



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:43 AM UTC

PDB ID : 1F8I / pdb_00001f8i
Title : CRYSTAL STRUCTURE OF ISOCITRATE LYASE:NITROPROPIONATE:GLYOXYLATE COMPLEX FROM MYCOBACTERIUM TUBERCULOSIS
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Deposited on : 2000-06-30
Resolution : 2.25 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)	:	2.49

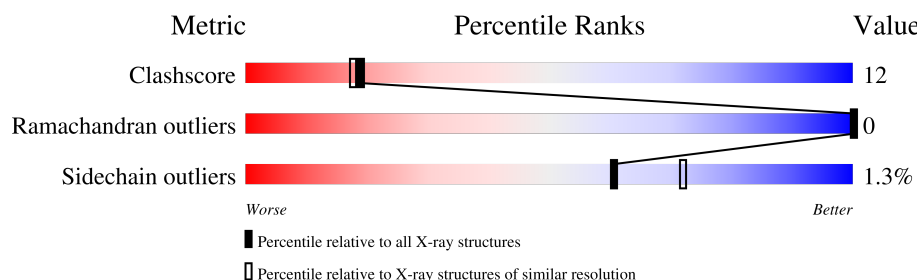
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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	429	79% 19% .
1	B	429	77% 21% .
1	C	429	75% 23% .
1	D	429	76% 22% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14340 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 ISOCITRATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3308	2078	575	647	8			
1	B	427	Total	C	N	O	S	0	0	0
			3308	2078	575	647	8			
1	C	427	Total	C	N	O	S	0	0	0
			3308	2078	575	647	8			
1	D	427	Total	C	N	O	S	0	0	0
			3308	2078	575	647	8			

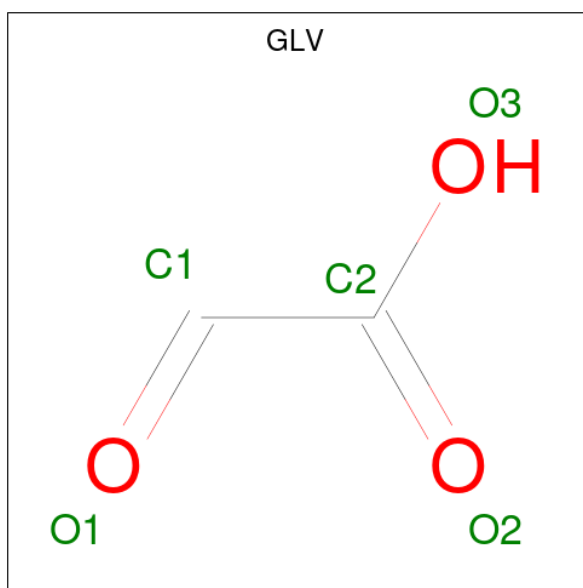
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	insertion	UNP P0A5H3
A	191	SER	CYS	engineered mutation	UNP P0A5H3
B	1	ALA	-	insertion	UNP P0A5H3
B	191	SER	CYS	engineered mutation	UNP P0A5H3
C	1	ALA	-	insertion	UNP P0A5H3
C	191	SER	CYS	engineered mutation	UNP P0A5H3
D	1	ALA	-	insertion	UNP P0A5H3
D	191	SER	CYS	engineered mutation	UNP P0A5H3

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

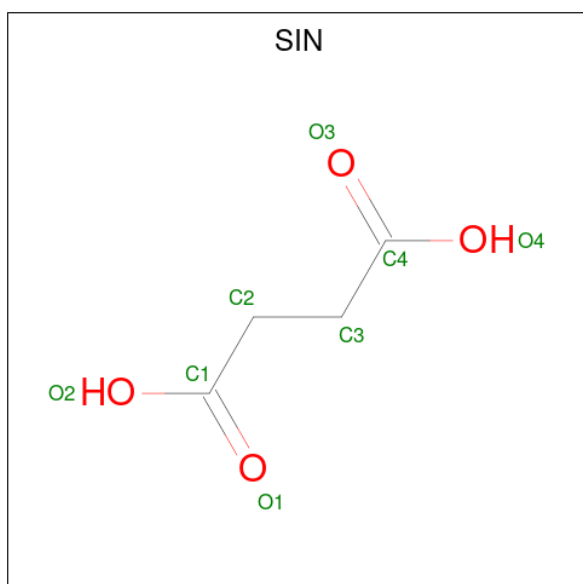
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GLYOXYLIC ACID (CCD ID: GLV) (formula: $C_2H_2O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	2	3		
3	B	1	Total	C	O	0	0
			5	2	3		
3	C	1	Total	C	O	0	0
			5	2	3		
3	D	1	Total	C	O	0	0
			5	2	3		

