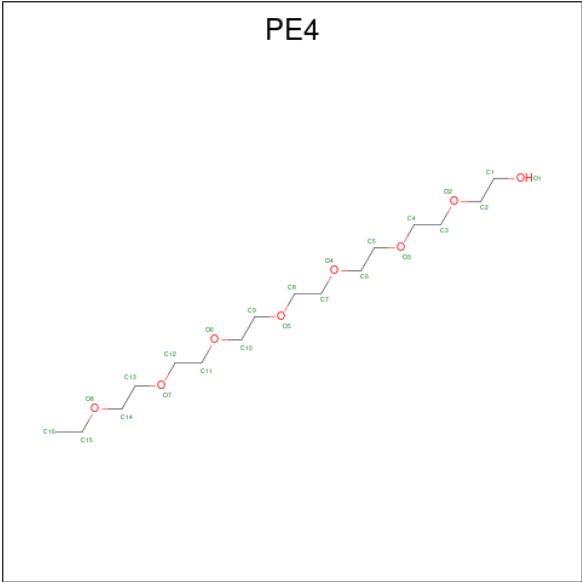
- Molecule 1 is a protein called Protein flp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2674	1692	458	518	6			
1	B	336	Total	C	N	O	S	0	0	0
			2658	1684	456	512	6			
1	C	329	Total	C	N	O	S	0	0	0
			2616	1658	447	505	6			
1	D	333	Total	C	N	O	S	0	0	0
			2642	1673	454	509	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MET	-	initiating methionine	UNP Q7A3Q5
B	29	MET	-	initiating methionine	UNP Q7A3Q5
C	29	MET	-	initiating methionine	UNP Q7A3Q5
D	29	MET	-	initiating methionine	UNP Q7A3Q5

- Molecule 2 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			24	16	8		

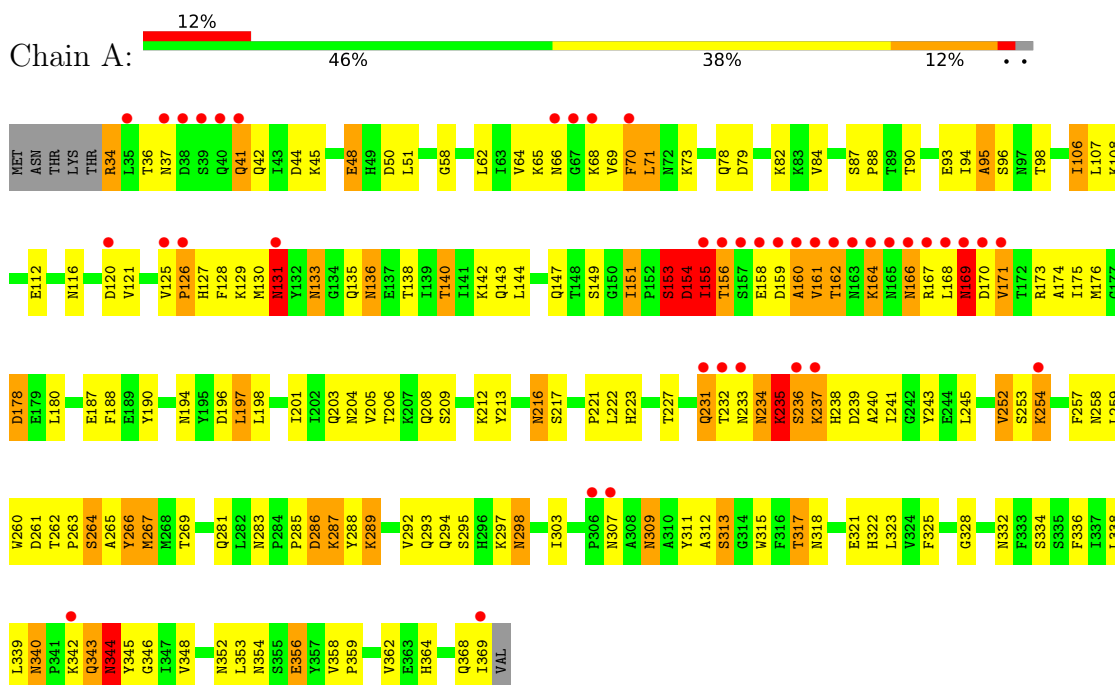
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	15	Total	O	0	0
			15	15		
3	C	6	Total	O	0	0
			6	6		
3	D	7	Total	O	0	0
			7	7		

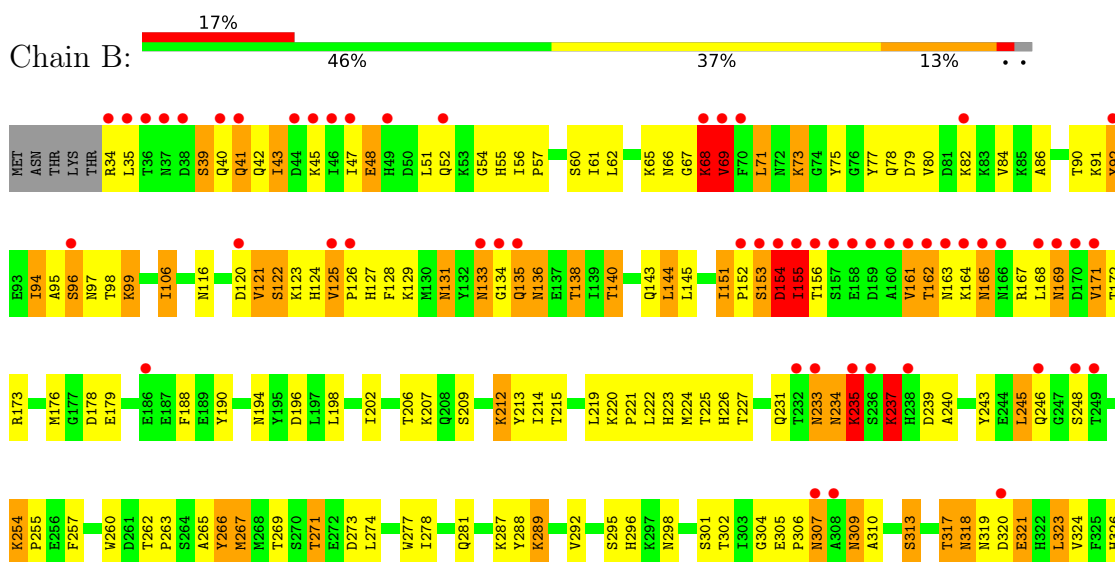
3 Residue-property plots

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: Protein flp

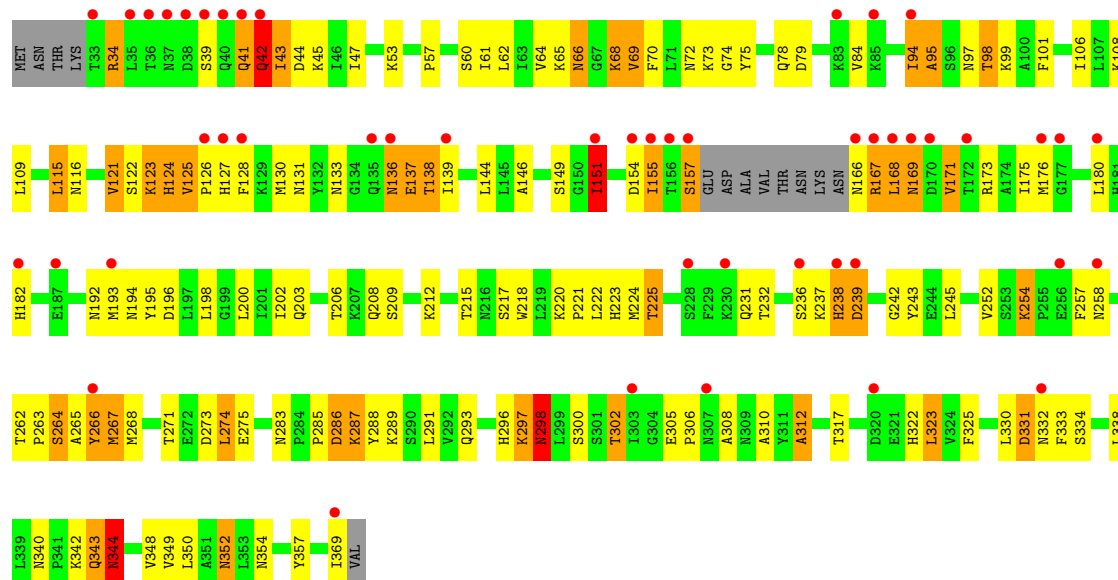


• Molecule 1: Protein flp

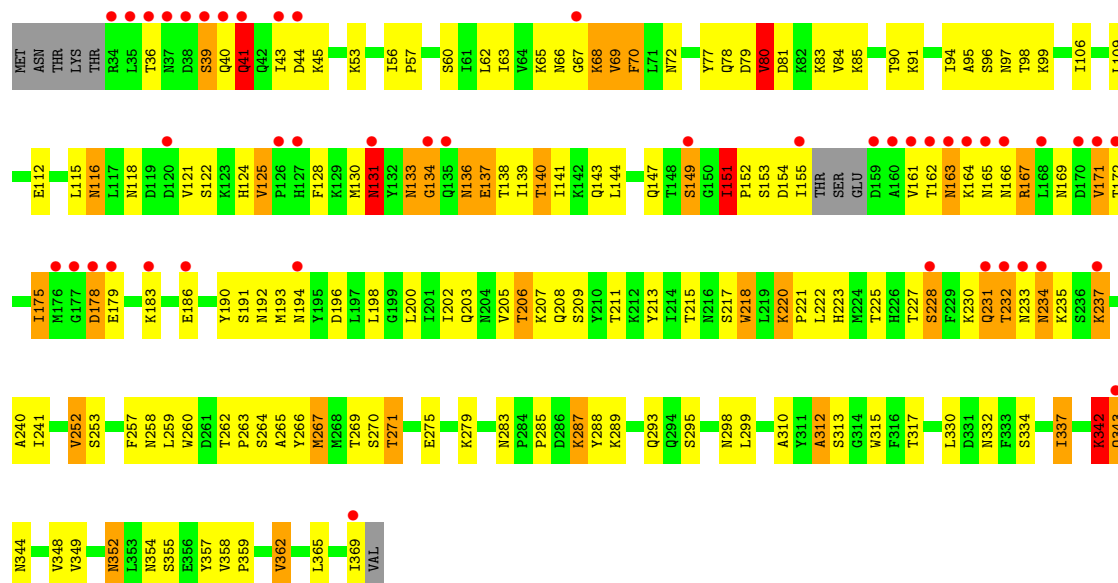




• Molecule 1: Protein flp



• Molecule 1: Protein flp



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	179.71Å 179.71Å 287.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.73 – 3.20 85.73 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (85.73-3.20) 96.4 (85.73-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.257 , 0.295 0.256 , 0.290	Depositor DCC
R_{free} test set	2315 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10649	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PE4

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	0.74	0/2734	1.14	23/3709 (0.6%)
1	B	0.75	0/2718	1.19	24/3689 (0.7%)
1	C	0.73	1/2675 (0.0%)	1.15	24/3629 (0.7%)
1	D	0.68	0/2701	1.09	18/3664 (0.5%)
All	All	0.73	1/10828 (0.0%)	1.14	89/14691 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	296	HIS	CG-ND1	-6.57	1.31	1.38

