



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 06:42 PM EDT

PDB ID : 1TLF / pdb_00001tlf
Title : UNPRECEDENTED QUATERNARY STRUCTURE OF E. COLI LAC RE-PRESSOR CORE TETRAMER: IMPLICATIONS FOR DNA LOOPING
Authors : Friedman, A.M.; Fischmann, T.O.; Steitz, T.A.
Deposited on : 1995-03-06
Resolution : 2.60 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

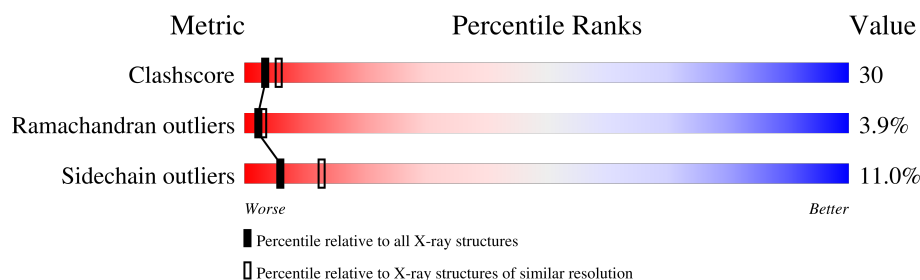
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	301	
1	B	301	
1	C	301	
1	D	301	

2 Entry composition [i](#)

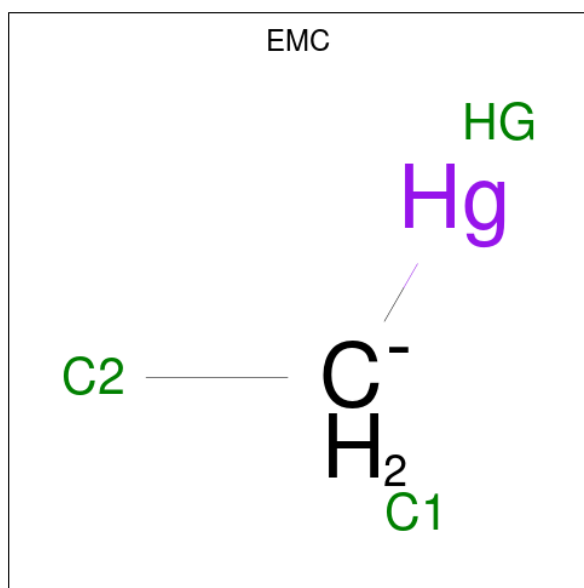
There are 3 unique types of molecules in this entry. The entry contains 10816 atoms, of which 1892 are hydrogens and 0 are deuteriums.

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 LAC REPRESSOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			
1	B	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			
1	C	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			
1	D	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			

- Molecule 2 is ETHYL MERCURY ION (CCD ID: EMC) (formula: C₂H₅Hg).



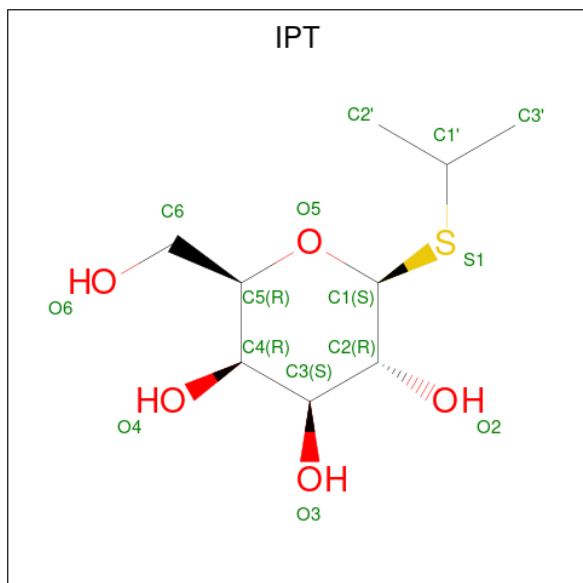
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	Hg	0	0
			3	2	1		
2	B	1	Total	C	Hg	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	Hg	0	0
			3	2	1		
2	D	1	Total	C	Hg	0	0
			3	2	1		

- Molecule 3 is 1-methylethyl 1-thio-beta-D-galactopyranoside (CCD ID: IPT) (formula: $C_9H_{18}O_5S$).



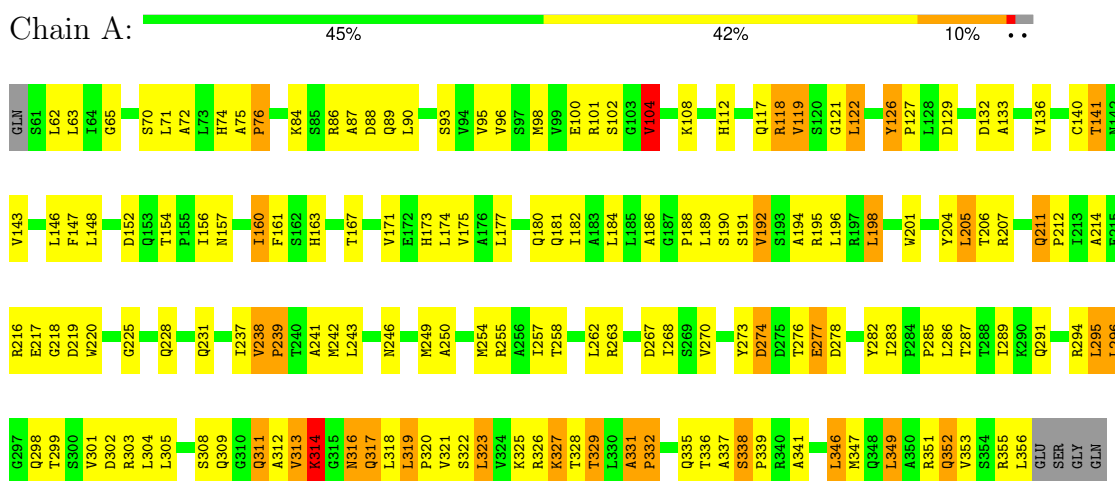
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	S	0	0
			26	9	11	5	1		
3	B	1	Total	C	H	O	S	0	0
			26	9	11	5	1		
3	C	1	Total	C	H	O	S	0	0
			26	9	11	5	1		
3	D	1	Total	C	H	O	S	0	0
			26	9	11	5	1		

3 Residue-property plots

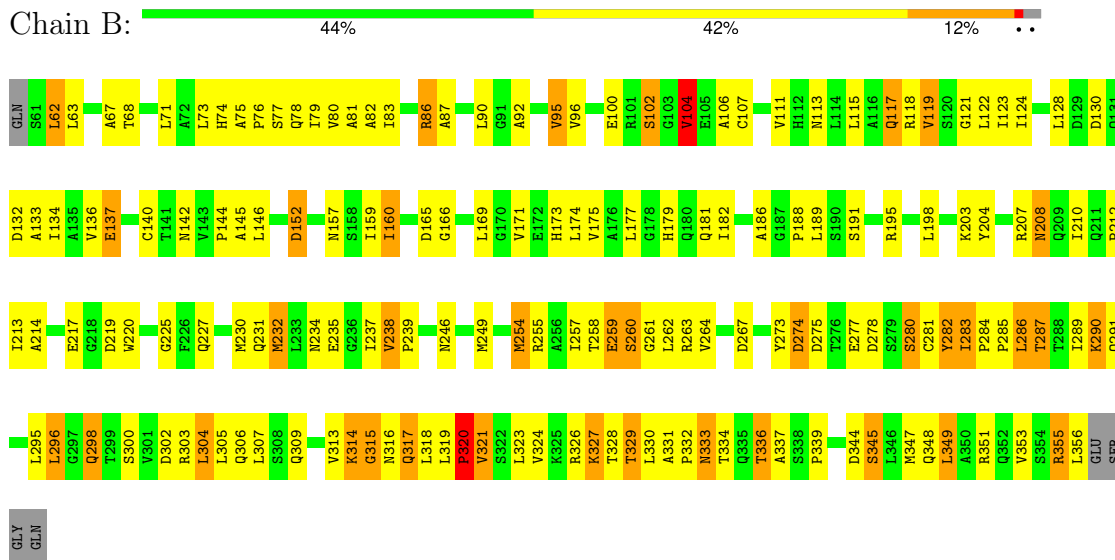
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: LAC REPRESSOR