- Molecule 4 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 4 4	0	0
4	B	1	Total C O 8 4 4	0	0
4	C	1	Total C O 8 4 4	0	0
4	D	1	Total C O 8 4 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	267	Total O 267 267	0	0
5	B	295	Total O 295 295	0	0
5	C	269	Total O 269 269	0	0
5	D	221	Total O 221 221	0	0

3 Residue-property plots

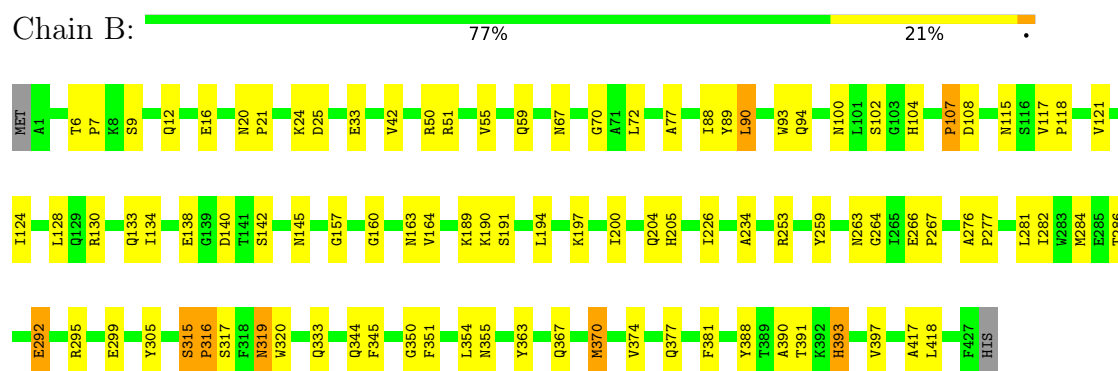
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