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	HIS	N-CA-C	-7.92	101.74	113.61
1	B	161	VAL	N-CA-C	7.64	119.76	108.45
1	D	80	VAL	N-CA-C	7.58	118.17	110.82
1	C	291	LEU	N-CA-C	-7.45	103.09	111.14
1	C	238	HIS	N-CA-C	7.34	121.08	112.72
1	A	159	ASP	N-CA-C	7.29	120.55	109.62
1	C	264	SER	N-CA-C	7.13	118.84	111.14
1	C	344	ASN	N-CA-C	6.94	120.74	111.30
1	D	186	GLU	N-CA-C	6.94	118.64	111.14
1	A	201	ILE	N-CA-C	-6.92	103.56	110.62
1	B	154	ASP	N-CA-C	6.91	118.69	108.60
1	C	266	TYR	N-CA-C	6.90	121.01	112.59
1	A	41	GLN	N-CA-C	6.76	118.42	108.14
1	C	333	PHE	N-CA-C	6.65	120.44	110.14
1	A	264	SER	N-CA-C	6.64	118.31	111.14
1	D	151	ILE	CA-C-N	6.62	126.64	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	151	ILE	C-N-CA	6.62	126.64	119.89
1	B	153	SER	N-CA-C	6.61	118.15	111.07
1	A	356	GLU	N-CA-C	-6.60	104.12	111.71
1	C	238	HIS	CB-CA-C	-6.51	100.20	110.94
1	C	298	ASN	N-CA-C	6.47	119.14	110.35
1	C	176	MET	N-CA-C	6.42	119.10	111.33
1	A	160	ALA	N-CA-C	6.37	120.20	111.54
1	A	95	ALA	CB-CA-C	-6.29	109.33	116.63
1	A	126	PRO	CB-CA-C	-6.25	101.25	111.56
1	C	95	ALA	CB-CA-C	-6.14	109.51	116.63
1	D	70	PHE	N-CA-C	-6.12	104.61	111.28
1	A	151	ILE	N-CA-C	6.10	113.88	108.63
1	A	344	ASN	N-CA-C	5.97	119.42	111.30
1	D	131	ASN	N-CA-C	5.94	118.21	109.24
1	C	42	GLN	N-CA-C	-5.93	105.63	112.92
1	A	126	PRO	N-CA-CB	-5.89	97.06	103.25
1	A	168	LEU	N-CA-C	5.88	118.30	110.53
1	B	135	GLN	N-CA-C	5.86	119.37	109.76
1	B	131	ASN	N-CA-C	5.81	118.94	109.24
1	B	68	LYS	N-CA-C	-5.80	101.81	110.23
1	B	266	TYR	N-CA-C	5.79	119.66	112.59
1	D	85	LYS	N-CA-C	5.79	118.62	110.23
1	D	41	GLN	N-CA-C	5.78	118.19	109.23
1	D	178	ASP	N-CA-C	5.77	118.20	110.35
1	C	124	HIS	N-CA-C	-5.73	106.06	113.16
1	D	77	TYR	N-CA-C	5.68	117.68	108.41
1	C	151	ILE	CA-C-N	5.67	125.67	119.89
1	C	151	ILE	C-N-CA	5.67	125.67	119.89
1	A	131	ASN	N-CA-C	5.64	118.27	109.52
1	A	153	SER	N-CA-C	5.63	120.15	112.04
1	A	135	GLN	N-CA-C	5.62	118.22	109.52
1	D	165	ASN	N-CA-C	-5.55	106.09	112.92
1	B	161	VAL	CB-CA-C	-5.53	101.14	110.71
1	C	123	LYS	N-CA-C	-5.50	106.70	113.41
1	B	237	LYS	CB-CA-C	-5.49	109.76	117.23
1	D	133	ASN	CB-CA-C	-5.48	110.27	116.63
1	D	39	SER	N-CA-C	-5.47	105.21	111.07
1	A	313	SER	N-CA-C	5.45	118.85	111.17
1	A	344	ASN	N-CA-CB	-5.45	103.83	111.62
1	D	342	LYS	N-CA-C	-5.42	102.85	110.50
1	B	144	LEU	N-CA-C	-5.40	104.81	111.40
1	A	126	PRO	N-CD-CG	-5.34	95.19	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	LYS	N-CA-C	5.33	117.63	109.95
1	B	39	SER	CB-CA-C	-5.33	110.45	116.63
1	A	266	TYR	N-CA-C	5.29	120.41	112.94
1	A	155	ILE	N-CA-C	5.28	120.33	109.34
1	B	355	SER	N-CA-C	5.26	117.24	108.99
1	C	116	ASN	N-CA-C	-5.26	102.41	110.14
1	C	254	LYS	CA-C-N	5.26	125.23	120.03
1	C	254	LYS	C-N-CA	5.26	125.23	120.03
1	D	237	LYS	CB-CA-C	-5.25	110.09	117.23
1	C	66	ASN	CB-CA-C	-5.22	109.03	116.34
1	D	134	GLY	N-CA-C	5.22	119.00	112.73
1	C	323	LEU	N-CA-C	5.20	117.37	108.90
1	B	71	LEU	N-CA-C	5.20	116.89	108.26
1	A	216	ASN	N-CA-C	5.16	116.59	111.07
1	B	133	ASN	CB-CA-C	-5.16	109.12	116.34
1	A	154	ASP	N-CA-C	5.16	116.13	108.60
1	C	245	LEU	N-CA-C	5.14	116.90	108.52
1	D	218	TRP	N-CA-C	5.13	118.99	112.12
1	B	151	ILE	CA-C-N	5.11	125.02	119.85
1	B	151	ILE	C-N-CA	5.11	125.02	119.85
1	B	304	GLY	N-CA-C	5.10	120.21	113.37
1	C	312	ALA	N-CA-C	5.10	116.48	107.61
1	C	296	HIS	N-CA-C	5.10	116.92	111.36
1	D	312	ALA	N-CA-C	5.09	115.74	107.23
1	B	69	VAL	N-CA-C	5.09	115.97	109.30
1	B	342	LYS	N-CA-C	-5.08	101.69	109.76
1	B	155	ILE	N-CA-C	5.06	119.87	109.34
1	A	235	LYS	N-CA-C	5.04	117.74	110.28
1	B	41	GLN	N-CA-C	5.04	117.36	108.75
1	C	133	ASN	CB-CA-C	-5.02	110.81	116.63
1	B	243	TYR	N-CA-C	5.00	117.60	109.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2674	0	2628	189	0
1	B	2658	0	2605	236	0
1	C	2616	0	2567	166	0
1	D	2642	0	2587	164	0
2	D	24	0	34	0	0
3	A	7	0	0	0	0
3	B	15	0	0	1	0
3	C	6	0	0	1	0
3	D	7	0	0	1	0
All	All	10649	0	10421	738	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 35.