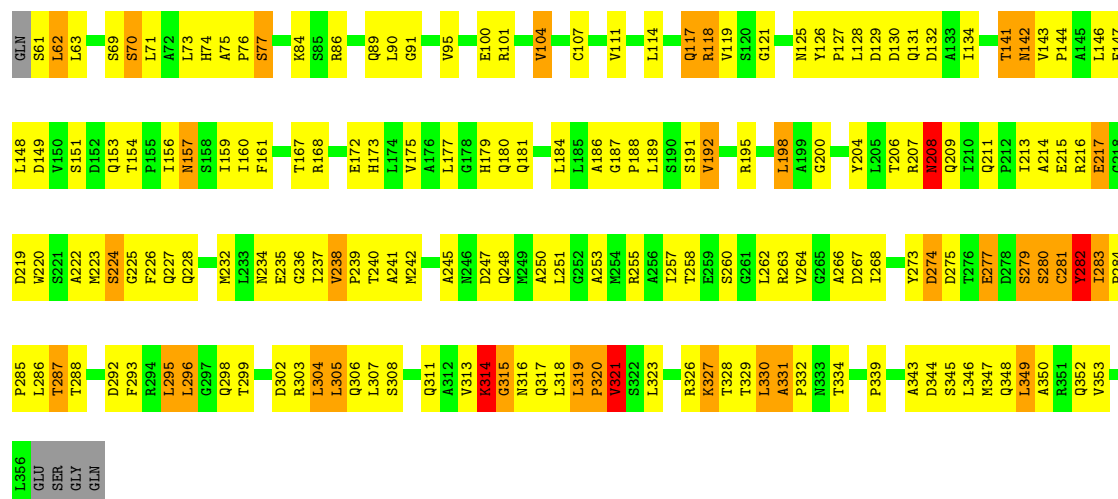


- Molecule 1: LAC REPRESSOR



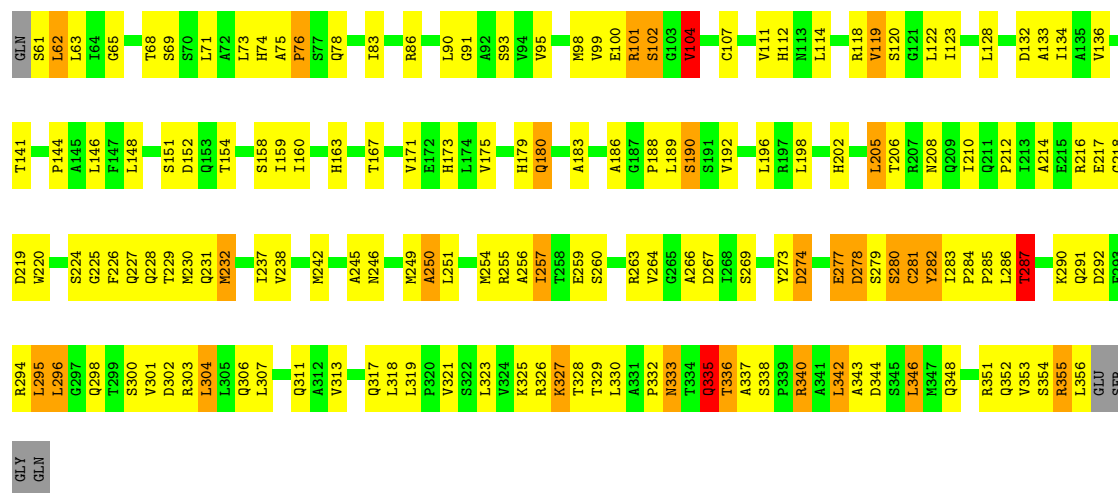
- Molecule 1: LAC REPRESSOR





Molecule 1: LAC REPRESSOR

Chain D: 45% 44% 9% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.16Å 64.73Å 117.94Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.222 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10816	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.70	0/2242	1.19	20/3048 (0.7%)
1	B	0.71	1/2242 (0.0%)	1.23	22/3048 (0.7%)
1	C	0.76	1/2242 (0.0%)	1.28	29/3048 (1.0%)
1	D	0.75	1/2242 (0.0%)	1.22	23/3048 (0.8%)
All	All	0.73	3/8968 (0.0%)	1.23	94/12192 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	232	MET	SD-CE	-7.24	1.61	1.79
1	C	223	MET	SD-CE	6.25	1.95	1.79
1	B	254	MET	SD-CE	-5.03	1.67	1.79

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	74	HIS	N-CA-C	9.73	122.90	111.71
1	B	319	LEU	CA-C-N	9.43	131.63	119.84
1	B	319	LEU	C-N-CA	9.43	131.63	119.84
1	C	280	SER	N-CA-C	-9.28	101.17	111.28
1	B	282	TYR	N-CA-C	-8.95	96.65	110.17
1	C	279	SER	N-CA-C	8.95	122.00	111.71
1	B	327	LYS	N-CA-C	8.66	122.36	112.57
1	C	240	THR	N-CA-C	-8.51	102.68	113.23
1	B	280	SER	N-CA-C	-8.32	97.49	109.96
1	C	331	ALA	N-CA-C	8.15	127.83	109.81
1	D	287	THR	N-CA-C	-7.94	96.61	109.96
1	C	331	ALA	C-N-CD	-7.81	103.42	120.60
1	B	336	THR	N-CA-C	7.70	120.75	111.82
1	D	208	ASN	N-CA-C	-7.66	102.45	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	LEU	CA-C-N	7.50	127.94	119.92
1	A	319	LEU	C-N-CA	7.50	127.94	119.92
1	D	280	SER	N-CA-C	-7.50	94.83	110.80
1	A	294	ARG	N-CA-C	-7.29	102.72	111.69
1	A	327	LYS	N-CA-C	7.24	121.42	112.59
1	B	67	ALA	N-CA-C	-7.23	96.95	108.73
1	B	104	VAL	CB-CA-C	-7.23	102.63	111.88
1	C	208	ASN	N-CA-C	-7.12	104.95	112.93
1	C	282	TYR	N-CA-C	-7.01	95.87	110.80
1	C	225	GLY	N-CA-C	-6.93	103.90	112.77
1	D	205	LEU	N-CA-C	-6.91	103.36	111.03
1	D	123	ILE	N-CA-C	-6.85	98.52	108.11
1	B	286	LEU	N-CA-C	6.73	119.66	108.96
1	D	327	LYS	N-CA-C	6.72	121.44	112.30
1	D	335	GLN	N-CA-C	-6.72	97.95	108.90
1	A	154	THR	CA-C-N	6.70	128.22	119.84
1	A	154	THR	C-N-CA	6.70	128.22	119.84
1	B	104	VAL	N-CA-C	6.63	117.32	110.36
1	A	190	SER	N-CA-C	-6.62	105.21	113.28
1	C	217	GLU	CA-C-O	6.53	128.63	121.06
1	C	159	ILE	N-CA-C	-6.49	98.10	107.78
1	C	319	LEU	CA-C-N	6.46	127.92	119.84
1	C	319	LEU	C-N-CA	6.46	127.92	119.84
1	B	315	GLY	N-CA-C	6.42	128.40	113.18
1	D	294	ARG	N-CA-C	-6.40	104.38	111.36
1	A	270	VAL	N-CA-C	6.38	117.49	108.17
1	A	314	LYS	N-CA-C	6.38	124.40	110.80
1	B	213	ILE	N-CA-C	-6.32	105.54	112.80
1	B	314	LYS	N-CA-C	6.26	124.14	110.80
1	D	190	SER	N-CA-C	-6.20	105.72	113.28
1	C	95	VAL	N-CA-C	-6.19	99.21	108.12
1	B	142	ASN	N-CA-C	6.18	120.13	112.47
1	B	225	GLY	N-CA-C	-6.14	105.06	112.49
1	A	287	THR	N-CA-C	-6.09	100.58	110.20
1	A	126	TYR	CA-C-N	6.06	127.68	120.23
1	A	126	TYR	C-N-CA	6.06	127.68	120.23
1	A	225	GLY	N-CA-C	-6.04	105.04	112.77
1	C	187	GLY	N-CA-C	-5.99	104.98	112.23
1	C	281	CYS	N-CA-C	-5.97	101.10	110.36
1	C	314	LYS	N-CA-C	5.93	123.43	110.80
1	D	232	MET	N-CA-C	-5.89	104.21	111.40
1	B	68	THR	N-CA-C	5.89	118.81	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	264	VAL	N-CA-C	-5.83	101.28	109.21
1	C	286	LEU	N-CA-C	5.81	118.14	109.25
1	C	315	GLY	N-CA-C	5.75	126.82	113.18
1	A	331	ALA	CA-C-N	5.74	127.02	119.84
1	A	331	ALA	C-N-CA	5.74	127.02	119.84
1	A	129	ASP	N-CA-C	-5.70	103.40	110.41
1	D	337	ALA	N-CA-C	5.63	118.12	110.35
1	D	338	SER	CA-C-N	5.62	125.08	119.24
1	D	338	SER	C-N-CA	5.62	125.08	119.24
1	B	82	ALA	N-CA-C	-5.60	105.08	111.07
1	A	278	ASP	N-CA-C	5.56	119.32	112.54
1	D	179	HIS	N-CA-C	5.55	117.75	109.25
1	C	281	CYS	CA-CB-SG	-5.54	101.65	114.40
1	C	349	LEU	N-CA-C	-5.54	105.32	111.36
1	D	282	TYR	N-CA-C	-5.54	101.52	110.32
1	B	320	PRO	N-CA-C	5.53	123.85	112.47
1	A	74	HIS	N-CA-C	5.50	117.36	111.36
1	B	278	ASP	N-CA-C	5.50	119.16	112.23
1	C	330	LEU	N-CA-C	-5.43	100.87	108.96
1	C	277	GLU	N-CA-C	5.37	122.23	110.80
1	B	290	LYS	N-CA-C	5.32	117.39	109.25
1	D	225	GLY	N-CA-C	-5.32	106.33	112.50
1	C	327	LYS	N-CA-C	5.31	121.58	113.61
1	D	250	ALA	N-CA-C	-5.31	105.39	111.07
1	D	99	VAL	N-CA-C	5.29	116.59	108.71
1	D	278	ASP	N-CA-C	5.28	122.05	110.80
1	C	74	HIS	N-CA-C	5.28	117.11	111.36
1	C	251	LEU	N-CA-C	-5.28	105.53	111.28
1	D	290	LYS	N-CA-C	5.27	117.32	109.25
1	B	74	HIS	N-CA-C	5.25	118.15	111.69
1	C	293	PHE	N-CA-C	-5.22	106.89	113.20
1	C	129	ASP	N-CA-C	-5.19	103.64	110.43
1	C	192	VAL	CB-CA-C	-5.12	105.41	111.81
1	D	134	ILE	N-CA-C	-5.09	105.36	110.30
1	B	133	ALA	N-CA-C	-5.06	105.68	111.14
1	C	266	ALA	N-CA-C	5.01	117.40	111.33
1	A	352	GLN	N-CA-C	-5.01	105.90	111.36
1	A	331	ALA	N-CA-C	-5.00	103.18	110.08