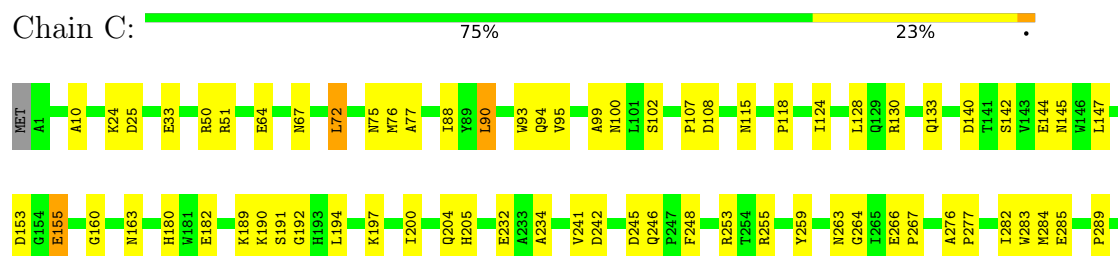
• Molecule 1: ISOCITRATE LYASE

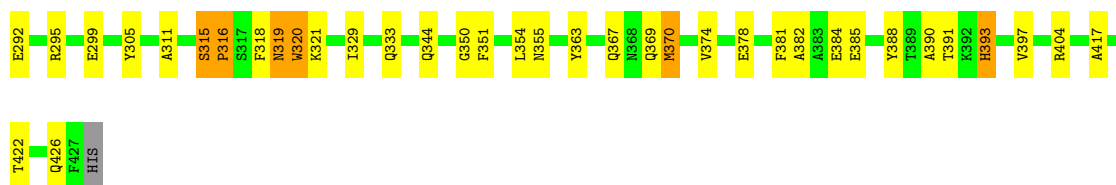


• Molecule 1: ISOCITRATE LYASE



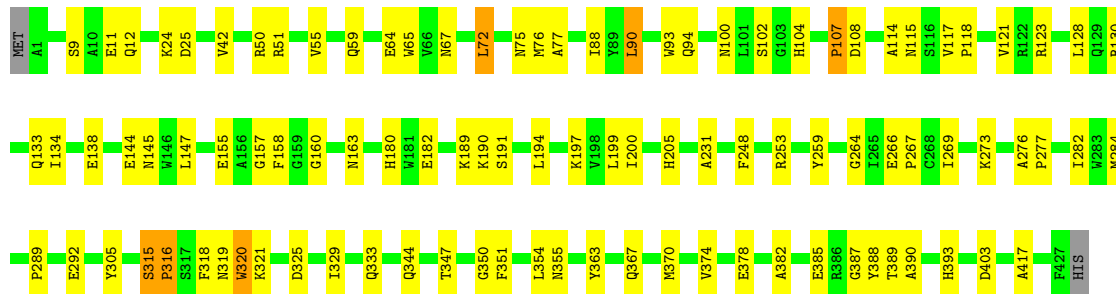
• Molecule 1: ISOCITRATE LYASE





• Molecule 1: ISOCITRATE LYASE

Chain D: 76% 22%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.29Å 129.02Å 166.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.02 – 2.25	Depositor
% Data completeness (in resolution range)	93.3 (35.02-2.25)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.166 , 0.210	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14340	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: SIN, MG, GLV

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	0.40	0/3379	0.90	12/4595 (0.3%)
1	B	0.40	0/3379	0.89	10/4595 (0.2%)
1	C	0.38	0/3379	0.89	11/4595 (0.2%)
1	D	0.38	0/3379	0.89	10/4595 (0.2%)
All	All	0.39	0/13516	0.89	43/18380 (0.2%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	315	SER	N-CA-C	9.26	121.60	109.83
1	B	315	SER	N-CA-C	8.06	121.35	109.50
1	A	315	SER	N-CA-C	8.00	121.26	109.50
1	A	320	TRP	N-CA-C	7.51	120.19	111.02
1	D	315	SER	N-CA-C	7.47	120.48	109.50
1	B	320	TRP	N-CA-C	7.03	119.60	111.02
1	D	347	THR	N-CA-C	6.67	119.11	111.11
1	B	417	ALA	N-CA-C	6.58	121.51	112.04
1	A	107	PRO	N-CA-C	-6.36	101.65	111.13
1	D	417	ALA	N-CA-C	6.25	121.03	112.04
1	B	107	PRO	N-CA-C	-6.01	102.17	111.13
1	D	107	PRO	N-CA-C	-5.96	102.25	111.13
1	B	316	PRO	N-CA-C	-5.93	107.09	114.20
1	A	114	ALA	N-CA-C	5.76	119.83	112.34
1	C	155	GLU	CB-CA-C	-5.70	109.99	116.54
1	C	417	ALA	N-CA-C	5.70	120.24	112.04
1	C	305	TYR	CA-C-N	5.63	125.74	119.32
1	C	305	TYR	C-N-CA	5.63	125.74	119.32
1	C	370	MET	N-CA-C	5.61	118.16	111.71
1	A	370	MET	N-CA-C	5.59	118.10	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	305	TYR	CA-C-N	5.56	125.66	119.32
1	D	305	TYR	C-N-CA	5.56	125.66	119.32
1	A	393	HIS	N-CA-C	5.38	117.89	111.71
1	A	417	ALA	N-CA-C	5.36	119.80	112.68
1	C	316	PRO	N-CA-C	-5.33	107.68	114.35
1	B	418	LEU	N-CA-C	5.33	117.09	111.28
1	C	393	HIS	N-CA-C	5.29	117.79	111.71
1	C	107	PRO	N-CA-C	-5.29	103.26	111.13
1	B	305	TYR	CA-C-N	5.26	125.32	119.32
1	B	305	TYR	C-N-CA	5.26	125.32	119.32
1	B	370	MET	N-CA-C	5.26	118.48	111.75
1	A	39	GLN	N-CA-C	5.25	119.67	113.16
1	A	408	THR	N-CA-C	-5.24	105.24	111.69
1	B	393	HIS	N-CA-C	5.24	117.73	111.71
1	C	320	TRP	N-CA-C	5.22	119.94	111.37
1	A	305	TYR	CA-C-N	5.20	125.25	119.32
1	A	305	TYR	C-N-CA	5.20	125.25	119.32
1	D	320	TRP	N-CA-C	5.20	119.90	111.37
1	D	114	ALA	N-CA-C	5.17	118.37	111.75
1	D	403	ASP	N-CA-C	-5.16	105.74	111.36
1	A	155	GLU	CB-CA-C	-5.15	110.62	116.54
1	C	64	GLU	N-CA-C	-5.10	105.72	111.28
1	D	316	PRO	N-CA-C	-5.06	107.81	114.03