All (738) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:SER:O	1:B:123:LYS:HG2	1.34	1.25
1:B:68:LYS:HB2	1:B:68:LYS:NZ	1.37	1.17
1:A:356:GLU:O	1:A:359:PRO:HD2	1.44	1.15
1:A:130:MET:HG2	1:A:180:LEU:HD21	1.30	1.11
1:B:318:ASN:HD22	1:B:318:ASN:C	1.54	1.11
1:C:137:GLU:HA	1:C:137:GLU:OE1	1.45	1.11
1:B:306:PRO:HA	3:B:408:HOH:O	1.50	1.10
1:B:125:VAL:HG11	1:B:128:PHE:HB2	1.31	1.10
1:B:323:LEU:HD12	1:B:323:LEU:H	1.04	1.09
1:D:125:VAL:HG11	1:D:128:PHE:HB2	1.33	1.09
1:D:155:ILE:HD13	1:D:193:MET:HE2	1.36	1.06
1:B:323:LEU:HD12	1:B:323:LEU:N	1.67	1.05
1:C:125:VAL:HG11	1:C:128:PHE:HB2	1.34	1.05
1:B:356:GLU:O	1:B:359:PRO:HD2	1.56	1.05
1:C:94:ILE:HG23	1:C:97:ASN:HB2	1.39	1.04
1:D:125:VAL:CG1	1:D:128:PHE:HB2	1.87	1.04
1:B:94:ILE:HG23	1:B:97:ASN:HB2	1.39	1.01
1:B:122:SER:O	1:B:123:LYS:CG	2.08	1.00
1:B:125:VAL:HG13	1:B:126:PRO:HD2	1.41	1.00
1:B:298:ASN:HD21	1:B:317:THR:HG21	1.29	0.98
1:B:106:ILE:HD12	1:B:198:LEU:HD22	1.45	0.97
1:C:98:THR:OG1	1:C:267:MET:HB3	1.64	0.97
1:C:298:ASN:H	1:C:298:ASN:ND2	1.51	0.97
1:A:334:SER:HB2	1:A:354:ASN:HA	1.46	0.96
1:B:68:LYS:HB2	1:B:68:LYS:HZ3	1.14	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:VAL:CG2	1:C:175:ILE:HG13	1.96	0.95
1:C:298:ASN:HA	1:C:312:ALA:HB2	1.47	0.95
1:B:68:LYS:NZ	1:B:68:LYS:CB	2.30	0.95
1:A:289:LYS:NZ	1:A:289:LYS:HB3	1.81	0.95
1:D:130:MET:CE	1:D:175:ILE:HB	1.96	0.94
1:C:151:ILE:HD11	1:C:193:MET:HB2	1.47	0.94
1:B:68:LYS:HB2	1:B:68:LYS:HZ2	1.22	0.94
1:B:131:ASN:HB3	1:B:136:ASN:HA	1.50	0.93
1:B:235:LYS:HB2	1:B:239:ASP:HB2	1.47	0.93
1:A:289:LYS:HB3	1:A:289:LYS:HZ3	1.31	0.92
1:A:233:ASN:HD21	1:A:254:LYS:HB2	1.32	0.92
1:B:255:PRO:HD3	1:B:332:ASN:HD21	1.32	0.92
1:B:255:PRO:HD3	1:B:332:ASN:ND2	1.84	0.91
1:D:140:THR:HG23	1:D:143:GLN:HG3	1.53	0.90
1:C:34:ARG:H	1:C:34:ARG:HD2	1.36	0.90
1:B:41:GLN:HB3	1:B:43:ILE:HD13	1.52	0.90
1:C:65:LYS:HG3	1:C:369:ILE:CG2	2.02	0.89
1:C:215:THR:O	1:C:220:LYS:HG2	1.72	0.89
1:D:83:LYS:O	1:D:83:LYS:HD3	1.73	0.88
1:C:121:VAL:HG11	1:C:128:PHE:CD2	2.09	0.88
1:A:127:HIS:O	1:B:207:LYS:HE3	1.74	0.87
1:C:217:SER:O	1:C:221:PRO:HG2	1.74	0.87
1:A:298:ASN:HA	1:A:312:ALA:HB2	1.54	0.87
1:B:155:ILE:HG22	1:B:155:ILE:O	1.72	0.87
1:C:130:MET:HE1	1:C:175:ILE:O	1.75	0.87
1:B:156:THR:HB	1:B:178:ASP:OD2	1.76	0.86
1:D:206:THR:HG21	1:D:213:TYR:HB2	1.56	0.86
1:B:334:SER:OG	1:B:354:ASN:HA	1.75	0.86
1:C:298:ASN:H	1:C:298:ASN:HD22	1.23	0.86
1:D:97:ASN:HD21	1:D:337:ILE:HB	1.38	0.86
1:D:202:ILE:O	1:D:206:THR:HB	1.76	0.85
1:A:171:VAL:HG22	1:A:171:VAL:O	1.76	0.85
1:A:166:ASN:HD21	1:A:173:ARG:NH2	1.75	0.85
1:A:154:ASP:OD1	1:A:155:ILE:HB	1.77	0.84
1:C:65:LYS:HB3	1:C:70:PHE:CD2	2.12	0.84
1:D:130:MET:HE1	1:D:175:ILE:HB	1.57	0.84
1:D:206:THR:HG22	1:D:208:GLN:HG2	1.57	0.84
1:A:206:THR:HG22	1:A:208:GLN:HG2	1.58	0.83
1:D:241:ILE:HG21	1:D:252:VAL:CG2	2.09	0.83
1:B:125:VAL:HG13	1:B:126:PRO:CD	2.08	0.83
1:A:166:ASN:ND2	1:A:173:ARG:NH2	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LYS:O	1:A:312:ALA:HB1	1.79	0.82
1:C:65:LYS:HG3	1:C:369:ILE:HG21	1.59	0.82
1:C:305:GLU:HG3	1:C:306:PRO:HD2	1.62	0.82
1:A:130:MET:CG	1:A:180:LEU:HD21	2.10	0.82
1:C:169:ASN:C	1:C:169:ASN:HD22	1.87	0.82
1:C:171:VAL:HG23	1:C:171:VAL:O	1.79	0.81
1:B:95:ALA:HA	1:B:265:ALA:O	1.80	0.81
1:B:342:LYS:O	1:B:343:GLN:HB2	1.79	0.80
1:C:171:VAL:HG23	1:C:175:ILE:HG13	1.61	0.80
1:B:133:ASN:CG	1:B:134:GLY:H	1.87	0.80
1:D:206:THR:CG2	1:D:208:GLN:HG2	2.10	0.80
1:B:318:ASN:C	1:B:318:ASN:ND2	2.30	0.80
1:A:151:ILE:HD12	1:A:194:ASN:ND2	1.97	0.80
1:C:298:ASN:ND2	1:C:298:ASN:N	2.28	0.80
1:A:98:THR:HG23	1:A:267:MET:HE3	1.63	0.79
1:B:106:ILE:CD1	1:B:198:LEU:HD22	2.12	0.79
1:A:171:VAL:O	1:A:171:VAL:CG2	2.30	0.79
1:B:323:LEU:N	1:B:323:LEU:CD1	2.44	0.79
1:A:289:LYS:NZ	1:A:289:LYS:CB	2.45	0.79
1:A:166:ASN:HD21	1:A:173:ARG:HH22	1.29	0.78
1:B:235:LYS:HB2	1:B:239:ASP:CB	2.12	0.78
1:C:171:VAL:CG2	1:C:171:VAL:O	2.30	0.78
1:B:318:ASN:ND2	1:B:321:GLU:H	1.81	0.78
1:D:259:LEU:O	1:D:262:THR:HG22	1.82	0.78
1:B:206:THR:HG21	1:B:213:TYR:CD1	2.18	0.78
1:A:169:ASN:O	1:A:171:VAL:HG12	1.83	0.78
1:A:79:ASP:HB3	1:A:84:VAL:HG12	1.65	0.78
1:D:241:ILE:CG2	1:D:252:VAL:HG22	2.14	0.78
1:B:234:ASN:HD22	1:B:234:ASN:C	1.92	0.77
1:B:323:LEU:H	1:B:323:LEU:CD1	1.93	0.77
1:B:92:TYR:HB3	1:B:333:PHE:CE2	2.19	0.77
1:A:36:THR:HG23	1:A:36:THR:O	1.83	0.77
1:C:151:ILE:HD11	1:C:193:MET:CB	2.13	0.77
1:A:161:VAL:HG13	1:A:162:THR:N	1.98	0.77
1:B:96:SER:HB2	1:B:328:GLY:HA2	1.67	0.77
1:B:309:ASN:H	1:B:309:ASN:HD22	1.30	0.76
1:B:198:LEU:O	1:B:202:ILE:HD12	1.86	0.76
1:D:171:VAL:CG1	1:D:260:TRP:HB2	2.15	0.76
1:C:69:VAL:CG2	1:C:69:VAL:O	2.34	0.76
1:B:162:THR:HG23	1:B:163:ASN:CB	2.16	0.76
1:A:166:ASN:CG	1:A:173:ARG:HH21	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:HA	1:B:127:HIS:CD2	2.21	0.75
1:D:161:VAL:HB	1:D:164:LYS:O	1.85	0.75
1:B:60:SER:HB3	1:B:271:THR:OG1	1.86	0.75
1:C:175:ILE:HG12	1:C:193:MET:HE3	1.69	0.75
1:A:154:ASP:OD1	1:A:154:ASP:C	2.30	0.74
1:A:154:ASP:O	1:A:155:ILE:HG22	1.87	0.74
1:A:233:ASN:ND2	1:A:254:LYS:HB2	2.02	0.74
1:B:125:VAL:CG1	1:B:128:PHE:HB2	2.15	0.74
1:D:155:ILE:CD1	1:D:193:MET:HE2	2.16	0.74
1:A:171:VAL:HB	1:A:260:TRP:CD2	2.23	0.74
1:D:116:ASN:HD22	1:D:118:ASN:H	1.36	0.73
1:D:136:ASN:C	1:D:136:ASN:ND2	2.43	0.73
1:D:334:SER:HB2	1:D:354:ASN:HA	1.69	0.73
1:C:298:ASN:HD22	1:C:298:ASN:N	1.86	0.73
1:D:40:GLN:O	1:D:41:GLN:NE2	2.21	0.73
1:B:79:ASP:HB3	1:B:84:VAL:HG12	1.70	0.73
1:A:205:VAL:HG22	1:B:127:HIS:NE2	2.04	0.73
1:B:136:ASN:C	1:B:136:ASN:ND2	2.47	0.73
1:B:318:ASN:HD21	1:B:321:GLU:H	1.34	0.73
1:B:298:ASN:ND2	1:B:317:THR:HG21	2.03	0.72
1:D:130:MET:HE2	1:D:175:ILE:HB	1.71	0.72
1:D:155:ILE:HD13	1:D:193:MET:CE	2.17	0.72
1:B:171:VAL:O	1:B:171:VAL:CG2	2.37	0.72
1:C:257:PHE:HB2	1:C:266:TYR:OH	1.89	0.72
1:A:254:LYS:HD2	1:A:254:LYS:O	1.90	0.72
1:A:309:ASN:HD22	1:A:309:ASN:H	1.33	0.72
1:B:122:SER:O	1:B:123:LYS:CB	2.38	0.71
1:B:334:SER:HG	1:B:354:ASN:HA	1.54	0.71
1:B:224:MET:HE1	1:B:277:TRP:HB2	1.71	0.71
1:A:151:ILE:HD12	1:A:194:ASN:HD21	1.55	0.71
1:A:212:LYS:HE2	1:A:216:ASN:HD21	1.56	0.71
1:C:289:LYS:O	1:C:293:GLN:HG3	1.90	0.71
1:A:285:PRO:HG2	1:A:288:TYR:HD2	1.54	0.71
1:A:297:LYS:O	1:A:312:ALA:CB	2.38	0.71
1:B:233:ASN:C	1:B:233:ASN:HD22	1.99	0.71
1:A:93:GLU:OE2	1:A:235:LYS:NZ	2.23	0.71
1:D:94:ILE:CD1	1:D:267:MET:HG2	2.21	0.71
1:C:121:VAL:CG1	1:C:128:PHE:CD2	2.74	0.70
1:D:97:ASN:ND2	1:D:337:ILE:HB	2.05	0.70
1:B:162:THR:HG23	1:B:163:ASN:HB2	1.73	0.70
1:D:171:VAL:HG11	1:D:260:TRP:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ASN:HD21	1:C:344:ASN:HD21	1.38	0.70
1:D:79:ASP:HB3	1:D:84:VAL:HG12	1.72	0.70
1:B:65:LYS:O	1:B:67:GLY:N	2.22	0.69
1:B:222:LEU:CD1	1:B:224:MET:HE3	2.22	0.69
1:A:79:ASP:HB3	1:A:84:VAL:CG1	2.22	0.69
1:A:298:ASN:HD21	1:A:317:THR:HG21	1.56	0.69
1:B:62:LEU:HB2	1:B:271:THR:HG22	1.75	0.69
1:B:79:ASP:HB3	1:B:84:VAL:CG1	2.22	0.69
1:D:79:ASP:HB3	1:D:84:VAL:CG1	2.22	0.69
1:A:283:ASN:HD21	1:A:344:ASN:HD21	1.41	0.69
1:A:283:ASN:ND2	1:A:344:ASN:HD21	1.91	0.68
1:D:203:GLN:HG3	1:D:209:SER:HA	1.74	0.68
1:A:125:VAL:CG1	1:A:128:PHE:HB2	2.22	0.68
1:A:161:VAL:CG1	1:A:162:THR:N	2.56	0.68
1:B:169:ASN:O	1:B:171:VAL:HG12	1.94	0.68
1:A:206:THR:HG21	1:A:213:TYR:CD1	2.28	0.68
1:B:69:VAL:CG2	1:B:69:VAL:O	2.42	0.68
1:D:151:ILE:HD11	1:D:193:MET:HB3	1.74	0.68
1:D:241:ILE:CG2	1:D:252:VAL:CG2	2.70	0.68
1:B:43:ILE:N	1:B:43:ILE:HD12	2.09	0.68
1:D:65:LYS:HE2	1:D:70:PHE:CE1	2.28	0.68
1:D:125:VAL:HG12	1:D:128:PHE:HB2	1.75	0.68
1:A:166:ASN:CG	1:A:173:ARG:NH2	2.52	0.67
1:C:34:ARG:HD2	1:C:34:ARG:N	2.08	0.67
1:C:65:LYS:HD2	1:C:70:PHE:HE2	1.58	0.67
1:B:68:LYS:HZ3	1:B:68:LYS:CB	1.98	0.67
1:B:156:THR:CB	1:B:178:ASP:OD2	2.43	0.67
1:B:97:ASN:ND2	1:B:335:SER:HB2	2.10	0.67
1:C:297:LYS:HG3	1:C:297:LYS:O	1.94	0.66
1:D:67:GLY:O	1:D:279:LYS:NZ	2.27	0.66
1:A:96:SER:HB3	1:A:328:GLY:HA2	1.77	0.66
1:A:153:SER:HB3	1:A:190:TYR:O	1.94	0.66
1:D:66:ASN:O	1:D:68:LYS:HD2	1.96	0.66
1:B:92:TYR:HB3	1:B:333:PHE:HE2	1.59	0.66
1:B:140:THR:HG23	1:B:143:GLN:CD	2.19	0.66
1:B:131:ASN:HB3	1:B:136:ASN:CA	2.23	0.66
1:C:94:ILE:HG23	1:C:97:ASN:CB	2.20	0.66
1:A:356:GLU:O	1:A:359:PRO:CD	2.35	0.66
1:B:136:ASN:ND2	1:B:136:ASN:O	2.29	0.66
1:D:91:LYS:NZ	1:D:228:SER:OG	2.29	0.66
1:A:235:LYS:HB3	1:A:239:ASP:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:VAL:CG1	1:C:128:PHE:HB2	2.21	0.65
1:D:196:ASP:HA	1:D:263:PRO:HG2	1.78	0.65
1:A:136:ASN:O	1:A:136:ASN:ND2	2.29	0.65
1:C:99:LYS:HE2	1:C:195:TYR:HB2	1.78	0.65
1:C:41:GLN:O	1:C:41:GLN:NE2	2.30	0.65
1:B:340:ASN:ND2	1:B:342:LYS:O	2.30	0.65
1:B:94:ILE:HG13	1:B:269:THR:HG22	1.79	0.65
1:B:165:ASN:O	1:B:165:ASN:ND2	2.30	0.65
1:B:222:LEU:HD13	1:B:224:MET:HE3	1.79	0.65
1:C:208:GLN:HE21	1:C:212:LYS:HD3	1.62	0.65
1:B:43:ILE:HD12	1:B:43:ILE:H	1.61	0.65
1:B:234:ASN:O	1:B:234:ASN:ND2	2.30	0.65
1:D:151:ILE:HD11	1:D:193:MET:CB	2.27	0.65
1:A:243:TYR:O	1:A:353:LEU:HD12	1.97	0.64
1:C:169:ASN:O	1:C:169:ASN:ND2	2.30	0.64
1:A:106:ILE:CD1	1:A:198:LEU:HD22	2.27	0.64
1:A:298:ASN:N	1:A:298:ASN:HD22	1.94	0.64
1:B:235:LYS:CB	1:B:239:ASP:CB	2.75	0.64
1:C:167:ARG:HD2	1:C:258:ASN:HA	1.79	0.64
1:A:222:LEU:O	1:A:223:HIS:HB2	1.97	0.64
1:A:253:SER:HB3	1:A:332:ASN:HB3	1.80	0.64
1:C:136:ASN:C	1:C:136:ASN:ND2	2.55	0.64
1:C:151:ILE:CD1	1:C:193:MET:HB2	2.26	0.64
1:D:130:MET:HE1	1:D:175:ILE:CB	2.27	0.64
1:D:136:ASN:ND2	1:D:136:ASN:O	2.30	0.64
1:D:233:ASN:ND2	1:D:233:ASN:O	2.30	0.64
1:C:65:LYS:HB3	1:C:70:PHE:CE2	2.32	0.64
1:B:106:ILE:HG13	1:B:202:ILE:HD11	1.80	0.64
1:B:255:PRO:CD	1:B:332:ASN:HD21	2.08	0.64
1:B:257:PHE:HB2	1:B:266:TYR:OH	1.98	0.64
1:C:94:ILE:CG2	1:C:97:ASN:HB2	2.23	0.64
1:C:137:GLU:OE1	1:C:137:GLU:CA	2.30	0.63
1:D:171:VAL:HG12	1:D:260:TRP:CB	2.28	0.63
1:A:166:ASN:OD1	1:A:173:ARG:NH2	2.25	0.63
1:C:136:ASN:ND2	1:C:136:ASN:O	2.30	0.63
1:C:125:VAL:HG13	1:C:126:PRO:HD2	1.80	0.63
1:D:136:ASN:C	1:D:136:ASN:HD22	2.05	0.63
1:A:292:VAL:O	1:A:295:SER:HB3	1.99	0.63
1:D:169:ASN:O	1:D:171:VAL:HG13	1.99	0.63
1:A:127:HIS:HB2	1:B:207:LYS:HE2	1.80	0.63
1:B:133:ASN:CG	1:B:134:GLY:N	2.52	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ASN:HB3	1:C:136:ASN:HA	1.80	0.63
1:B:125:VAL:HG12	1:B:128:PHE:H	1.63	0.62
1:B:138:THR:HG22	1:B:138:THR:O	1.99	0.62
1:B:292:VAL:O	1:B:295:SER:HB3	1.99	0.62
1:A:131:ASN:HB3	1:A:136:ASN:HA	1.81	0.62
1:C:286:ASP:OD2	1:C:286:ASP:N	2.32	0.62
1:D:287:LYS:HE2	1:D:288:TYR:CE2	2.34	0.62
1:C:95:ALA:HA	1:C:265:ALA:O	1.99	0.62
1:C:131:ASN:HA	1:C:136:ASN:HA	1.81	0.62
1:C:169:ASN:O	1:C:171:VAL:HG12	1.99	0.62
1:C:323:LEU:HD22	1:C:338:LEU:HD11	1.79	0.62
1:A:125:VAL:HG11	1:A:128:PHE:HB2	1.82	0.62
1:B:133:ASN:OD1	1:B:134:GLY:N	2.33	0.62
1:A:227:THR:HG23	1:A:269:THR:HB	1.82	0.62
1:B:321:GLU:HB3	1:B:323:LEU:HD11	1.81	0.62
1:C:98:THR:HG22	1:C:263:PRO:O	2.00	0.62
1:D:147:GLN:OE1	1:D:190:TYR:HA	2.00	0.62