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	2213	462	2265	145	0
1	B	2213	462	2265	136	0
1	C	2213	462	2266	170	0
1	D	2213	462	2265	140	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	1	0
2	D	3	0	0	0	0
3	A	15	11	18	0	0
3	B	15	11	18	0	0
3	C	15	11	18	0	0
3	D	15	11	18	1	0
All	All	8924	1892	9133	541	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 30.

All (541) 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:A:189:LEU:HD11	1:A:217:GLU:OE2	1.26	1.34
1:D:189:LEU:HD11	1:D:217:GLU:OE2	1.17	1.32
1:C:189:LEU:CD2	1:C:217:GLU:OE2	1.79	1.30
1:C:189:LEU:HD21	1:C:217:GLU:OE2	1.09	1.24
1:A:189:LEU:HG	1:A:217:GLU:OE1	1.41	1.19
1:B:186:ALA:HB3	1:B:217:GLU:HG2	1.25	1.17
1:C:186:ALA:HB3	1:C:217:GLU:HG2	1.21	1.16
1:D:189:LEU:CD1	1:D:217:GLU:OE2	1.95	1.14
1:C:189:LEU:HG	1:C:217:GLU:OE1	1.51	1.07
1:A:189:LEU:CD1	1:A:217:GLU:OE2	2.03	1.06
1:D:189:LEU:HG	1:D:217:GLU:OE1	1.54	1.06
1:D:86:ARG:HG2	1:D:301:VAL:HB	1.39	1.05
1:C:281:CYS:SG	1:C:282:TYR:N	2.29	1.02
1:D:295:LEU:HD13	1:D:319:LEU:HD22	1.46	0.96
1:C:71:LEU:HD13	1:D:71:LEU:HD13	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:HD3	1:B:281:CYS:HA	1.47	0.95
1:C:189:LEU:CD2	1:C:217:GLU:CD	2.38	0.95
1:A:189:LEU:HG	1:A:217:GLU:CD	1.91	0.95
1:C:189:LEU:HG	1:C:217:GLU:CD	1.93	0.94
1:B:146:LEU:HD11	1:B:159:ILE:HG13	1.48	0.91
1:C:104:VAL:HG13	1:C:132:ASP:HB3	1.53	0.91
1:B:104:VAL:HG13	1:B:132:ASP:HB3	1.52	0.90
1:A:218:GLY:HA3	1:A:249:MET:HE1	1.54	0.90
1:C:255:ARG:HG2	1:D:281:CYS:HA	1.52	0.89
1:C:177:LEU:HB3	1:C:331:ALA:CB	2.03	0.89
1:C:62:LEU:HD13	1:C:305:LEU:HD21	1.53	0.88
1:C:189:LEU:CG	1:C:217:GLU:OE1	2.20	0.88
1:B:177:LEU:HD11	1:B:329:THR:HG23	1.56	0.87
1:D:189:LEU:HG	1:D:217:GLU:CD	1.99	0.86
1:B:86:ARG:HG3	1:B:298:GLN:HA	1.56	0.86
1:C:177:LEU:HB3	1:C:331:ALA:HB3	1.56	0.85
1:D:189:LEU:CG	1:D:217:GLU:OE1	2.24	0.85
1:A:71:LEU:O	1:B:77:SER:HB3	1.77	0.84
1:A:255:ARG:HG2	1:B:281:CYS:HB2	1.59	0.84
1:D:351:ARG:HH11	1:D:351:ARG:HB3	1.42	0.84
1:B:173:HIS:CE1	1:B:329:THR:HG21	2.14	0.83
1:C:189:LEU:CG	1:C:217:GLU:OE2	2.27	0.82
1:B:230:MET:HE3	1:B:230:MET:HA	1.62	0.82
1:D:189:LEU:CD1	1:D:217:GLU:CD	2.53	0.81
1:C:186:ALA:HB3	1:C:217:GLU:CG	2.07	0.81
1:D:254:MET:HA	1:D:257:ILE:HD12	1.62	0.81
1:A:84:LYS:HE3	1:B:100:GLU:HG3	1.62	0.80
1:A:216:ARG:HB3	1:A:228:GLN:HE21	1.47	0.80
1:A:285:PRO:HG3	1:B:255:ARG:NH1	1.96	0.80
1:A:189:LEU:CG	1:A:217:GLU:CD	2.55	0.80
1:A:189:LEU:CG	1:A:217:GLU:OE1	2.28	0.79
1:C:148:LEU:HD13	1:C:296:LEU:HD11	1.61	0.79
1:C:189:LEU:CG	1:C:217:GLU:CD	2.56	0.78
1:B:203:LYS:O	1:B:207:ARG:HG2	1.86	0.76
1:D:189:LEU:CG	1:D:217:GLU:CD	2.59	0.76
1:A:119:VAL:HG11	1:A:122:LEU:HD23	1.67	0.75
1:A:201:TRP:O	1:A:205:LEU:HB2	1.87	0.75
1:B:75:ALA:HB3	1:B:76:PRO:HD3	1.68	0.75
1:A:148:LEU:HD13	1:A:296:LEU:HD11	1.67	0.75
1:A:75:ALA:HB3	1:A:76:PRO:HD3	1.68	0.74
1:A:205:LEU:HD13	1:A:212:PRO:HD3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:MET:SD	1:C:347:MET:SD	2.87	0.72
1:D:188:PRO:HD3	1:D:219:ASP:HA	1.71	0.72
1:D:230:MET:HE1	1:D:260:SER:OG	1.89	0.72
1:C:224:SER:HA	1:C:227:GLN:HG2	1.70	0.72
1:C:306:GLN:HB3	1:C:311:GLN:HB3	1.72	0.72
1:A:160:ILE:HD12	1:A:161:PHE:O	1.90	0.72
1:B:320:PRO:O	1:B:321:VAL:HB	1.89	0.71
1:D:351:ARG:HB3	1:D:351:ARG:NH1	2.06	0.70
1:C:189:LEU:HD21	1:C:217:GLU:CD	2.09	0.70
1:D:266:ALA:HA	1:D:330:LEU:HD23	1.74	0.70
1:B:349:LEU:O	1:B:353:VAL:HG23	1.92	0.70
1:C:69:SER:HB2	1:C:101:ARG:CZ	2.21	0.70
1:A:117:GLN:O	1:A:118:ARG:HB3	1.91	0.69
1:A:214:ALA:HB2	1:A:237:ILE:HG21	1.73	0.69
1:B:165:ASP:O	1:B:169:LEU:HG	1.91	0.69
1:D:186:ALA:HB3	1:D:217:GLU:HG2	1.74	0.69
1:A:218:GLY:HA3	1:A:249:MET:CE	2.22	0.68
1:C:186:ALA:CB	1:C:217:GLU:HG2	2.12	0.68
1:A:274:ASP:HB3	1:A:276:THR:HG23	1.76	0.68
1:A:303:ARG:NH1	1:A:317:GLN:HG2	2.09	0.68
1:B:351:ARG:HD2	1:B:355:ARG:HH22	1.59	0.68
1:C:232:MET:HE1	1:C:242:MET:HE3	1.74	0.67
1:B:152:ASP:HA	1:B:316:ASN:HD21	1.60	0.67
1:D:173:HIS:HE1	1:D:329:THR:OG1	1.77	0.67
1:D:86:ARG:HG2	1:D:301:VAL:CB	2.22	0.67
1:B:144:PRO:HB3	1:B:307:LEU:HG	1.76	0.67
1:A:152:ASP:HB2	1:A:318:LEU:HD21	1.75	0.67
1:D:205:LEU:HD13	1:D:212:PRO:HG3	1.77	0.67
1:A:346:LEU:HD23	1:D:346:LEU:HD12	1.75	0.66
1:C:86:ARG:NH2	1:C:90:LEU:HD21	2.09	0.66
1:D:175:VAL:HG12	1:D:210:ILE:HD12	1.75	0.66
1:A:173:HIS:CE1	1:A:329:THR:HG21	2.30	0.66
1:D:189:LEU:CD1	1:D:217:GLU:OE1	2.44	0.66
1:C:179:HIS:NE2	1:C:331:ALA:HB2	2.10	0.66
1:C:189:LEU:CD2	1:C:217:GLU:OE1	2.42	0.66
1:A:346:LEU:HD21	1:C:346:LEU:HD21	1.78	0.65
1:C:285:PRO:HD2	1:C:327:LYS:HB2	1.78	0.65
1:A:152:ASP:HB3	1:A:160:ILE:HD11	1.77	0.65
1:B:152:ASP:HA	1:B:316:ASN:ND2	2.12	0.65
1:C:191:SER:O	1:C:195:ARG:HG3	1.96	0.65
1:A:189:LEU:CG	1:A:217:GLU:OE2	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:GLY:HA3	1:D:249:MET:CE	2.27	0.64
1:A:285:PRO:O	1:A:328:THR:HG23	1.97	0.64
1:B:232:MET:HG2	1:B:237:ILE:HB	1.80	0.64
1:A:132:ASP:O	1:A:136:VAL:HG23	1.99	0.63
1:D:218:GLY:HA3	1:D:249:MET:HE1	1.80	0.63
1:A:250:ALA:O	1:A:254:MET:HG3	1.96	0.63
1:B:307:LEU:HD13	1:B:313:VAL:HG22	1.80	0.63
1:B:264:VAL:HG11	1:B:328:THR:HG22	1.80	0.63
1:D:189:LEU:CG	1:D:217:GLU:OE2	2.47	0.63
1:B:230:MET:HE1	1:B:260:SER:OG	1.99	0.63
1:A:262:LEU:HD13	1:A:268:ILE:HD11	1.80	0.62
1:A:355:ARG:CD	1:B:334:THR:HB	2.29	0.62
1:C:281:CYS:O	1:C:282:TYR:HB2	1.99	0.62
1:B:90:LEU:HD11	1:B:302:ASP:OD1	1.99	0.62
1:A:96:VAL:HB	1:B:96:VAL:HB	1.82	0.62
1:B:273:TYR:HE1	1:B:291:GLN:NE2	1.97	0.62
1:B:246:ASN:HA	1:B:273:TYR:O	1.98	0.62
1:C:329:THR:O	1:C:330:LEU:HD12	2.00	0.62
1:D:353:VAL:O	1:D:356:LEU:HB3	1.99	0.62
1:A:285:PRO:HD2	1:A:327:LYS:HB2	1.82	0.62
1:B:171:VAL:O	1:B:175:VAL:HG13	2.00	0.62
1:A:188:PRO:HG3	1:A:219:ASP:HA	1.82	0.61
1:C:214:ALA:HB2	1:C:237:ILE:HG21	1.81	0.61
1:A:242:MET:CE	1:A:257:ILE:HD11	2.30	0.61
1:A:255:ARG:HH11	1:B:281:CYS:HA	1.64	0.61
1:B:189:LEU:HD13	1:B:195:ARG:HG2	1.81	0.61
1:C:100:GLU:CD	1:C:100:GLU:H	2.08	0.61
1:C:295:LEU:HD13	1:C:319:LEU:HD22	1.81	0.61
1:D:111:VAL:HG13	1:D:122:LEU:HD22	1.81	0.61
1:B:246:ASN:OD1	1:B:249:MET:HG3	2.01	0.61
1:A:117:GLN:NE2	1:B:117:GLN:HG3	2.16	0.60