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	3308	0	3193	78	0
1	B	3308	0	3193	80	0
1	C	3308	0	3193	91	0
1	D	3308	0	3193	83	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	1	0	0
3	B	5	0	1	0	0
3	C	5	0	1	0	0
3	D	5	0	1	0	0
4	A	8	0	4	1	0
4	B	8	0	4	1	0
4	C	8	0	4	0	0
4	D	8	0	4	1	0
5	A	267	0	0	7	0
5	B	295	0	0	3	0
5	C	269	0	0	5	0
5	D	221	0	0	3	0
All	All	14340	0	12792	308	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 12.

All (308) 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:160:GLY:H	1:A:163:ASN:HD22	1.26	0.83
1:C:108:ASP:HB3	1:C:191:SER:HB2	1.62	0.82
1:B:42:VAL:HG21	1:C:147:LEU:HD12	1.61	0.82
1:C:100:ASN:HD22	1:C:102:SER:H	1.33	0.76
1:B:190:LYS:HB2	1:B:197:LYS:HG2	1.67	0.76
1:C:130:ARG:HH11	1:C:133:GLN:HE22	1.34	0.76
1:A:147:LEU:HD12	1:D:42:VAL:HG21	1.68	0.76
1:C:190:LYS:HB2	1:C:197:LYS:HG2	1.67	0.75
1:C:94:GLN:NE2	1:C:351:PHE:H	1.84	0.75
1:A:190:LYS:HB2	1:A:197:LYS:HG2	1.71	0.72
1:B:108:ASP:HB3	1:B:191:SER:HB2	1.70	0.72
1:D:160:GLY:H	1:D:163:ASN:HD22	1.39	0.70
1:B:9:SER:OG	1:B:12:GLN:HG3	1.93	0.69
1:C:355:ASN:HD21	1:D:75:ASN:HD22	1.42	0.68
1:A:160:GLY:N	1:A:163:ASN:HD22	1.91	0.67
1:B:77:ALA:HB1	1:B:88:ILE:HD13	1.77	0.67
1:B:94:GLN:NE2	1:B:351:PHE:H	1.93	0.67
1:D:108:ASP:HB3	1:D:191:SER:HB2	1.75	0.67
1:A:77:ALA:HB1	1:A:88:ILE:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ASN:HD22	1:B:102:SER:H	1.42	0.66
1:D:190:LYS:HB2	1:D:197:LYS:HG2	1.76	0.66
1:D:94:GLN:NE2	1:D:351:PHE:H	1.93	0.66
1:A:160:GLY:H	1:A:163:ASN:ND2	1.94	0.65
1:D:100:ASN:HD22	1:D:102:SER:H	1.44	0.65
1:B:130:ARG:HH11	1:B:133:GLN:HE22	1.45	0.64
1:C:51:ARG:HH12	1:C:145:ASN:HD21	1.46	0.64
1:A:100:ASN:HD22	1:A:102:SER:H	1.45	0.64
1:D:51:ARG:HH12	1:D:145:ASN:HD21	1.46	0.64
1:A:42:VAL:HG21	1:D:147:LEU:HD12	1.80	0.63
1:A:276:ALA:HB3	1:A:277:PRO:HD3	1.81	0.63
1:B:160:GLY:H	1:B:163:ASN:HD22	1.46	0.63
1:C:100:ASN:ND2	1:C:102:SER:H	1.96	0.63
1:A:354:LEU:HD23	1:A:354:LEU:C	2.23	0.62