1:B:220:LYS:HB2	1:B:221:PRO:HD3	1.82	0.62
1:C:65:LYS:CG	1:C:369:ILE:HG21	2.29	0.61
1:C:78:GLN:HE22	1:C:238:HIS:HA	1.64	0.61
1:B:163:ASN:CG	1:B:164:LYS:H	2.08	0.61
1:A:217:SER:O	1:A:221:PRO:HG2	2.00	0.61
1:C:65:LYS:HG3	1:C:369:ILE:HG23	1.82	0.61
1:C:298:ASN:HB3	1:C:310:ALA:HB1	1.83	0.61
1:D:137:GLU:OE2	1:D:183:LYS:HE3	2.01	0.61
1:D:234:ASN:C	1:D:234:ASN:OD1	2.43	0.61
1:C:257:PHE:CB	1:C:266:TYR:OH	2.48	0.61
1:A:36:THR:O	1:A:36:THR:CG2	2.48	0.61
1:A:262:THR:N	1:A:263:PRO:HD2	2.15	0.61
1:D:137:GLU:OE1	1:D:137:GLU:HA	2.00	0.61
1:D:167:ARG:HB3	1:D:258:ASN:HD22	1.66	0.61
1:B:154:ASP:C	1:B:154:ASP:OD1	2.44	0.60
1:B:47:ILE:HG21	1:B:75:TYR:CD1	2.36	0.60
1:B:224:MET:CE	1:B:277:TRP:HB2	2.31	0.60
1:D:90:THR:CG2	1:D:240:ALA:HB2	2.31	0.60
1:D:202:ILE:CG2	1:D:213:TYR:HD2	2.14	0.60
1:A:136:ASN:ND2	1:A:136:ASN:C	2.59	0.60
1:B:171:VAL:O	1:B:171:VAL:HG22	2.02	0.60
1:D:213:TYR:CE1	1:D:217:SER:CB	2.84	0.60
1:D:232:THR:O	1:D:233:ASN:HB3	2.01	0.60
1:A:173:ARG:CD	1:B:207:LYS:O	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:HIS:CD2	1:B:248:SER:HB3	2.37	0.60
1:D:171:VAL:HG23	1:D:175:ILE:HD11	1.83	0.60
1:B:55:HIS:HD2	1:B:248:SER:HB3	1.66	0.60
1:C:47:ILE:HG21	1:C:75:TYR:CD2	2.37	0.60
1:C:130:MET:HG2	1:C:180:LEU:HD21	1.83	0.60
1:B:155:ILE:O	1:B:155:ILE:CG2	2.46	0.60
1:A:130:MET:HE3	1:A:178:ASP:O	2.02	0.59
1:B:245:LEU:HD22	1:B:353:LEU:HD11	1.84	0.59
1:A:286:ASP:HA	1:A:289:LYS:HG3	1.84	0.59
1:B:56:ILE:HG12	1:B:353:LEU:HD23	1.83	0.59
1:B:154:ASP:OD1	1:B:155:ILE:HG13	2.02	0.59
1:B:171:VAL:HB	1:B:260:TRP:CD2	2.37	0.59
1:A:231:GLN:O	1:A:232:THR:HB	2.03	0.59
1:D:65:LYS:HE2	1:D:70:PHE:CD1	2.38	0.59
1:D:109:LEU:HB3	1:D:115:LEU:HD23	1.82	0.59
1:A:34:ARG:HD2	1:A:34:ARG:N	2.17	0.59
1:C:331:ASP:OD2	1:C:331:ASP:N	2.30	0.59
1:B:96:SER:O	1:B:99:LYS:HG3	2.02	0.59
1:A:171:VAL:HB	1:A:260:TRP:CE3	2.37	0.59
1:B:235:LYS:CB	1:B:239:ASP:HB3	2.32	0.59
1:D:222:LEU:O	1:D:223:HIS:HB2	2.01	0.59
1:D:213:TYR:CE1	1:D:217:SER:HB2	2.37	0.59
1:A:204:ASN:HB3	1:B:126:PRO:HB2	1.85	0.59
1:C:123:LYS:HG3	1:C:124:HIS:CD2	2.37	0.59
1:B:131:ASN:CB	1:B:136:ASN:HA	2.27	0.59
1:B:161:VAL:O	1:B:161:VAL:HG13	2.03	0.58
1:C:155:ILE:HD11	1:C:157:SER:OG	2.03	0.58
1:B:305:GLU:HA	1:B:305:GLU:OE1	2.02	0.58
1:A:161:VAL:HG13	1:A:162:THR:H	1.69	0.58
1:A:318:ASN:ND2	1:A:321:GLU:HB2	2.17	0.58
1:C:283:ASN:ND2	1:C:344:ASN:HD21	2.00	0.58
1:D:62:LEU:HB2	1:D:271:THR:HG22	1.85	0.58
1:B:262:THR:HA	1:B:266:TYR:HB2	1.85	0.58
1:B:305:GLU:CD	1:B:306:PRO:HD2	2.28	0.58
1:C:65:LYS:CB	1:C:70:PHE:HD2	2.16	0.58
1:C:98:THR:OG1	1:C:267:MET:CB	2.48	0.58
1:B:43:ILE:H	1:B:43:ILE:CD1	2.16	0.58
1:A:232:THR:O	1:A:233:ASN:HB3	2.04	0.58
1:A:323:LEU:HD22	1:A:338:LEU:HD11	1.86	0.58
1:B:120:ASP:OD1	1:B:121:VAL:N	2.37	0.58
1:A:241:ILE:CG2	1:A:252:VAL:HG23	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:VAL:O	1:C:69:VAL:HG23	2.03	0.57
1:B:90:THR:CG2	1:B:240:ALA:HB2	2.34	0.57
1:C:167:ARG:O	1:C:167:ARG:HG3	2.04	0.57
1:D:106:ILE:CD1	1:D:198:LEU:HD22	2.34	0.57
1:A:94:ILE:CD1	1:A:267:MET:HG2	2.34	0.57
1:B:131:ASN:O	1:B:179:GLU:HG3	2.05	0.57
1:D:140:THR:HG23	1:D:143:GLN:CG	2.32	0.57
1:A:130:MET:HG2	1:A:180:LEU:CD2	2.20	0.57
1:D:315:TRP:HZ3	1:D:337:ILE:CG2	2.18	0.57
1:A:90:THR:CG2	1:A:240:ALA:HB2	2.35	0.57
1:A:125:VAL:HG13	1:A:126:PRO:HD2	1.85	0.57
1:A:140:THR:HG23	1:A:143:GLN:CD	2.30	0.57
1:B:169:ASN:HD22	1:B:169:ASN:C	2.12	0.57
1:B:145:LEU:HD22	1:B:313:SER:HB3	1.86	0.56
1:D:130:MET:HE1	1:D:175:ILE:CG2	2.36	0.56
1:D:153:SER:HA	1:D:191:SER:HB2	1.87	0.56
1:D:289:LYS:O	1:D:293:GLN:HG3	2.05	0.56
1:D:171:VAL:CG1	1:D:260:TRP:CB	2.82	0.56
1:D:218:TRP:C	1:D:221:PRO:HD2	2.31	0.56
1:C:257:PHE:HB2	1:C:266:TYR:CZ	2.41	0.56
1:C:262:THR:HA	1:C:266:TYR:HB2	1.87	0.56
1:A:289:LYS:CB	1:A:289:LYS:HZ2	2.18	0.56
1:A:95:ALA:O	1:A:265:ALA:HA	2.06	0.56
1:A:106:ILE:HD12	1:A:198:LEU:HD22	1.87	0.56
1:A:175:ILE:CD1	1:A:197:LEU:HD13	2.36	0.56
1:A:281:GLN:HG2	1:A:339:LEU:CD1	2.36	0.56
1:A:233:ASN:HD21	1:A:254:LYS:CB	2.14	0.56
1:A:356:GLU:C	1:A:359:PRO:HD2	2.25	0.56
1:C:68:LYS:CD	1:C:69:VAL:H	2.18	0.56
1:D:94:ILE:HD11	1:D:267:MET:HG2	1.87	0.55
1:B:234:ASN:C	1:B:234:ASN:ND2	2.55	0.55
1:C:218:TRP:C	1:C:221:PRO:HD2	2.31	0.55
1:C:342:LYS:O	1:C:343:GLN:HB2	2.04	0.55
1:A:171:VAL:HB	1:A:260:TRP:CG	2.41	0.55
1:A:62:LEU:HB3	1:A:348:VAL:HB	1.89	0.55
1:A:257:PHE:HB2	1:A:266:TYR:OH	2.07	0.55
1:A:309:ASN:H	1:A:309:ASN:ND2	2.04	0.55
1:A:262:THR:HA	1:A:266:TYR:HB2	1.87	0.55
1:B:129:LYS:O	1:B:176:MET:HE3	2.06	0.55
1:B:60:SER:CB	1:B:92:TYR:OH	2.54	0.55
1:D:285:PRO:HG2	1:D:288:TYR:HD2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:VAL:O	1:C:69:VAL:HG22	2.05	0.55
1:D:206:THR:HG21	1:D:213:TYR:CB	2.34	0.54
1:C:155:ILE:HG13	1:C:157:SER:N	2.22	0.54
1:A:140:THR:HG23	1:A:143:GLN:CG	2.38	0.54
1:C:151:ILE:CD1	1:C:193:MET:CB	2.85	0.54
1:B:140:THR:HG23	1:B:143:GLN:CG	2.38	0.54
1:C:121:VAL:HG11	1:C:128:PHE:CE2	2.42	0.54
1:C:198:LEU:O	1:C:202:ILE:HG12	2.07	0.54
1:A:295:SER:O	1:A:313:SER:HB2	2.07	0.54
1:A:37:ASN:N	1:A:70:PHE:O	2.36	0.54
1:A:140:THR:HG23	1:A:143:GLN:HG3	1.89	0.54
1:B:78:GLN:NE2	1:B:90:THR:OG1	2.40	0.54
1:B:94:ILE:HG13	1:B:269:THR:CG2	2.37	0.54
1:C:262:THR:N	1:C:263:PRO:CD	2.71	0.54
1:D:220:LYS:N	1:D:221:PRO:CD	2.70	0.54
1:D:137:GLU:OE1	1:D:137:GLU:CA	2.55	0.53
1:B:56:ILE:HA	1:B:353:LEU:CD2	2.39	0.53
1:C:42:GLN:C	1:C:42:GLN:CD	2.76	0.53
1:A:64:VAL:O	1:A:345:TYR:HA	2.09	0.53
1:A:286:ASP:HA	1:A:289:LYS:CG	2.37	0.53
1:B:40:GLN:O	1:B:41:GLN:NE2	2.41	0.53
1:B:94:ILE:CG2	1:B:97:ASN:HB2	2.27	0.53
1:C:203:GLN:HG3	1:C:209:SER:HA	1.90	0.53
1:A:130:MET:HE1	1:A:175:ILE:O	2.08	0.53
1:B:97:ASN:HD22	1:B:335:SER:HB2	1.72	0.53
1:D:67:GLY:N	1:D:344:ASN:OD1	2.41	0.53
1:A:321:GLU:O	1:A:322:HIS:HB2	2.08	0.53
1:C:65:LYS:CG	1:C:369:ILE:CG2	2.82	0.53
1:D:352:ASN:C	1:D:352:ASN:HD22	2.16	0.53
1:B:318:ASN:HD22	1:B:319:ASN:N	2.03	0.53
1:A:289:LYS:O	1:A:293:GLN:HG3	2.09	0.53
1:B:222:LEU:HD13	1:B:224:MET:CE	2.38	0.53
1:B:222:LEU:O	1:B:223:HIS:HB2	2.09	0.53
1:C:65:LYS:CB	1:C:70:PHE:CD2	2.85	0.53
1:C:334:SER:HB3	1:C:354:ASN:HA	1.91	0.53
1:D:83:LYS:O	1:D:83:LYS:CD	2.52	0.53
1:A:65:LYS:HG2	1:A:70:PHE:CD1	2.44	0.53
1:B:94:ILE:HD13	1:B:97:ASN:HB3	1.91	0.52
1:B:98:THR:OG1	1:B:267:MET:HB3	2.09	0.52
1:B:164:LYS:CG	1:B:164:LYS:O	2.58	0.52
1:D:60:SER:HB3	1:D:271:THR:OG1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ARG:HB2	1:D:259:LEU:H	1.74	0.52
1:B:140:THR:HG23	1:B:143:GLN:HG3	1.90	0.52
1:C:274:LEU:O	1:C:275:GLU:C	2.53	0.52
1:D:144:LEU:HB2	1:D:198:LEU:HD21	1.92	0.52
1:A:42:GLN:O	1:A:45:LYS:HG2	2.10	0.52
1:C:101:PHE:CD2	1:C:267:MET:HE1	2.45	0.52
1:C:101:PHE:CD2	1:C:267:MET:CE	2.93	0.52
1:C:297:LYS:O	1:C:297:LYS:CG	2.58	0.52
1:D:230:LYS:HE2	1:D:257:PHE:CD1	2.45	0.52
1:D:62:LEU:HB3	1:D:348:VAL:HB	1.91	0.52
1:C:242:GLY:HA3	1:C:332:ASN:HB2	1.91	0.52
1:D:298:ASN:OD1	1:D:310:ALA:HB3	2.10	0.52
1:B:246:GLN:OE1	1:B:246:GLN:HA	2.09	0.52
1:C:64:VAL:HA	1:C:69:VAL:HA	1.91	0.52
1:C:106:ILE:HG12	1:C:202:ILE:HD11	1.92	0.52
1:D:109:LEU:HB2	1:D:115:LEU:HD21	1.91	0.52
1:A:149:SER:OG	1:A:151:ILE:HD12	2.09	0.52
1:B:309:ASN:H	1:B:309:ASN:ND2	2.05	0.52
1:B:222:LEU:HD12	1:B:224:MET:HE3	1.92	0.52
1:B:237:LYS:N	1:B:237:LYS:HD3	2.22	0.52
1:C:61:ILE:HG13	1:C:349:VAL:HG22	1.91	0.51
1:B:47:ILE:O	1:B:51:LEU:HG	2.09	0.51
1:B:162:THR:HG23	1:B:163:ASN:N	2.22	0.51
1:B:257:PHE:HD2	1:B:266:TYR:CE2	2.28	0.51
1:B:361:LEU:HD12	1:B:361:LEU:O	2.11	0.51
1:C:79:ASP:HB3	1:C:84:VAL:HG12	1.91	0.51
1:C:283:ASN:HD21	1:C:344:ASN:ND2	2.05	0.51
1:A:147:GLN:HE21	1:A:311:TYR:HE2	1.57	0.51
1:B:39:SER:OG	1:B:40:GLN:N	2.42	0.51
1:B:153:SER:HB2	1:B:190:TYR:O	2.10	0.51
1:C:139:ILE:HG21	1:C:144:LEU:CD2	2.40	0.51
1:A:58:GLY:CA	1:A:352:ASN:HD21	2.23	0.51
1:D:109:LEU:CB	1:D:115:LEU:CD2	2.89	0.51
1:B:164:LYS:O	1:B:164:LYS:HG3	2.09	0.51
1:D:230:LYS:HE2	1:D:257:PHE:CE1	2.46	0.51
1:A:160:ALA:O	1:A:161:VAL:HG23	2.10	0.51
1:C:131:ASN:CA	1:C:136:ASN:HA	2.40	0.51
1:A:71:LEU:HD11	1:A:73:LYS:CB	2.41	0.51
1:C:285:PRO:HG2	1:C:288:TYR:HD2	1.76	0.51
1:B:60:SER:HB2	1:B:92:TYR:OH	2.11	0.50
1:C:239:ASP:N	1:C:239:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ALA:HB2	1:C:325:PHE:CZ	2.46	0.50
1:D:162:THR:CG2	1:D:163:ASN:N	2.74	0.50
1:A:196:ASP:HA	1:A:263:PRO:HG2	1.92	0.50
1:C:68:LYS:HD3	1:C:69:VAL:HG13	1.94	0.50
1:C:206:THR:HG22	1:C:208:GLN:HB3	1.93	0.50
1:D:342:LYS:O	1:D:343:GLN:HB2	2.11	0.50
1:A:78:GLN:HG2	1:A:84:VAL:HG13	1.94	0.50
1:A:358:VAL:HB	1:A:359:PRO:HD3	1.93	0.50
1:B:202:ILE:O	1:B:206:THR:HB	2.12	0.50
1:B:206:THR:CG2	1:B:213:TYR:CD1	2.92	0.50
1:C:68:LYS:HD2	1:C:69:VAL:H	1.76	0.50
1:D:154:ASP:OD1	1:D:154:ASP:O	2.30	0.50
1:D:349:VAL:CG1	1:D:358:VAL:HG13	2.42	0.50
1:A:298:ASN:ND2	1:A:317:THR:HG21	2.26	0.50
1:B:209:SER:OG	1:B:212:LYS:HB2	2.11	0.50
1:D:315:TRP:HZ3	1:D:337:ILE:HG21	1.76	0.50
1:C:271:THR:HG23	1:C:350:LEU:HD12	1.94	0.50
1:B:227:THR:HG23	1:B:269:THR:HB	1.94	0.50
1:C:62:LEU:HB3	1:C:348:VAL:HB	1.94	0.50
1:D:344:ASN:OD1	1:D:344:ASN:O	2.30	0.50
1:A:94:ILE:HD11	1:A:267:MET:HG2	1.94	0.50
1:B:334:SER:HB2	1:B:358:VAL:HG21	1.94	0.50
1:C:138:THR:O	1:C:138:THR:HG22	2.12	0.50
1:D:162:THR:HG23	1:D:163:ASN:N	2.27	0.50
1:A:125:VAL:HG12	1:A:128:PHE:HB2	1.91	0.49
1:A:167:ARG:O	1:A:259:LEU:HB2	2.12	0.49
1:A:206:THR:HG22	1:A:208:GLN:CG	2.36	0.49
1:B:298:ASN:N	1:B:298:ASN:HD22	2.10	0.49
1:C:154:ASP:OD1	1:C:154:ASP:O	2.30	0.49
1:B:128:PHE:HD1	1:B:172:THR:HG23	1.76	0.49
1:B:307:ASN:O	1:B:307:ASN:ND2	2.30	0.49
1:C:95:ALA:HB2	1:C:330:LEU:HG	1.94	0.49
1:B:125:VAL:CG1	1:B:126:PRO:HD2	2.28	0.49
1:D:95:ALA:HB2	1:D:330:LEU:HG	1.94	0.49
1:B:68:LYS:CB	1:B:68:LYS:HZ2	2.08	0.49
1:C:267:MET:HG3	1:C:268:MET:N	2.27	0.49
1:B:97:ASN:ND2	1:B:335:SER:CB	2.75	0.49
1:B:356:GLU:C	1:B:359:PRO:HD2	2.34	0.49
1:B:171:VAL:O	1:B:171:VAL:HG23	2.12	0.49
1:B:281:GLN:HG2	1:B:339:LEU:HD13	1.95	0.49
1:D:128:PHE:CZ	1:D:130:MET:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ASN:O	1:D:198:LEU:HG	2.12	0.49
1:D:213:TYR:CD1	1:D:217:SER:HB2	2.48	0.49
1:C:149:SER:OG	1:C:194:ASN:ND2	2.42	0.49
1:D:359:PRO:O	1:D:362:VAL:HG22	2.12	0.49
1:B:226:HIS:HD2	1:B:273:ASP:OD1	1.95	0.48
1:C:139:ILE:CG2	1:C:144:LEU:CD2	2.91	0.48
1:C:155:ILE:HG13	1:C:157:SER:H	1.77	0.48
1:B:55:HIS:CD2	1:B:248:SER:CB	2.96	0.48
1:B:156:THR:CG2	1:B:178:ASP:OD2	2.61	0.48
1:C:131:ASN:CB	1:C:136:ASN:HA	2.43	0.48
1:A:203:GLN:HG3	1:A:209:SER:HA	1.94	0.48
1:B:43:ILE:N	1:B:43:ILE:CD1	2.74	0.48
1:B:235:LYS:HB3	1:B:239:ASP:HB3	1.95	0.48
1:B:62:LEU:HB3	1:B:348:VAL:HB	1.95	0.48
1:B:342:LYS:O	1:B:343:GLN:CB	2.55	0.48
1:D:149:SER:HB2	1:D:151:ILE:HG22	1.94	0.48
1:D:233:ASN:O	1:D:233:ASN:CG	2.56	0.48
1:B:153:SER:CB	1:B:190:TYR:O	2.62	0.48
1:C:155:ILE:HG22	1:C:193:MET:HE2	1.95	0.48
1:A:173:ARG:HD2	1:B:207:LYS:O	2.13	0.48
1:B:171:VAL:HB	1:B:260:TRP:CE3	2.49	0.48