1:D:306:GLN:HB3	1:D:311:GLN:O	2.02	0.60
1:D:227:GLN:O	1:D:231:GLN:HG2	2.02	0.60
1:A:171:VAL:O	1:A:175:VAL:HG13	2.02	0.60
1:B:104:VAL:HG13	1:B:132:ASP:CB	2.29	0.60
1:A:104:VAL:HG22	1:A:132:ASP:CG	2.27	0.59
1:A:255:ARG:HG2	1:B:281:CYS:CB	2.31	0.59
1:C:348:GLN:O	1:C:352:GLN:HG3	2.01	0.59
1:D:148:LEU:HD21	1:D:300:SER:OG	2.01	0.59
1:D:68:THR:HG21	1:D:71:LEU:HD21	1.83	0.59
1:B:173:HIS:HE1	1:B:329:THR:HG21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:HIS:HE2	1:C:331:ALA:HB2	1.68	0.59
1:B:111:VAL:HG21	1:B:136:VAL:HG13	1.85	0.59
1:D:148:LEU:HD22	1:D:296:LEU:HD21	1.85	0.59
1:D:214:ALA:HB2	1:D:237:ILE:HG21	1.85	0.59
1:A:255:ARG:CG	1:B:281:CYS:HB2	2.31	0.59
1:A:323:LEU:HD21	1:A:325:LYS:HG3	1.85	0.58
1:B:177:LEU:HD11	1:B:329:THR:CG2	2.31	0.58
1:A:283:ILE:HB	1:B:283:ILE:HG13	1.85	0.58
1:A:313:VAL:HG23	1:A:314:LYS:H	1.68	0.58
1:B:121:GLY:HA3	1:B:304:LEU:HD11	1.84	0.58
1:C:160:ILE:HG13	1:C:318:LEU:HD23	1.85	0.58
1:D:340:ARG:NH1	1:D:343:ALA:HB3	2.18	0.58
1:A:285:PRO:HB2	1:A:326:ARG:HB3	1.85	0.58
1:B:79:ILE:O	1:B:83:ILE:HG13	2.03	0.58
1:A:352:GLN:HG2	1:A:355:ARG:HH22	1.69	0.58
1:C:273:TYR:O	1:C:274:ASP:HB2	2.03	0.58
1:C:234:ASN:ND2	1:D:351:ARG:NH2	2.51	0.58
1:D:86:ARG:HD3	1:D:302:ASP:OD1	2.04	0.58
1:C:303:ARG:NH1	1:C:317:GLN:HG3	2.19	0.57
1:A:86:ARG:HG2	1:A:298:GLN:HA	1.86	0.57
1:B:290:LYS:O	1:B:321:VAL:HA	2.05	0.57
1:C:126:TYR:CD1	1:C:127:PRO:HD2	2.39	0.57
1:B:289:ILE:HD13	1:B:323:LEU:HD13	1.85	0.57
1:C:238:VAL:HG23	1:C:268:ILE:HD11	1.85	0.57
1:D:173:HIS:CD2	1:D:323:LEU:HD21	2.40	0.57
1:A:186:ALA:HB2	1:A:198:LEU:HG	1.87	0.57
1:A:189:LEU:CD1	1:A:217:GLU:CD	2.74	0.57
1:A:216:ARG:NH1	1:A:231:GLN:HB3	2.19	0.57
1:B:107:CYS:SG	1:B:128:LEU:HD11	2.44	0.57
1:D:107:CYS:O	1:D:111:VAL:HG23	2.05	0.57
1:A:295:LEU:HD13	1:A:299:THR:HG21	1.87	0.57
1:C:121:GLY:HA3	1:C:304:LEU:HD11	1.86	0.57
1:A:313:VAL:HG23	1:A:314:LYS:N	2.20	0.57
1:A:317:GLN:HE21	1:A:317:GLN:HA	1.69	0.57
1:A:349:LEU:HD11	1:B:345:SER:HB2	1.87	0.57
1:B:351:ARG:HD2	1:B:355:ARG:NH2	2.19	0.57
1:D:73:LEU:O	1:D:76:PRO:HD2	2.05	0.57
1:B:102:SER:HB2	1:B:106:ALA:HB2	1.86	0.57
1:D:152:ASP:HB3	1:D:160:ILE:HD11	1.87	0.56
1:B:134:ILE:O	1:B:137:GLU:HB3	2.05	0.56
1:C:151:SER:C	1:C:153:GLN:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:GLU:HA	1:C:175:VAL:HG22	1.85	0.56
1:D:279:SER:C	1:D:280:SER:O	2.43	0.56
1:A:62:LEU:HD21	1:A:305:LEU:HD22	1.87	0.56
1:B:286:LEU:O	1:B:326:ARG:HD2	2.06	0.56
1:B:63:LEU:HD12	1:B:119:VAL:HA	1.87	0.56
1:C:69:SER:HB3	1:C:126:TYR:CD1	2.39	0.56
1:D:224:SER:OG	1:D:249:MET:HE3	2.05	0.56
1:C:147:PHE:CD1	1:C:156:ILE:HD12	2.41	0.56
1:C:117:GLN:O	1:C:118:ARG:HB3	2.05	0.56
1:A:163:HIS:CD2	1:A:163:HIS:H	2.22	0.56
1:B:182:ILE:O	1:B:212:PRO:HA	2.06	0.56
1:B:285:PRO:HG2	1:B:327:LYS:HB2	1.87	0.55
1:A:206:THR:HG22	1:A:211:GLN:OE1	2.06	0.55
1:D:348:GLN:O	1:D:352:GLN:HG3	2.06	0.55
1:D:86:ARG:HD2	1:D:298:GLN:HB2	1.88	0.55
1:A:63:LEU:HD23	1:A:93:SER:HB2	1.87	0.55
1:C:189:LEU:HD23	1:C:217:GLU:CD	2.29	0.55
1:C:216:ARG:HD3	1:C:228:GLN:HE21	1.71	0.55
1:A:173:HIS:O	1:A:177:LEU:HG	2.07	0.55
1:A:121:GLY:HA3	1:A:304:LEU:HD11	1.87	0.55
1:C:86:ARG:HG2	1:C:298:GLN:HA	1.89	0.55
1:C:295:LEU:HD22	1:C:299:THR:HG23	1.87	0.55
1:D:273:TYR:O	1:D:274:ASP:HB2	2.07	0.55
1:A:191:SER:HB3	1:A:194:ALA:HB3	1.89	0.55
1:D:280:SER:C	1:D:282:TYR:H	2.15	0.55
1:C:287:THR:HG21	1:C:329:THR:HB	1.89	0.54
1:D:335:GLN:O	1:D:336:THR:HB	2.05	0.54
1:A:152:ASP:CB	1:A:318:LEU:HD21	2.37	0.54
1:A:263:ARG:O	1:A:267:ASP:HB2	2.07	0.54
1:C:234:ASN:HD21	1:D:351:ARG:NH2	2.05	0.54
1:A:312:ALA:O	1:A:313:VAL:HG13	2.07	0.54
1:B:287:THR:HA	1:B:324:VAL:O	2.07	0.54
1:A:86:ARG:HH11	1:A:89:GLN:NE2	2.05	0.54
1:D:101:ARG:HH22	3:D:998:IPT:C6	2.20	0.54
1:C:281:CYS:SG	1:D:251:LEU:HG	2.48	0.54
1:A:347:MET:O	1:A:351:ARG:HG2	2.08	0.54
1:B:238:VAL:HG22	1:B:238:VAL:O	2.08	0.53
1:C:234:ASN:HD21	1:D:351:ARG:HH21	1.57	0.53
1:A:71:LEU:HD13	1:B:71:LEU:HD13	1.90	0.53
1:A:118:ARG:HG2	1:A:119:VAL:N	2.23	0.53
1:D:188:PRO:C	1:D:190:SER:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ARG:HD2	1:C:317:GLN:OE1	2.09	0.53
1:A:104:VAL:HG22	1:A:132:ASP:OD2	2.08	0.53
1:C:329:THR:O	1:C:329:THR:HG23	2.07	0.53
1:C:349:LEU:HD12	1:D:342:LEU:HD12	1.90	0.53
1:D:280:SER:O	1:D:282:TYR:N	2.42	0.53
1:C:111:VAL:HA	1:C:114:LEU:HD12	1.90	0.53
1:C:219:ASP:O	1:C:220:TRP:HB2	2.09	0.53
1:A:192:VAL:O	1:A:196:LEU:HG	2.10	0.52
1:A:204:TYR:HA	1:A:207:ARG:HB2	1.91	0.52
1:C:141:THR:O	1:C:143:VAL:HG23	2.09	0.52
1:A:86:ARG:HH11	1:A:89:GLN:HE22	1.57	0.52
1:A:191:SER:HB3	1:A:194:ALA:CB	2.38	0.52
1:C:224:SER:O	1:C:227:GLN:HG2	2.10	0.52
1:D:132:ASP:O	1:D:136:VAL:HG23	2.09	0.52
1:C:101:ARG:HA	1:C:126:TYR:OH	2.09	0.52
1:C:161:PHE:HB3	1:C:321:VAL:HG23	1.91	0.52
1:A:323:LEU:HD21	1:A:325:LYS:HE3	1.92	0.52
1:B:204:TYR:O	1:B:207:ARG:HB2	2.10	0.52
1:B:264:VAL:CG1	1:B:328:THR:HG22	2.39	0.52
1:C:295:LEU:HD22	1:C:299:THR:CG2	2.38	0.52
1:A:104:VAL:O	1:A:108:LYS:HG3	2.10	0.52
1:B:287:THR:HB	1:B:326:ARG:H	1.74	0.52
1:C:126:TYR:CG	1:C:127:PRO:HD2	2.45	0.52
1:D:173:HIS:CE1	1:D:329:THR:OG1	2.60	0.52
1:D:354:SER:C	1:D:356:LEU:H	2.17	0.52
1:A:295:LEU:O	1:A:299:THR:HG23	2.09	0.52
1:C:227:GLN:HG3	1:C:228:GLN:N	2.24	0.52
1:A:273:TYR:O	1:A:274:ASP:HB2	2.10	0.52
1:C:86:ARG:CZ	1:C:90:LEU:HD21	2.39	0.52
1:C:255:ARG:CG	1:D:281:CYS:HA	2.33	0.52
1:A:157:ASN:ND2	1:A:314:LYS:HA	2.25	0.51
1:B:307:LEU:HD13	1:B:313:VAL:CG2	2.40	0.51
1:C:179:HIS:NE2	1:C:331:ALA:CB	2.73	0.51
1:D:205:LEU:CD1	1:D:212:PRO:HG3	2.41	0.51
1:C:260:SER:O	1:D:355:ARG:NH2	2.43	0.51
1:A:238:VAL:O	1:A:238:VAL:HG22	2.09	0.51
1:B:336:THR:O	1:B:337:ALA:HB3	2.10	0.51
1:D:273:TYR:HE1	1:D:291:GLN:NE2	2.09	0.51
1:B:303:ARG:NH2	1:B:314:LYS:O	2.43	0.51
1:C:189:LEU:HD23	1:C:217:GLU:OE1	2.10	0.51
1:D:61:SER:N	1:D:91:GLY:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:LEU:O	1:D:326:ARG:HD2	2.10	0.51
1:B:124:ILE:HD12	1:B:124:ILE:N	2.25	0.51
1:C:71:LEU:CD1	1:D:71:LEU:HD13	2.29	0.51
1:C:239:PRO:HB2	1:C:241:ALA:O	2.11	0.51
1:C:118:ARG:O	1:C:118:ARG:HG2	2.10	0.51
1:C:296:LEU:HD13	1:C:296:LEU:O	2.11	0.51
1:C:343:ALA:O	1:C:347:MET:HG2	2.11	0.51
1:A:355:ARG:HH21	1:B:336:THR:HA	1.76	0.50
1:B:351:ARG:HB3	1:B:355:ARG:NH1	2.27	0.50
1:C:61:SER:N	1:C:91:GLY:O	2.43	0.50
1:B:353:VAL:O	1:B:356:LEU:HG	2.11	0.50
1:C:281:CYS:O	1:C:282:TYR:CB	2.59	0.50
1:C:247:ASP:O	1:C:250:ALA:HB3	2.11	0.50
1:A:184:LEU:CD2	1:A:243:LEU:HD12	2.42	0.50
1:A:355:ARG:HG2	1:A:355:ARG:O	2.12	0.50
1:B:235:GLU:HG3	1:B:237:ILE:HG12	1.94	0.50
1:D:256:ALA:HA	1:D:259:GLU:HB2	1.93	0.50
1:D:285:PRO:HD2	1:D:327:LYS:HB2	1.93	0.50
1:C:326:ARG:C	1:C:327:LYS:HD2	2.37	0.50
1:D:167:THR:O	1:D:171:VAL:HG23	2.11	0.50
1:C:161:PHE:CZ	1:C:296:LEU:HB2	2.47	0.50
1:D:202:HIS:O	1:D:206:THR:HG23	2.12	0.50
1:B:140:CYS:SG	1:B:145:ALA:HB2	2.52	0.49
1:C:264:VAL:HG11	1:C:328:THR:HG22	1.93	0.49
1:A:174:LEU:HD22	1:A:241:ALA:HB1	1.95	0.49
1:B:86:ARG:CG	1:B:298:GLN:HA	2.36	0.49
1:C:344:ASP:O	1:C:347:MET:HB2	2.13	0.49
1:B:208:ASN:H	1:B:208:ASN:HD22	1.61	0.49
1:C:146:LEU:HD11	1:C:303:ARG:HD3	1.93	0.49
1:C:222:ALA:HA	1:C:248:GLN:O	2.12	0.49
1:C:188:PRO:HD3	1:C:219:ASP:HA	1.95	0.49
1:D:263:ARG:HD3	1:D:267:ASP:OD2	2.13	0.49
1:A:352:GLN:HG2	1:A:355:ARG:NH2	2.26	0.49
1:C:349:LEU:O	1:C:353:VAL:HG23	2.12	0.49
1:A:295:LEU:HD13	1:A:299:THR:CG2	2.43	0.48
1:C:90:LEU:HD11	1:C:302:ASP:OD1	2.13	0.48
1:A:167:THR:HG22	1:A:201:TRP:CD1	2.48	0.48
1:B:273:TYR:O	1:B:274:ASP:CB	2.61	0.48
1:D:280:SER:O	1:D:281:CYS:HB2	2.13	0.48
1:D:295:LEU:CD1	1:D:319:LEU:HD22	2.31	0.48
1:A:148:LEU:HD13	1:A:296:LEU:CD1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:HB3	1:A:326:ARG:HD3	1.95	0.48
1:B:177:LEU:CD1	1:B:329:THR:HG23	2.34	0.48
1:C:279:SER:O	1:C:281:CYS:O	2.31	0.48
1:C:232:MET:HG2	1:C:237:ILE:HB	1.95	0.48
1:D:63:LEU:HD23	1:D:93:SER:HB2	1.95	0.48
1:C:245:ALA:O	1:C:273:TYR:HB3	2.14	0.48
1:D:303:ARG:O	1:D:307:LEU:HD13	2.13	0.48
1:B:119:VAL:HG11	1:B:122:LEU:CD2	2.44	0.48
1:D:188:PRO:HD2	1:D:220:TRP:CE2	2.49	0.48
1:A:192:VAL:HG13	1:A:195:ARG:NH2	2.28	0.48
1:B:273:TYR:O	1:B:274:ASP:HB2	2.14	0.48
1:C:125:ASN:HB2	1:C:148:LEU:HD12	1.96	0.48
1:C:69:SER:HB3	1:C:126:TYR:HD1	1.77	0.47
1:A:346:LEU:CD2	1:C:346:LEU:HD21	2.43	0.47
1:C:173:HIS:HE1	1:C:329:THR:HG21	1.80	0.47
1:C:181:GLN:HB3	1:C:213:ILE:HD13	1.95	0.47
1:B:146:LEU:HD21	1:B:300:SER:HA	1.97	0.47
1:C:73:LEU:HD12	1:C:101:ARG:NH2	2.30	0.47
1:D:75:ALA:HB3	1:D:76:PRO:HD3	1.96	0.47
1:A:356:LEU:HA	1:B:336:THR:OG1	2.15	0.47
1:C:107:CYS:SG	1:C:128:LEU:HD11	2.54	0.47
1:A:98:MET:HE1	1:B:81:ALA:HA	1.97	0.47
1:B:260:SER:HB2	1:B:262:LEU:HD12	1.97	0.47
1:B:284:PRO:HG2	1:B:328:THR:HG22	1.97	0.47
1:B:336:THR:HG23	1:B:337:ALA:O	2.15	0.47
1:C:206:THR:HG22	1:C:211:GLN:NE2	2.29	0.47
1:D:100:GLU:O	1:D:102:SER:N	2.48	0.47
1:D:284:PRO:HG2	1:D:328:THR:HG22	1.95	0.47
1:A:263:ARG:H	1:A:267:ASP:HB2	1.80	0.47
1:B:208:ASN:O	1:B:210:ILE:HG13	2.14	0.47
1:B:119:VAL:HG13	1:B:121:GLY:O	2.15	0.47
1:D:218:GLY:CA	1:D:249:MET:HE1	2.43	0.47
1:B:234:ASN:HB3	1:C:226:PHE:HE1	1.80	0.47
1:C:69:SER:O	1:C:70:SER:C	2.57	0.47
1:A:317:GLN:HE21	1:A:317:GLN:CA	2.29	0.46
1:C:279:SER:C	1:C:281:CYS:O	2.58	0.46
1:A:100:GLU:C	1:A:102:SER:H	2.23	0.46
1:C:281:CYS:SG	1:D:255:ARG:HB2	2.55	0.46
1:D:183:ALA:CB	1:D:232:MET:HE1	2.45	0.46
1:A:289:ILE:HA	1:A:322:SER:O	2.15	0.46
1:A:316:ASN:OD1	1:A:318:LEU:HD22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:HIS:CE1	1:C:329:THR:HG21	2.51	0.46
1:D:175:VAL:CG1	1:D:210:ILE:HD12	2.44	0.46
1:A:254:MET:HE1	1:A:282:TYR:HB3	1.97	0.46
1:C:255:ARG:HH11	1:D:281:CYS:H	1.63	0.46
1:C:303:ARG:HH12	1:C:317:GLN:HG3	1.79	0.46
1:D:188:PRO:C	1:D:190:SER:N	2.73	0.46
1:D:344:ASP:O	1:D:348:GLN:HG3	2.16	0.46
1:A:173:HIS:HE1	1:A:329:THR:HG21	1.78	0.46
1:B:214:ALA:HB2	1:B:237:ILE:HG21	1.97	0.46
1:C:303:ARG:HE	1:C:313:VAL:HG21	1.80	0.46
1:D:104:VAL:HG13	1:D:132:ASP:HB3	1.96	0.46
1:D:214:ALA:HB3	1:D:232:MET:HE3	1.96	0.46
1:B:179:HIS:ND1	1:B:332:PRO:HG3	2.31	0.46
1:B:339:PRO:HB3	1:C:353:VAL:O	2.15	0.46
1:C:263:ARG:HD3	1:C:267:ASP:OD1	2.15	0.46
1:A:65:GLY:O	1:A:122:LEU:HA	2.16	0.46
1:A:309:GLN:HB3	1:A:311:GLN:OE1	2.16	0.46
1:B:78:GLN:HE22	1:B:277:GLU:H	1.64	0.46
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.76	0.46
1:C:144:PRO:HB2	1:C:307:LEU:HD23	1.98	0.46
1:A:133:ALA:HB1	1:A:156:ILE:HD13	1.97	0.46
1:C:75:ALA:HB3	1:C:76:PRO:HD3	1.98	0.46
1:C:216:ARG:HH11	1:C:228:GLN:NE2	2.14	0.46
1:D:283:ILE:HA	1:D:284:PRO:HA	1.83	0.46
1:C:234:ASN:C	1:C:236:GLY:H	2.23	0.46
1:B:123:ILE:HA	1:B:146:LEU:O	2.16	0.46
1:B:145:ALA:O	1:B:157:ASN:HB2	2.16	0.46
1:B:263:ARG:O	1:B:267:ASP:HB2	2.16	0.45
1:C:168:ARG:HG2	1:C:168:ARG:HH11	1.81	0.45
1:D:186:ALA:O	1:D:217:GLU:HA	2.16	0.45
1:D:226:PHE:CD1	1:D:255:ARG:HG3	2.50	0.45
1:D:278:ASP:O	1:D:280:SER:O	2.35	0.45
1:A:220:TRP:HE3	1:A:246:ASN:ND2	2.14	0.45
1:D:186:ALA:HA	1:D:245:ALA:HB2	1.99	0.45
1:D:280:SER:C	1:D:282:TYR:N	2.75	0.45
1:B:254:MET:HE2	1:B:286:LEU:HD13	1.97	0.45
1:B:280:SER:O	1:B:281:CYS:SG	2.75	0.45
1:C:258:THR:HG21	1:D:283:ILE:HD13	1.98	0.45
1:D:86:ARG:HD2	1:D:298:GLN:CB	2.46	0.45
1:D:100:GLU:H	1:D:100:GLU:CD	2.25	0.45
1:A:182:ILE:O	1:A:212:PRO:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASP:HA	1:A:291:GLN:HG3	1.98	0.45
1:C:287:THR:HG22	1:C:328:THR:OG1	2.16	0.45
1:A:95:VAL:HG23	1:B:95:VAL:HG13	1.99	0.45
1:D:78:GLN:HE22	1:D:277:GLU:H	1.65	0.45
1:D:151:SER:HA	1:D:196:LEU:HD11	1.99	0.45
1:B:87:ALA:HA	1:B:92:ALA:HB3	1.98	0.45
1:B:332:PRO:O	1:B:333:ASN:C	2.60	0.45
1:A:219:ASP:O	1:A:220:TRP:HB2	2.16	0.45
1:A:254:MET:O	1:A:258:THR:HG23	2.17	0.45
1:C:283:ILE:HD11	1:D:255:ARG:HA	1.98	0.45
1:C:339:PRO:HG3	1:D:356:LEU:HD21	1.98	0.45
1:D:146:LEU:HD21	1:D:159:ILE:HD12	1.98	0.45
1:B:287:THR:HG21	1:B:329:THR:HB	1.99	0.44
1:C:90:LEU:HD23	1:C:90:LEU:N	2.32	0.44
1:D:273:TYR:O	1:D:274:ASP:CB	2.65	0.44
1:A:117:GLN:CD	1:B:117:GLN:HG3	2.42	0.44
1:A:186:ALA:HB3	1:A:217:GLU:HG2	1.99	0.44
1:A:218:GLY:CA	1:A:249:MET:HE1	2.34	0.44
1:A:323:LEU:CD2	1:A:325:LYS:HE3	2.47	0.44
1:B:255:ARG:O	1:B:259:GLU:HB2	2.18	0.44
1:C:228:GLN:NE2	1:C:228:GLN:HA	2.32	0.44
1:D:163:HIS:CE1	1:D:196:LEU:HD22	2.53	0.44