1:A:196:ASP:HA	1:A:263:PRO:CG	2.43	0.48
1:B:94:ILE:HD13	1:B:97:ASN:CB	2.44	0.48
1:B:287:LYS:HG3	1:B:288:TYR:CD2	2.49	0.48
1:C:169:ASN:C	1:C:169:ASN:ND2	2.54	0.48
1:C:322:HIS:O	1:C:340:ASN:ND2	2.46	0.48
1:D:222:LEU:O	1:D:223:HIS:CB	2.60	0.48
1:B:48:GLU:O	1:B:52:GLN:HG3	2.13	0.48
1:D:262:THR:HG23	1:D:263:PRO:HD3	1.96	0.48
1:B:69:VAL:O	1:B:69:VAL:HG22	2.12	0.48
1:C:72:ASN:ND2	1:C:275:GLU:OE2	2.47	0.48
1:C:222:LEU:O	1:C:223:HIS:HB2	2.14	0.48
1:A:162:THR:HB	1:A:164:LYS:O	2.13	0.47
1:A:261:ASP:C	1:A:263:PRO:HD2	2.40	0.47
1:B:342:LYS:HD2	1:B:342:LYS:HA	1.67	0.47
1:A:205:VAL:CG2	1:B:127:HIS:NE2	2.75	0.47
1:A:209:SER:H	1:B:164:LYS:NZ	2.12	0.47
1:A:232:THR:HG22	1:A:234:ASN:H	1.77	0.47
1:A:281:GLN:HG2	1:A:339:LEU:HD13	1.95	0.47
1:D:109:LEU:HB2	1:D:115:LEU:CD2	2.44	0.47
1:A:359:PRO:O	1:A:362:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ILE:CG2	1:D:213:TYR:CD2	2.96	0.47
1:A:311:TYR:CD1	1:A:315:TRP:O	2.67	0.47
1:B:301:SER:HA	1:B:310:ALA:HA	1.97	0.47
1:D:287:LYS:CE	1:D:288:TYR:CE2	2.96	0.47
1:B:125:VAL:CG1	1:B:128:PHE:H	2.27	0.47
1:D:56:ILE:HD11	1:D:355:SER:HB3	1.96	0.47
1:A:127:HIS:O	1:B:207:LYS:CE	2.55	0.47
1:B:92:TYR:N	1:B:92:TYR:CD1	2.82	0.47
1:C:79:ASP:HB3	1:C:84:VAL:CG1	2.45	0.47
1:C:130:MET:HE1	1:C:175:ILE:HG22	1.96	0.47
1:D:262:THR:N	1:D:263:PRO:HD2	2.29	0.47
1:D:298:ASN:HA	1:D:312:ALA:HB2	1.96	0.47
1:B:94:ILE:HG22	1:B:95:ALA:N	2.29	0.47
1:D:63:ILE:HD11	1:D:365:LEU:HD22	1.96	0.47
1:A:287:LYS:HB2	1:A:287:LYS:HE2	1.64	0.47
1:D:115:LEU:CD1	1:D:141:ILE:HD13	2.45	0.47
1:C:42:GLN:HB2	1:C:45:LYS:HD3	1.97	0.46
1:A:169:ASN:O	1:A:171:VAL:N	2.47	0.46
1:B:48:GLU:OE1	1:B:75:TYR:CD2	2.68	0.46
1:B:134:GLY:HA3	1:C:344:ASN:HB2	1.96	0.46
1:B:262:THR:HG22	1:B:266:TYR:HB2	1.97	0.46
1:C:42:GLN:H	1:C:42:GLN:NE2	2.13	0.46
1:C:243:TYR:CE1	1:C:252:VAL:HG12	2.50	0.46
1:D:265:ALA:O	1:D:266:TYR:HB2	2.15	0.46
1:D:287:LYS:HB2	1:D:287:LYS:HE3	1.47	0.46
1:B:162:THR:HG23	1:B:163:ASN:HB3	1.95	0.46
1:D:72:ASN:ND2	1:D:275:GLU:OE2	2.48	0.46
1:C:65:LYS:CD	1:C:70:PHE:HE2	2.25	0.46
1:D:171:VAL:HG12	1:D:260:TRP:HB3	1.97	0.46
1:A:147:GLN:HG3	1:A:311:TYR:CD2	2.50	0.46
1:B:226:HIS:HB2	1:B:273:ASP:OD2	2.15	0.46
1:D:41:GLN:NE2	1:D:41:GLN:HA	2.29	0.46
1:D:96:SER:O	1:D:99:LYS:HG3	2.15	0.46
1:C:41:GLN:H	1:C:41:GLN:HE21	1.64	0.46
1:C:42:GLN:OE1	1:C:43:ILE:N	2.49	0.46
1:D:109:LEU:CB	1:D:115:LEU:HD23	2.44	0.46
1:D:315:TRP:CZ3	1:D:337:ILE:HG21	2.50	0.46
1:A:368:GLN:C	1:A:369:ILE:HG13	2.41	0.46
1:D:62:LEU:CD1	1:D:69:VAL:HG12	2.46	0.46
1:D:91:LYS:HG2	1:D:270:SER:HB3	1.97	0.46
1:A:336:PHE:CD1	1:A:362:VAL:HG11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ALA:HB1	1:C:300:SER:HB3	1.99	0.46
1:D:109:LEU:HB3	1:D:115:LEU:CD2	2.44	0.46
1:A:155:ILE:O	1:A:155:ILE:HG23	2.16	0.45
1:A:236:SER:OG	1:A:237:LYS:N	2.49	0.45
1:B:188:PHE:CD1	1:B:188:PHE:C	2.94	0.45
1:B:42:GLN:H	1:B:42:GLN:CD	2.24	0.45
1:C:60:SER:HA	1:C:74:GLY:HA2	1.98	0.45
1:C:99:LYS:HE2	1:C:195:TYR:CB	2.46	0.45
1:C:171:VAL:CG2	1:C:175:ILE:CG1	2.83	0.45
1:A:120:ASP:HB3	1:A:138:THR:HG23	1.98	0.45
1:D:231:GLN:HE21	1:D:231:GLN:HB3	1.62	0.45
1:A:166:ASN:O	1:A:260:TRP:CZ3	2.70	0.45
1:A:241:ILE:CG2	1:A:252:VAL:CG2	2.94	0.45
1:A:340:ASN:ND2	1:A:342:LYS:O	2.49	0.45
1:C:68:LYS:CD	1:C:69:VAL:HG13	2.47	0.45
1:C:131:ASN:HB3	1:C:136:ASN:CA	2.46	0.45
1:D:167:ARG:HD2	1:D:258:ASN:HA	1.97	0.45
1:D:220:LYS:HB2	1:D:221:PRO:HD3	1.97	0.45
1:B:60:SER:C	1:B:61:ILE:HD12	2.41	0.45
1:B:309:ASN:ND2	1:B:317:THR:O	2.50	0.45
1:C:308:ALA:HB2	1:C:325:PHE:HZ	1.81	0.45
1:B:54:GLY:O	1:B:55:HIS:HB2	2.17	0.45
1:C:42:GLN:C	1:C:42:GLN:OE1	2.60	0.45
1:C:123:LYS:HB2	1:C:123:LYS:HE3	1.68	0.45
1:D:206:THR:CG2	1:D:208:GLN:CG	2.89	0.45
1:B:56:ILE:HA	1:B:353:LEU:HD23	1.98	0.45
1:D:45:LYS:HB2	1:D:45:LYS:HE3	1.69	0.45
1:B:215:THR:HA	1:B:219:LEU:HB2	1.98	0.45
1:C:330:LEU:O	1:C:331:ASP:C	2.60	0.45
1:B:194:ASN:O	1:B:198:LEU:HG	2.18	0.44
1:C:168:LEU:HD13	1:C:168:LEU:HA	1.63	0.44
1:B:98:THR:O	1:B:98:THR:HG22	2.17	0.44
1:C:130:MET:CE	1:C:175:ILE:HG22	2.47	0.44
1:D:337:ILE:HD12	1:D:348:VAL:HG13	1.99	0.44
1:A:50:ASP:OD2	1:A:364:HIS:HD2	2.00	0.44
1:A:175:ILE:HD12	1:A:197:LEU:HD13	1.99	0.44
1:B:125:VAL:CG1	1:B:126:PRO:CD	2.90	0.44
1:C:57:PRO:HB2	1:C:352:ASN:OD1	2.18	0.44
1:D:137:GLU:OE1	1:D:138:THR:N	2.50	0.44
1:A:258:ASN:HD22	1:A:258:ASN:N	2.14	0.44
1:C:99:LYS:HE2	1:C:195:TYR:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASP:O	1:A:48:GLU:HB2	2.18	0.44
1:A:325:PHE:HB3	1:A:338:LEU:HD12	1.99	0.44
1:D:283:ASN:ND2	1:D:344:ASN:HD21	2.16	0.44
1:A:204:ASN:OD1	1:B:126:PRO:HB3	2.17	0.44
1:D:80:VAL:HG12	1:D:81:ASP:N	2.33	0.44
1:C:302:THR:O	1:C:302:THR:HG22	2.18	0.43
1:D:166:ASN:HD22	1:D:166:ASN:HA	1.63	0.43
1:A:241:ILE:HG21	1:A:252:VAL:HG23	1.99	0.43
1:B:274:LEU:O	1:B:278:ILE:HG12	2.18	0.43
1:C:325:PHE:HB3	1:C:338:LEU:HD12	1.99	0.43
1:A:131:ASN:HB3	1:A:136:ASN:CA	2.48	0.43
1:A:222:LEU:O	1:A:223:HIS:CB	2.65	0.43
1:A:281:GLN:HG2	1:A:339:LEU:HD11	2.00	0.43
1:B:57:PRO:HD3	1:B:353:LEU:HD22	2.00	0.43
1:C:305:GLU:HG3	1:C:306:PRO:CD	2.41	0.43
1:A:267:MET:HE2	1:A:267:MET:HB2	1.80	0.43
1:C:167:ARG:HB3	3:C:402:HOH:O	2.18	0.43
1:C:236:SER:O	1:C:237:LYS:HB2	2.18	0.43
1:D:192:ASN:O	1:D:264:SER:OG	2.37	0.43
1:D:267:MET:HB2	1:D:267:MET:HE2	1.65	0.43
1:D:283:ASN:HD21	1:D:344:ASN:HD21	1.66	0.43
1:B:214:ILE:HG22	1:B:219:LEU:HG	2.00	0.43
1:B:318:ASN:ND2	1:B:320:ASP:N	2.66	0.43
1:B:358:VAL:HB	1:B:359:PRO:HD3	2.01	0.43
1:D:234:ASN:OD1	1:D:235:LYS:N	2.52	0.43
1:C:98:THR:HG1	1:C:267:MET:HB3	1.75	0.43
1:C:298:ASN:OD1	1:C:310:ALA:HB3	2.18	0.43
1:D:206:THR:HG22	1:D:208:GLN:CG	2.38	0.43
1:D:262:THR:N	1:D:263:PRO:CD	2.81	0.43
1:A:196:ASP:OD1	1:A:263:PRO:HG2	2.18	0.43
1:A:336:PHE:CE1	1:A:362:VAL:HG21	2.53	0.43
1:B:169:ASN:O	1:B:169:ASN:ND2	2.30	0.43
1:D:106:ILE:HD12	1:D:198:LEU:HD22	1.99	0.43
1:D:115:LEU:HD12	1:D:141:ILE:CD1	2.49	0.43
1:A:58:GLY:N	1:A:352:ASN:HD21	2.17	0.43
1:A:68:LYS:HD2	1:A:68:LYS:HA	1.85	0.43
1:B:144:LEU:HB2	1:B:198:LEU:HD21	2.01	0.43
1:A:71:LEU:HD11	1:A:73:LYS:HB3	2.00	0.42
1:A:342:LYS:O	1:A:343:GLN:HB2	2.19	0.42
1:B:309:ASN:ND2	1:B:318:ASN:HA	2.34	0.42
1:C:121:VAL:CG1	1:C:122:SER:N	2.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:VAL:O	1:C:252:VAL:HG23	2.19	0.42
1:A:262:THR:N	1:A:263:PRO:CD	2.81	0.42
1:B:71:LEU:HD11	1:B:73:LYS:HB2	2.00	0.42
1:C:131:ASN:OD1	1:C:131:ASN:N	2.52	0.42
1:D:153:SER:HA	1:D:191:SER:CB	2.48	0.42
1:A:71:LEU:HD11	1:A:73:LYS:HB2	2.00	0.42
1:B:62:LEU:HB2	1:B:271:THR:CG2	2.45	0.42
1:B:77:TYR:HB2	1:B:80:VAL:HG12	2.01	0.42
1:A:257:PHE:HB2	1:A:266:TYR:CZ	2.55	0.42
1:B:220:LYS:HB2	1:B:221:PRO:CD	2.47	0.42
1:B:254:LYS:HG3	1:B:254:LYS:O	2.19	0.42
1:D:164:LYS:HD3	1:D:164:LYS:HA	1.74	0.42
1:D:227:THR:HG23	1:D:269:THR:HB	2.02	0.42
1:D:230:LYS:HB3	1:D:266:TYR:HB3	2.01	0.42
1:A:156:THR:HG21	1:A:178:ASP:OD2	2.19	0.42
1:B:140:THR:CG2	1:B:143:GLN:CD	2.89	0.42
1:B:219:LEU:O	1:B:224:MET:N	2.51	0.42
1:C:166:ASN:O	1:C:167:ARG:HB3	2.20	0.42
1:D:98:THR:HG23	1:D:267:MET:HE3	2.00	0.42
1:D:78:GLN:HG3	1:D:240:ALA:HA	2.00	0.42
1:A:149:SER:OG	1:A:194:ASN:ND2	2.50	0.42
1:B:92:TYR:HB3	1:B:333:PHE:CD2	2.53	0.42
1:B:196:ASP:HA	1:B:263:PRO:HG2	2.01	0.42
1:C:106:ILE:HD13	1:C:202:ILE:HD13	2.01	0.42
1:C:109:LEU:CB	1:C:115:LEU:HD21	2.49	0.42
1:D:169:ASN:HB2	3:D:504:HOH:O	2.20	0.42
1:A:209:SER:H	1:B:164:LYS:HZ1	1.67	0.42
1:B:94:ILE:HG23	1:B:97:ASN:CB	2.29	0.42
1:D:53:LYS:HD3	1:D:357:TYR:CE1	2.55	0.42
1:A:188:PHE:CD1	1:A:188:PHE:C	2.97	0.42
1:B:56:ILE:HA	1:B:353:LEU:HD22	2.02	0.42
1:B:95:ALA:HB2	1:B:330:LEU:HD12	2.02	0.42
1:B:281:GLN:HG2	1:B:339:LEU:CD1	2.50	0.42
1:C:109:LEU:HB2	1:C:115:LEU:HD21	2.02	0.42
1:D:121:VAL:HG23	1:D:139:ILE:O	2.19	0.42
1:D:124:HIS:ND1	1:D:205:VAL:CG2	2.83	0.42
1:C:192:ASN:HD22	1:C:192:ASN:HA	1.72	0.42
1:C:196:ASP:OD1	1:C:264:SER:OG	2.38	0.42
1:A:58:GLY:O	1:A:352:ASN:ND2	2.53	0.41
1:B:219:LEU:HD13	1:B:227:THR:HB	2.02	0.41
1:D:133:ASN:HB3	1:D:134:GLY:H	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:LEU:HD12	1:D:313:SER:H	1.85	0.41
1:A:64:VAL:O	1:A:346:GLY:N	2.45	0.41
1:B:47:ILE:HG21	1:B:75:TYR:CE1	2.55	0.41
1:C:101:PHE:CD2	1:C:267:MET:HE3	2.55	0.41
1:D:131:ASN:O	1:D:179:GLU:HG3	2.20	0.41
1:A:285:PRO:HG2	1:A:288:TYR:CD2	2.44	0.41
1:A:289:LYS:HZ2	1:A:289:LYS:HB2	1.86	0.41
1:B:125:VAL:CG1	1:B:126:PRO:N	2.79	0.41
1:A:87:SER:HB2	1:A:88:PRO:CD	2.51	0.41
1:A:133:ASN:HD22	1:A:133:ASN:HA	1.56	0.41
1:A:154:ASP:OD1	1:A:154:ASP:O	2.38	0.41
1:A:257:PHE:C	1:A:258:ASN:HD22	2.27	0.41
1:A:303:ILE:O	1:A:303:ILE:HG13	2.21	0.41
1:B:151:ILE:HA	1:B:152:PRO:HD3	1.77	0.41
1:B:235:LYS:CB	1:B:239:ASP:HB2	2.31	0.41
1:A:131:ASN:HA	1:A:136:ASN:HA	2.03	0.41
1:B:287:LYS:HE3	1:D:112:GLU:OE2	2.20	0.41
1:C:44:ASP:OD2	1:C:73:LYS:HE2	2.20	0.41
1:C:223:HIS:O	1:C:225:THR:HG22	2.20	0.41
1:D:96:SER:C	1:D:98:THR:N	2.78	0.41
1:A:166:ASN:ND2	1:A:170:ASP:O	2.53	0.41
1:A:286:ASP:OD2	1:A:286:ASP:N	2.32	0.41
1:A:121:VAL:HG21	1:A:144:LEU:HD11	2.03	0.41
1:B:47:ILE:HD11	1:B:365:LEU:HD21	2.02	0.41
1:C:206:THR:HG22	1:C:208:GLN:CB	2.50	0.41
1:D:298:ASN:ND2	1:D:298:ASN:H	2.18	0.41
1:B:78:GLN:HB3	1:B:86:ALA:HA	2.03	0.41
1:A:94:ILE:HD11	1:A:267:MET:CG	2.51	0.41
1:B:296:HIS:CD2	1:B:324:VAL:HG11	2.56	0.41
1:C:53:LYS:HB3	1:C:357:TYR:CE2	2.56	0.41
1:D:235:LYS:HD3	1:D:240:ALA:O	2.21	0.41
1:D:342:LYS:O	1:D:343:GLN:CB	2.68	0.41
1:B:318:ASN:HB3	1:B:323:LEU:HD13	2.02	0.40
1:D:151:ILE:HA	1:D:152:PRO:HD3	1.87	0.40
1:D:253:SER:HB3	1:D:332:ASN:HB3	2.03	0.40
1:A:107:LEU:HD22	1:A:294:GLN:CD	2.46	0.40
1:A:142:LYS:HB2	1:A:142:LYS:HE3	1.93	0.40
1:A:204:ASN:C	1:B:127:HIS:HD2	2.29	0.40
1:B:60:SER:HB2	1:B:92:TYR:CE1	2.57	0.40
1:B:326:HIS:HD2	1:B:327:SER:O	2.04	0.40
1:C:287:LYS:HE2	1:C:287:LYS:HB2	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ILE:HG22	1:D:252:VAL:HG22	1.98	0.40
1:A:108:LYS:NZ	1:A:112:GLU:OE2	2.55	0.40
1:A:205:VAL:CA	1:B:127:HIS:CD2	2.99	0.40
1:A:342:LYS:O	1:A:343:GLN:CB	2.70	0.40
1:B:163:ASN:CG	1:B:164:LYS:N	2.73	0.40
1:B:235:LYS:HB3	1:B:235:LYS:HE3	1.85	0.40
1:B:289:LYS:HB2	1:B:289:LYS:HE3	1.63	0.40
1:C:126:PRO:HG2	1:C:127:HIS:H	1.86	0.40
1:C:224:MET:HG2	1:C:273:ASP:HB3	2.04	0.40
1:D:198:LEU:O	1:D:202:ILE:HG13	2.20	0.40
1:A:34:ARG:N	1:A:34:ARG:CD	2.85	0.40
1:D:94:ILE:HG12	1:D:267:MET:HG2	2.02	0.40
1:A:171:VAL:HG23	1:A:174:ALA:HB3	2.02	0.40
1:A:173:ARG:HG2	1:B:207:LYS:O	2.21	0.40
1:D:57:PRO:HD2	1:D:352:ASN:ND2	2.37	0.40
1:D:215:THR:O	1:D:220:LYS:CG	2.70	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	334/342 (98%)	320 (96%)	12 (4%)	2 (1%)	21	56
1	B	334/342 (98%)	321 (96%)	12 (4%)	1 (0%)	36	68
1	C	325/342 (95%)	315 (97%)	10 (3%)	0	100	100
1	D	329/342 (96%)	320 (97%)	9 (3%)	0	100	100
All	All	1322/1368 (97%)	1276 (96%)	43 (3%)	3 (0%)	43	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ILE
1	B	66	ASN
1	A	169	ASN