1:A:147:PHE:CD1	1:A:156:ILE:HD12	2.53	0.44
1:C:281:CYS:SG	1:D:251:LEU:HD11	2.58	0.44
1:C:303:ARG:HE	1:C:313:VAL:CG2	2.31	0.44
1:C:349:LEU:HD13	1:C:349:LEU:HA	1.83	0.44
1:D:128:LEU:O	1:D:192:VAL:HG21	2.18	0.44
1:D:133:ALA:HB3	1:D:154:THR:HG21	2.00	0.44
1:A:98:MET:SD	1:B:80:VAL:HG12	2.58	0.44
1:B:219:ASP:O	1:B:220:TRP:HB2	2.17	0.44
1:C:347:MET:O	1:C:350:ALA:HB3	2.18	0.44
1:D:63:LEU:O	1:D:120:SER:N	2.50	0.44
1:D:246:ASN:OD1	1:D:249:MET:HG3	2.18	0.44
1:D:332:PRO:O	1:D:333:ASN:C	2.61	0.44
1:A:242:MET:HE3	1:A:257:ILE:HD11	1.98	0.43
1:C:160:ILE:O	1:C:319:LEU:N	2.48	0.43
1:C:305:LEU:O	1:C:308:SER:HB3	2.18	0.43
1:A:304:LEU:C	1:A:304:LEU:HD13	2.43	0.43
1:B:160:ILE:O	1:B:318:LEU:HA	2.18	0.43
1:B:166:GLY:HA3	1:B:273:TYR:OH	2.18	0.43
1:B:186:ALA:HB3	1:B:217:GLU:CG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:SER:H	1:C:101:ARG:HE	1.66	0.43
1:C:154:THR:HG22	1:C:156:ILE:HG12	2.00	0.43
1:C:167:THR:CB	1:C:200:GLY:HA3	2.47	0.43
1:C:273:TYR:O	1:C:274:ASP:CB	2.64	0.43
1:C:285:PRO:HB2	1:C:326:ARG:HB3	1.98	0.43
1:D:250:ALA:O	1:D:254:MET:HG3	2.18	0.43
1:A:283:ILE:O	1:B:283:ILE:HG13	2.18	0.43
1:A:286:LEU:O	1:A:326:ARG:HD2	2.18	0.43
1:B:227:GLN:O	1:B:231:GLN:HG3	2.18	0.43
1:B:306:GLN:HA	1:B:309:GLN:HB3	2.00	0.43
1:C:126:TYR:O	1:C:149:ASP:HB3	2.18	0.43
1:B:115:LEU:C	1:B:117:GLN:H	2.26	0.43
1:C:326:ARG:HH21	2:C:999:EMC:C1	2.30	0.43
1:D:160:ILE:O	1:D:318:LEU:HA	2.18	0.43
1:A:90:LEU:HD11	1:A:302:ASP:OD1	2.18	0.43
1:B:177:LEU:HB3	1:B:331:ALA:HA	2.00	0.43
1:C:141:THR:C	1:C:143:VAL:H	2.26	0.43
1:C:224:SER:CA	1:C:227:GLN:HG2	2.42	0.43
1:C:253:ALA:O	1:C:257:ILE:HG13	2.19	0.43
1:A:63:LEU:HD12	1:A:119:VAL:HA	2.00	0.43
1:B:258:THR:O	1:B:261:GLY:N	2.52	0.43
1:C:104:VAL:HG13	1:C:132:ASP:CB	2.36	0.43
1:C:283:ILE:HA	1:C:284:PRO:HA	1.93	0.43
1:B:300:SER:O	1:B:304:LEU:HB2	2.17	0.43
1:A:126:TYR:HA	1:A:127:PRO:HD3	1.77	0.43
1:B:344:ASP:O	1:B:348:GLN:HG3	2.19	0.43
1:C:319:LEU:HA	1:C:320:PRO:HD3	1.90	0.43
1:D:296:LEU:HD22	1:D:296:LEU:O	2.19	0.43
1:C:207:ARG:C	1:C:209:GLN:H	2.26	0.43
1:B:305:LEU:O	1:B:309:GLN:N	2.51	0.42
1:C:89:GLN:C	1:C:91:GLY:H	2.25	0.42
1:C:157:ASN:OD1	1:C:307:LEU:HD21	2.19	0.42
1:D:63:LEU:HB3	1:D:119:VAL:HA	2.01	0.42
1:D:254:MET:HE1	1:D:282:TYR:HB3	2.00	0.42
1:B:208:ASN:ND2	1:B:208:ASN:N	2.67	0.42
1:C:198:LEU:HD11	1:C:215:GLU:OE2	2.19	0.42
1:A:346:LEU:HD21	1:C:346:LEU:CD2	2.48	0.42
1:B:235:GLU:HG3	1:B:237:ILE:CG1	2.49	0.42
1:C:77:SER:HB2	1:D:71:LEU:O	2.20	0.42
1:C:157:ASN:HA	1:C:314:LYS:O	2.18	0.42
1:C:281:CYS:HA	1:D:255:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:VAL:O	1:A:356:LEU:HB3	2.19	0.42
1:C:144:PRO:HG3	1:C:308:SER:HA	2.01	0.42
1:D:63:LEU:HD23	1:D:63:LEU:HA	1.86	0.42
1:D:114:LEU:HB3	1:D:119:VAL:HG21	2.00	0.42
1:B:345:SER:HA	1:B:348:GLN:NE2	2.35	0.42
1:C:107:CYS:O	1:C:111:VAL:HG23	2.20	0.42
1:C:287:THR:HB	1:C:326:ARG:H	1.83	0.42
1:D:65:GLY:O	1:D:122:LEU:HA	2.18	0.42
1:B:302:ASP:O	1:B:306:GLN:HG3	2.19	0.42
1:C:69:SER:HB2	1:C:101:ARG:NH2	2.34	0.42
1:D:189:LEU:HD12	1:D:217:GLU:OE1	2.18	0.42
1:B:73:LEU:HD23	1:B:73:LEU:HA	1.74	0.42
1:B:174:LEU:O	1:B:179:HIS:HB2	2.20	0.42
1:B:179:HIS:CE1	1:B:332:PRO:HG3	2.55	0.42
1:B:188:PRO:HD2	1:B:220:TRP:CE2	2.55	0.42
1:A:346:LEU:HG	1:B:349:LEU:HD23	2.02	0.41
1:A:349:LEU:O	1:A:353:VAL:HG23	2.20	0.41
1:B:284:PRO:HG2	1:B:328:THR:CG2	2.49	0.41
1:C:184:LEU:HD13	1:C:198:LEU:CD2	2.51	0.41
1:D:304:LEU:O	1:D:307:LEU:HB2	2.20	0.41
1:A:70:SER:C	1:A:72:ALA:H	2.28	0.41
1:A:246:ASN:OD1	1:A:249:MET:HG3	2.20	0.41
1:B:316:ASN:OD1	1:B:317:GLN:N	2.52	0.41
1:C:117:GLN:O	1:C:118:ARG:CB	2.67	0.41
1:C:172:GLU:O	1:C:175:VAL:HG22	2.20	0.41
1:C:292:ASP:HB3	1:C:295:LEU:HB2	2.02	0.41
1:A:160:ILE:O	1:A:318:LEU:HA	2.20	0.41
1:C:168:ARG:HD3	1:C:204:TYR:CE2	2.55	0.41
1:D:86:ARG:NH2	1:D:90:LEU:HD21	2.34	0.41
1:A:255:ARG:HD3	1:B:281:CYS:CA	2.35	0.41
1:A:305:LEU:O	1:A:308:SER:HB3	2.20	0.41
1:C:84:LYS:HE2	1:D:98:MET:O	2.20	0.41
1:A:238:VAL:HA	1:A:239:PRO:HD2	1.80	0.41
1:B:62:LEU:HD13	1:B:305:LEU:HD22	2.03	0.41
1:C:273:TYR:N	1:C:288:THR:OG1	2.54	0.41
1:C:296:LEU:HD13	1:C:296:LEU:C	2.45	0.41
1:C:305:LEU:HD22	1:C:305:LEU:HA	1.85	0.41
1:D:216:ARG:HB3	1:D:228:GLN:HE21	1.86	0.41
1:D:287:THR:HG23	1:D:325:LYS:HA	2.01	0.41
1:D:69:SER:HB3	1:D:101:ARG:HH21	1.85	0.41
1:D:146:LEU:HD11	1:D:159:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:VAL:HG11	1:D:317:GLN:NE2	2.36	0.41
1:A:285:PRO:HG3	1:B:255:ARG:HH12	1.82	0.41
1:A:313:VAL:CG2	1:A:314:LYS:H	2.32	0.41
1:B:257:ILE:O	1:B:262:LEU:HB2	2.20	0.41
1:D:256:ALA:O	1:D:257:ILE:C	2.63	0.41
1:B:289:ILE:CG2	1:B:321:VAL:HG13	2.51	0.41
1:D:180:GLN:H	1:D:180:GLN:CD	2.29	0.41
1:A:167:THR:O	1:A:171:VAL:HG23	2.21	0.41
1:A:338:SER:O	1:A:341:ALA:HB3	2.21	0.41
1:B:191:SER:O	1:B:195:ARG:HG3	2.21	0.41
1:C:151:SER:C	1:C:153:GLN:N	2.77	0.41
1:C:232:MET:O	1:C:235:GLU:HB2	2.20	0.41
1:C:257:ILE:HG23	1:C:262:LEU:HB2	2.03	0.41
1:D:219:ASP:O	1:D:220:TRP:HB2	2.21	0.41
1:D:291:GLN:HG2	1:D:321:VAL:HG23	2.03	0.41
1:A:140:CYS:O	1:A:141:THR:C	2.63	0.41
1:A:319:LEU:HA	1:A:320:PRO:HD3	1.78	0.41
1:B:181:GLN:O	1:B:239:PRO:HB2	2.20	0.41
1:A:146:LEU:HD12	1:A:157:ASN:HB2	2.02	0.40
1:B:291:GLN:HG2	1:B:321:VAL:HG22	2.04	0.40
1:C:126:TYR:C	1:C:149:ASP:HB3	2.45	0.40
1:D:242:MET:N	1:D:269:SER:O	2.53	0.40
1:D:254:MET:HE1	1:D:282:TYR:CD2	2.55	0.40
1:D:62:LEU:HB2	1:D:120:SER:OG	2.21	0.40
1:D:175:VAL:HG12	1:D:210:ILE:CD1	2.46	0.40
1:D:229:THR:O	1:D:232:MET:HB3	2.21	0.40
1:A:87:ALA:O	1:A:88:ASP:C	2.63	0.40
1:A:121:GLY:HA2	1:A:143:VAL:HG12	2.03	0.40
1:B:115:LEU:C	1:B:117:GLN:N	2.79	0.40
1:D:144:PRO:HB2	1:D:307:LEU:HB3	2.03	0.40
1:D:335:GLN:HE21	1:D:335:GLN:HB2	1.73	0.40
1:A:331:ALA:O	1:A:332:PRO:O	2.39	0.40
1:C:208:ASN:N	1:C:208:ASN:HD22	2.18	0.40
1:C:345:SER:O	1:C:349:LEU:HD23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/301 (98%)	258 (88%)	22 (8%)	14 (5%)	2	2
1	B	294/301 (98%)	259 (88%)	26 (9%)	9 (3%)	3	5
1	C	294/301 (98%)	253 (86%)	29 (10%)	12 (4%)	2	3
1	D	294/301 (98%)	255 (87%)	28 (10%)	11 (4%)	2	3
All	All	1176/1204 (98%)	1025 (87%)	105 (9%)	46 (4%)	2	3

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	VAL
1	A	274	ASP
1	A	313	VAL
1	A	314	LYS
1	A	332	PRO
1	B	274	ASP
1	C	141	THR
1	C	274	ASP
1	C	282	TYR
1	C	321	VAL
1	D	104	VAL
1	D	141	THR
1	D	274	ASP
1	D	277	GLU
1	A	119	VAL
1	A	141	THR
1	A	277	GLU
1	A	337	ALA
1	B	130	ASP
1	B	259	GLU
1	B	275	ASP
1	B	320	PRO

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Mol	Chain	Res	Type
1	B	333	ASN
1	C	142	ASN
1	C	315	GLY
1	D	101	ARG
1	D	119	VAL
1	D	292	ASP
1	A	118	ARG
1	A	336	THR
1	B	321	VAL
1	C	70	SER
1	C	275	ASP
1	C	314	LYS
1	D	333	ASN
1	D	355	ARG
1	A	338	SER
1	C	277	GLU
1	C	332	PRO
1	D	281	CYS
1	A	101	ARG
1	A	239	PRO
1	B	62	LEU
1	C	118	ARG
1	B	315	GLY
1	D	257	ILE

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	242/246 (98%)	216 (89%)	26 (11%)	6	14
1	B	242/246 (98%)	212 (88%)	30 (12%)	4	9
1	C	242/246 (98%)	213 (88%)	29 (12%)	5	10
1	D	242/246 (98%)	221 (91%)	21 (9%)	9	21
All	All	968/984 (98%)	862 (89%)	106 (11%)	6	13