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	301/309 (97%)	249 (83%)	52 (17%)	2	10
1	B	297/309 (96%)	241 (81%)	56 (19%)	1	9
1	C	294/309 (95%)	250 (85%)	44 (15%)	3	15
1	D	295/309 (96%)	249 (84%)	46 (16%)	2	13
All	All	1187/1236 (96%)	989 (83%)	198 (17%)	2	11

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	41	GLN
1	A	48	GLU
1	A	51	LEU
1	A	66	ASN
1	A	69	VAL
1	A	70	PHE
1	A	71	LEU
1	A	82	LYS
1	A	106	ILE
1	A	116	ASN
1	A	129	LYS
1	A	131	ASN
1	A	133	ASN
1	A	136	ASN
1	A	140	THR
1	A	153	SER
1	A	154	ASP
1	A	155	ILE

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Mol	Chain	Res	Type
1	A	156	THR
1	A	158	GLU
1	A	161	VAL
1	A	162	THR
1	A	164	LYS
1	A	166	ASN
1	A	169	ASN
1	A	171	VAL
1	A	176	MET
1	A	178	ASP
1	A	187	GLU
1	A	197	LEU
1	A	231	GLN
1	A	234	ASN
1	A	235	LYS
1	A	236	SER
1	A	237	LYS
1	A	238	HIS
1	A	245	LEU
1	A	252	VAL
1	A	254	LYS
1	A	264	SER
1	A	267	MET
1	A	286	ASP
1	A	287	LYS
1	A	289	LYS
1	A	298	ASN
1	A	307	ASN
1	A	309	ASN
1	A	317	THR
1	A	340	ASN
1	A	343	GLN
1	A	344	ASN
1	B	34	ARG
1	B	35	LEU
1	B	43	ILE
1	B	45	LYS
1	B	48	GLU
1	B	68	LYS
1	B	69	VAL
1	B	73	LYS
1	B	82	LYS

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Mol	Chain	Res	Type
1	B	91	LYS
1	B	92	TYR
1	B	94	ILE
1	B	96	SER
1	B	99	LYS
1	B	106	ILE
1	B	116	ASN
1	B	121	VAL
1	B	122	SER
1	B	125	VAL
1	B	135	GLN
1	B	136	ASN
1	B	138	THR
1	B	140	THR
1	B	154	ASP
1	B	155	ILE
1	B	162	THR
1	B	165	ASN
1	B	167	ARG
1	B	168	LEU
1	B	169	ASN
1	B	171	VAL
1	B	173	ARG
1	B	212	LYS
1	B	225	THR
1	B	231	GLN
1	B	233	ASN
1	B	234	ASN
1	B	235	LYS
1	B	237	LYS
1	B	245	LEU
1	B	254	LYS
1	B	267	MET
1	B	271	THR
1	B	289	LYS
1	B	302	THR
1	B	307	ASN
1	B	309	ASN
1	B	313	SER
1	B	317	THR
1	B	318	ASN
1	B	321	GLU

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Mol	Chain	Res	Type
1	B	323	LEU
1	B	342	LYS
1	B	343	GLN
1	B	362	VAL
1	B	367	THR
1	C	34	ARG
1	C	39	SER
1	C	41	GLN
1	C	42	GLN
1	C	43	ILE
1	C	66	ASN
1	C	68	LYS
1	C	69	VAL
1	C	94	ILE
1	C	98	THR
1	C	108	LYS
1	C	115	LEU
1	C	121	VAL
1	C	125	VAL
1	C	136	ASN
1	C	137	GLU
1	C	138	THR
1	C	151	ILE
1	C	155	ILE
1	C	157	SER
1	C	167	ARG
1	C	168	LEU
1	C	169	ASN
1	C	171	VAL
1	C	173	ARG
1	C	182	HIS
1	C	200	LEU
1	C	225	THR
1	C	231	GLN
1	C	232	THR
1	C	239	ASP
1	C	254	LYS
1	C	267	MET
1	C	274	LEU
1	C	286	ASP
1	C	287	LYS
1	C	297	LYS

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Mol	Chain	Res	Type
1	C	298	ASN
1	C	302	THR
1	C	317	THR
1	C	331	ASP
1	C	343	GLN
1	C	344	ASN
1	C	352	ASN
1	D	36	THR
1	D	39	SER
1	D	41	GLN
1	D	43	ILE
1	D	44	ASP
1	D	68	LYS
1	D	69	VAL
1	D	80	VAL
1	D	116	ASN
1	D	122	SER
1	D	125	VAL
1	D	131	ASN
1	D	136	ASN
1	D	137	GLU
1	D	140	THR
1	D	149	SER
1	D	151	ILE
1	D	163	ASN
1	D	167	ARG
1	D	171	VAL
1	D	172	THR
1	D	175	ILE
1	D	178	ASP
1	D	200	LEU
1	D	206	THR
1	D	207	LYS
1	D	211	THR
1	D	220	LYS
1	D	225	THR
1	D	228	SER
1	D	231	GLN
1	D	232	THR
1	D	234	ASN
1	D	237	LYS
1	D	252	VAL

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Mol	Chain	Res	Type
1	D	267	MET
1	D	271	THR
1	D	287	LYS
1	D	295	SER
1	D	317	THR
1	D	337	ILE
1	D	342	LYS
1	D	343	GLN
1	D	352	ASN
1	D	362	VAL
1	D	369	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	66	ASN
1	A	97	ASN
1	A	118	ASN
1	A	124	HIS
1	A	133	ASN
1	A	136	ASN
1	A	192	ASN
1	A	194	ASN
1	A	208	GLN
1	A	216	ASN
1	A	226	HIS
1	A	258	ASN
1	A	283	ASN
1	A	294	GLN
1	A	298	ASN
1	A	309	ASN
1	A	319	ASN
1	A	322	HIS
1	A	326	HIS
1	A	340	ASN
1	A	352	ASN
1	A	354	ASN
1	A	364	HIS
1	A	366	ASN
1	A	368	GLN
1	B	66	ASN