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	PRO
1	A	104	VAL
1	A	112	HIS
1	A	122	LEU
1	A	160	ILE
1	A	180	GLN
1	A	181	GLN
1	A	192	VAL
1	A	198	LEU
1	A	205	LEU
1	A	211	GLN
1	A	238	VAL
1	A	277	GLU
1	A	295	LEU
1	A	296	LEU
1	A	301	VAL
1	A	311	GLN
1	A	316	ASN
1	A	317	GLN
1	A	321	VAL
1	A	323	LEU
1	A	329	THR
1	A	335	GLN
1	A	339	PRO
1	A	346	LEU
1	A	349	LEU
1	B	86	ARG
1	B	95	VAL
1	B	102	SER
1	B	104	VAL
1	B	113	ASN
1	B	117	GLN
1	B	118	ARG
1	B	119	VAL
1	B	137	GLU
1	B	152	ASP
1	B	160	ILE
1	B	198	LEU
1	B	208	ASN
1	B	232	MET
1	B	238	VAL
1	B	260	SER

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Mol	Chain	Res	Type
1	B	282	TYR
1	B	283	ILE
1	B	287	THR
1	B	295	LEU
1	B	296	LEU
1	B	298	GLN
1	B	304	LEU
1	B	317	GLN
1	B	320	PRO
1	B	329	THR
1	B	330	LEU
1	B	345	SER
1	B	349	LEU
1	B	355	ARG
1	C	62	LEU
1	C	63	LEU
1	C	77	SER
1	C	104	VAL
1	C	117	GLN
1	C	119	VAL
1	C	130	ASP
1	C	131	GLN
1	C	134	ILE
1	C	142	ASN
1	C	157	ASN
1	C	180	GLN
1	C	192	VAL
1	C	198	LEU
1	C	208	ASN
1	C	224	SER
1	C	238	VAL
1	C	280	SER
1	C	283	ILE
1	C	287	THR
1	C	295	LEU
1	C	296	LEU
1	C	304	LEU
1	C	305	LEU
1	C	316	ASN
1	C	320	PRO
1	C	321	VAL
1	C	323	LEU

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Mol	Chain	Res	Type
1	C	334	THR
1	D	62	LEU
1	D	76	PRO
1	D	83	ILE
1	D	95	VAL
1	D	102	SER
1	D	104	VAL
1	D	112	HIS
1	D	118	ARG
1	D	158	SER
1	D	180	GLN
1	D	198	LEU
1	D	238	VAL
1	D	287	THR
1	D	295	LEU
1	D	296	LEU
1	D	304	LEU
1	D	335	GLN
1	D	336	THR
1	D	340	ARG
1	D	342	LEU
1	D	346	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	89	GLN
1	A	112	HIS
1	A	125	ASN
1	A	131	GLN
1	A	142	ASN
1	A	173	HIS
1	A	227	GLN
1	A	228	GLN
1	A	234	ASN
1	A	298	GLN
1	A	309	GLN
1	A	317	GLN
1	B	78	GLN
1	B	113	ASN
1	B	117	GLN

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Mol	Chain	Res	Type
1	B	125	ASN
1	B	173	HIS
1	B	181	GLN
1	B	208	ASN
1	B	227	GLN
1	B	228	GLN
1	B	234	ASN
1	B	291	GLN
1	B	309	GLN
1	B	333	ASN
1	B	335	GLN
1	B	348	GLN
1	C	78	GLN
1	C	125	ASN
1	C	131	GLN
1	C	173	HIS
1	C	208	ASN
1	C	227	GLN
1	C	228	GLN
1	C	234	ASN
1	C	291	GLN
1	C	316	ASN
1	D	78	GLN
1	D	157	ASN
1	D	163	HIS
1	D	173	HIS
1	D	227	GLN
1	D	228	GLN
1	D	234	ASN
1	D	291	GLN
1	D	335	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EMC	D	999	1	1,2,2	0.41	0	-		
3	IPT	B	998	-	15,15,15	1.18	1 (6%)	18,21,21	0.48	0
2	EMC	A	999	1	1,2,2	0.48	0	-		
2	EMC	C	999	-	1,2,2	0.47	0	-		
3	IPT	D	998	-	15,15,15	1.06	1 (6%)	18,21,21	0.93	1 (5%)
3	IPT	A	998	-	15,15,15	0.44	0	18,21,21	0.70	0
2	EMC	B	999	1	1,2,2	0.79	0	-		
3	IPT	C	998	-	15,15,15	0.96	1 (6%)	18,21,21	0.62	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	IPT	C	998	-	-	1/6/26/26	0/1/1/1
3	IPT	D	998	-	-	3/6/26/26	0/1/1/1
3	IPT	A	998	-	-	0/6/26/26	0/1/1/1
3	IPT	B	998	-	-	1/6/26/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	998	IPT	C1-S1	-3.55	1.73	1.80
3	B	998	IPT	C1-S1	-3.37	1.73	1.80
3	C	998	IPT	C1-S1	-3.35	1.73	1.80

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	998	IPT	C6-C5-C4	2.04	118.02	113.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	998	IPT	C4-C5-C6-O6
3	D	998	IPT	C3'-C1'-S1-C1
3	C	998	IPT	C4-C5-C6-O6
3	B	998	IPT	C2'-C1'-S1-C1
3	D	998	IPT	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	999	EMC	1	0
3	D	998	IPT	1	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.