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Mol	Chain	Res	Type
1	B	78	GLN
1	B	97	ASN
1	B	111	GLN
1	B	127	HIS
1	B	131	ASN
1	B	165	ASN
1	B	192	ASN
1	B	204	ASN
1	B	226	HIS
1	B	231	GLN
1	B	234	ASN
1	B	238	HIS
1	B	281	GLN
1	B	294	GLN
1	B	298	ASN
1	B	309	ASN
1	B	318	ASN
1	B	319	ASN
1	B	326	HIS
1	B	340	ASN
1	B	344	ASN
1	B	366	ASN
1	B	368	GLN
1	C	41	GLN
1	C	66	ASN
1	C	78	GLN
1	C	97	ASN
1	C	111	GLN
1	C	166	ASN
1	C	169	ASN
1	C	182	HIS
1	C	192	ASN
1	C	194	ASN
1	C	204	ASN
1	C	231	GLN
1	C	233	ASN
1	C	258	ASN
1	C	276	HIS
1	C	283	ASN
1	C	293	GLN
1	C	296	HIS
1	C	318	ASN

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Mol	Chain	Res	Type
1	C	340	ASN
1	C	368	GLN
1	D	49	HIS
1	D	97	ASN
1	D	116	ASN
1	D	127	HIS
1	D	163	ASN
1	D	166	ASN
1	D	169	ASN
1	D	181	HIS
1	D	182	HIS
1	D	204	ASN
1	D	223	HIS
1	D	231	GLN
1	D	246	GLN
1	D	258	ASN
1	D	283	ASN
1	D	307	ASN
1	D	309	ASN
1	D	319	ASN
1	D	322	HIS
1	D	340	ASN
1	D	352	ASN
1	D	364	HIS
1	D	366	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PE4	D	401	-	23,23,23	0.66	0	22,22,22	0.31	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
2	PE4	D	401	-	-	14/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

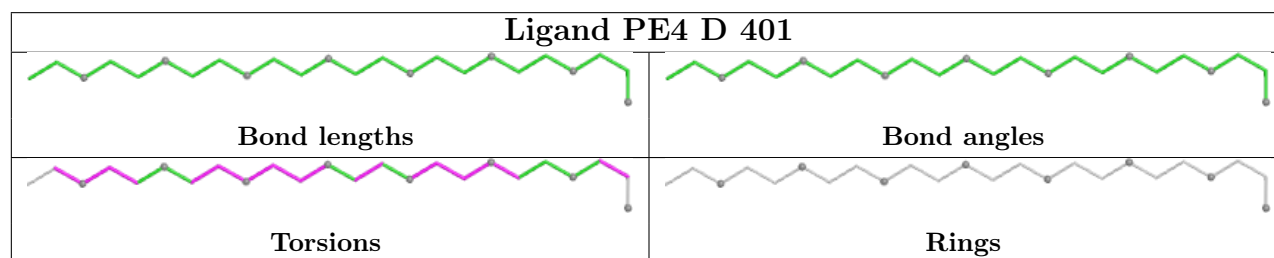
All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	PE4	O7-C13-C14-O8
2	D	401	PE4	O1-C1-C2-O2
2	D	401	PE4	O6-C10-C9-O5
2	D	401	PE4	O3-C5-C6-O4
2	D	401	PE4	O4-C7-C8-O5
2	D	401	PE4	C5-C6-O4-C7
2	D	401	PE4	C3-C4-O3-C5
2	D	401	PE4	O6-C11-C12-O7
2	D	401	PE4	C12-C11-O6-C10
2	D	401	PE4	C10-C9-O5-C8
2	D	401	PE4	C9-C10-O6-C11
2	D	401	PE4	C6-C5-O3-C4
2	D	401	PE4	C16-C15-O8-C14
2	D	401	PE4	C13-C14-O8-C15

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	336/342 (98%)	0.76	41 (12%) 8 6	29, 47, 79, 98	0
1	B	336/342 (98%)	1.13	57 (16%) 4 3	31, 55, 86, 100	0
1	C	329/342 (96%)	1.01	48 (14%) 6 4	37, 60, 99, 116	0
1	D	333/342 (97%)	1.01	46 (13%) 6 5	36, 54, 93, 104	0
All	All	1334/1368 (97%)	0.98	192 (14%) 6 5	29, 53, 91, 116	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	ASN	8.4
1	B	162	THR	7.4
1	A	161	VAL	7.1
1	A	162	THR	6.7
1	D	39	SER	6.5
1	A	159	ASP	6.3
1	B	161	VAL	5.8
1	A	156	THR	5.8
1	C	168	LEU	5.6
1	A	160	ALA	5.5
1	A	158	GLU	5.4
1	A	232	THR	5.4
1	B	233	ASN	5.3
1	D	40	GLN	5.3
1	C	40	GLN	5.2
1	D	232	THR	4.9
1	D	162	THR	4.9
1	D	165	ASN	4.7
1	B	160	ALA	4.7
1	C	169	ASN	4.6
1	C	172	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	37	ASN	4.4
1	D	163	ASN	4.4
1	A	40	GLN	4.3
1	B	232	THR	4.3
1	A	164	LYS	4.3
1	B	157	SER	4.3
1	D	178	ASP	4.3
1	B	158	GLU	4.2
1	D	155	ILE	4.1
1	D	159	ASP	4.1
1	B	126	PRO	4.1
1	A	157	SER	4.0
1	D	120	ASP	4.0
1	D	126	PRO	4.0
1	B	155	ILE	4.0
1	B	35	LEU	4.0
1	C	154	ASP	4.0
1	B	168	LEU	4.0
1	B	163	ASN	3.9
1	C	166	ASN	3.9
1	C	35	LEU	3.9
1	A	120	ASP	3.9
1	C	126	PRO	3.8
1	B	159	ASP	3.8
1	C	37	ASN	3.8
1	D	176	MET	3.8
1	D	168	LEU	3.8
1	D	134	GLY	3.7
1	B	171	VAL	3.7
1	B	169	ASN	3.6
1	D	41	GLN	3.6
1	B	166	ASN	3.6
1	B	153	SER	3.6
1	B	69	VAL	3.5
1	C	127	HIS	3.5
1	D	233	ASN	3.4
1	B	156	THR	3.4
1	D	166	ASN	3.3
1	C	156	THR	3.3
1	C	157	SER	3.3
1	C	176	MET	3.3
1	A	306	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	186	GLU	3.3
1	C	155	ILE	3.3
1	C	39	SER	3.3
1	B	34	ARG	3.3
1	D	131	ASN	3.3
1	C	332	ASN	3.2
1	C	94	ILE	3.2
1	A	168	LEU	3.1
1	D	186	GLU	3.1
1	B	46	ILE	3.1
1	A	35	LEU	3.0
1	B	154	ASP	3.0
1	D	170	ASP	3.0
1	A	37	ASN	3.0
1	A	131	ASN	3.0
1	D	164	LYS	3.0
1	D	161	VAL	3.0
1	D	228	SER	3.0
1	C	187	GLU	2.9
1	D	369	ILE	2.9
1	B	40	GLN	2.9
1	C	41	GLN	2.9
1	A	169	ASN	2.9
1	B	68	LYS	2.9
1	A	126	PRO	2.8
1	C	33	THR	2.8
1	C	38	ASP	2.8
1	B	37	ASN	2.8
1	D	127	HIS	2.8
1	B	248	SER	2.8
1	C	36	THR	2.8
1	A	66	ASN	2.7
1	A	163	ASN	2.7
1	B	307	ASN	2.7
1	C	307	ASN	2.7
1	B	38	ASP	2.7
1	C	83	LYS	2.7
1	A	39	SER	2.7
1	B	44	ASP	2.7
1	B	320	ASP	2.7
1	B	41	GLN	2.7
1	C	177	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	38	ASP	2.7
1	A	369	ILE	2.7
1	A	155	ILE	2.6
1	C	135	GLN	2.6
1	C	256	GLU	2.6
1	C	236	SER	2.6
1	C	136	ASN	2.6
1	A	233	ASN	2.6
1	C	128	PHE	2.6
1	C	193	MET	2.6
1	C	239	ASP	2.6
1	D	231	GLN	2.6
1	D	194	ASN	2.6
1	B	49	HIS	2.6
1	B	170	ASP	2.6
1	B	125	VAL	2.6
1	D	343	GLN	2.5
1	C	85	LYS	2.5
1	C	151	ILE	2.5
1	B	133	ASN	2.5
1	B	164	LYS	2.4
1	C	258	ASN	2.4
1	A	67	GLY	2.4
1	B	96	SER	2.4
1	B	70	PHE	2.4
1	D	36	THR	2.4
1	C	182	HIS	2.4
1	C	238	HIS	2.4
1	D	160	ALA	2.4
1	C	167	ARG	2.4
1	A	236	SER	2.4
1	D	149	SER	2.4
1	B	165	ASN	2.4
1	A	170	ASP	2.4
1	B	238	HIS	2.4
1	D	34	ARG	2.4
1	A	38	ASP	2.4
1	D	35	LEU	2.4
1	D	44	ASP	2.3
1	A	41	GLN	2.3
1	B	308	ALA	2.3
1	A	307	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	135	GLN	2.3
1	B	246	GLN	2.3
1	A	125	VAL	2.3
1	A	171	VAL	2.3
1	A	254	LYS	2.3
1	C	369	ILE	2.3
1	D	172	THR	2.3
1	D	179	GLU	2.3
1	D	67	GLY	2.3
1	D	135	GLN	2.3
1	B	92	TYR	2.2
1	A	165	ASN	2.2
1	C	42	GLN	2.2
1	C	228	SER	2.2
1	A	231	GLN	2.2
1	C	139	ILE	2.2
1	C	170	ASP	2.2
1	B	235	LYS	2.2
1	B	134	GLY	2.2
1	C	180	LEU	2.2
1	D	177	GLY	2.2
1	D	183	LYS	2.2
1	B	120	ASP	2.2
1	B	82	LYS	2.1
1	B	335	SER	2.1
1	D	237	LYS	2.1
1	C	320	ASP	2.1
1	B	236	SER	2.1
1	A	68	LYS	2.1
1	A	237	LYS	2.1
1	A	342	LYS	2.1
1	C	230	LYS	2.1
1	C	266	TYR	2.1
1	A	70	PHE	2.1
1	C	303	ILE	2.1
1	B	36	THR	2.1
1	B	52	GLN	2.1
1	B	152	PRO	2.1
1	A	167	ARG	2.1
1	D	171	VAL	2.0
1	D	43	ILE	2.0
1	D	234	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	249	THR	2.0
1	B	45	LYS	2.0
1	B	47	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

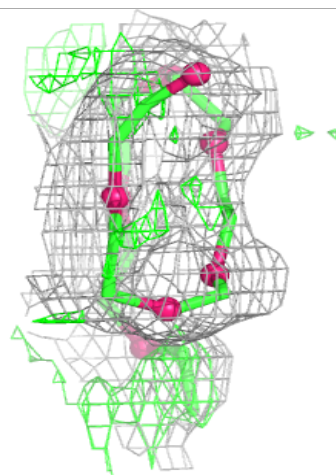
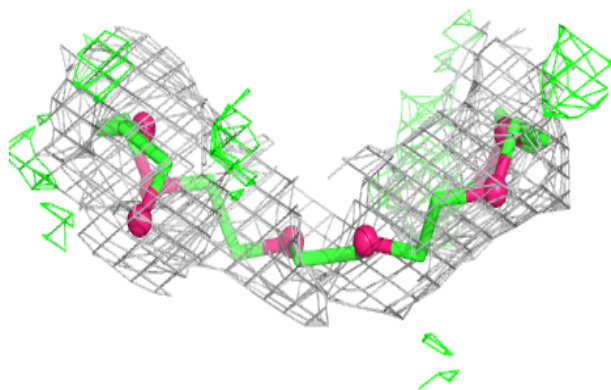
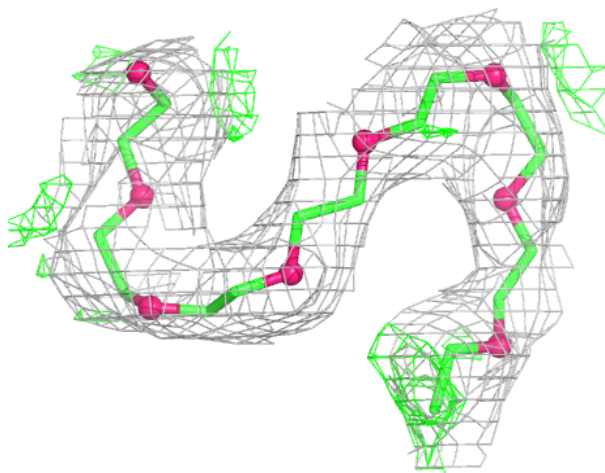
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PE4	D	401	24/24	0.77	0.25	94,98,99,99	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 PE4 D 401:

$2mF_o-DF_c$ (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.