1:A:388:TYR:CZ	1:A:390:ALA:HB3	2.34	0.62
1:A:94:GLN:HE22	1:A:350:GLY:H	1.48	0.62
1:D:77:ALA:HB1	1:D:88:ILE:HD13	1.80	0.62
1:A:130:ARG:HH11	1:A:133:GLN:HE22	1.44	0.62
1:C:160:GLY:H	1:C:163:ASN:HD22	1.46	0.62
1:C:374:VAL:HG21	1:D:329:ILE:HG21	1.82	0.62
1:B:388:TYR:CZ	1:B:390:ALA:HB3	2.35	0.61
1:B:130:ARG:HD3	1:B:133:GLN:NE2	2.14	0.61
1:C:24:LYS:HE3	1:C:25:ASP:OD2	1.99	0.61
1:D:266:GLU:HB3	1:D:267:PRO:HD3	1.81	0.61
1:C:333:GLN:HA	1:C:344:GLN:HE22	1.66	0.61
1:C:130:ARG:NH1	1:C:133:GLN:HE22	1.97	0.60
1:C:130:ARG:HH11	1:C:133:GLN:NE2	1.98	0.60
1:A:319:ASN:HD22	1:A:319:ASN:C	2.09	0.60
1:A:94:GLN:NE2	1:A:351:PHE:H	2.00	0.60
1:A:180:HIS:HD2	5:A:1023:HOH:O	1.84	0.60
1:A:264:GLY:O	1:A:267:PRO:HD2	2.02	0.59
1:C:370:MET:O	1:C:374:VAL:HG23	2.02	0.59
1:D:333:GLN:HA	1:D:344:GLN:HE22	1.67	0.59
1:A:333:GLN:CB	1:A:344:GLN:HE22	2.15	0.59
1:C:94:GLN:HE21	1:C:351:PHE:H	1.51	0.59
1:A:75:ASN:HD22	1:B:355:ASN:HD21	1.51	0.58
1:A:15:GLN:HA	5:A:1563:HOH:O	2.04	0.58
1:B:266:GLU:HB3	1:B:267:PRO:HD3	1.85	0.57
1:A:9:SER:OG	1:A:12:GLN:HG3	2.05	0.57
1:B:333:GLN:HA	1:B:344:GLN:HE22	1.69	0.57
1:A:100:ASN:ND2	1:A:102:SER:H	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:CD1	1:B:128:LEU:HD11	2.35	0.57
1:C:388:TYR:CZ	1:C:390:ALA:HB3	2.39	0.57
1:C:266:GLU:HB3	1:C:267:PRO:HD3	1.86	0.57
1:C:77:ALA:HB1	1:C:88:ILE:HD13	1.87	0.56
1:B:100:ASN:ND2	1:B:102:SER:H	2.03	0.56
5:B:1364:HOH:O	1:D:104:HIS:HE1	1.89	0.56
1:A:191:SER:HB3	1:A:194:LEU:HG	1.87	0.56
1:B:55:VAL:O	1:B:59:GLN:HG3	2.06	0.55
1:D:180:HIS:HD2	5:D:1028:HOH:O	1.88	0.55
1:C:370:MET:HE2	1:D:320:TRP:CZ2	2.41	0.55
1:A:94:GLN:HE22	1:A:350:GLY:N	2.03	0.55
1:C:295:ARG:O	1:C:299:GLU:HG3	2.07	0.55
1:B:319:ASN:C	1:B:319:ASN:HD22	2.15	0.55
1:C:381:PHE:CD1	1:C:391:THR:HG21	2.42	0.54
1:D:354:LEU:C	1:D:354:LEU:HD23	2.31	0.54
1:A:266:GLU:HB3	1:A:267:PRO:HD3	1.90	0.54
1:A:67:ASN:HA	1:A:344:GLN:O	2.08	0.54
1:B:264:GLY:O	1:B:267:PRO:HD2	2.08	0.54
1:D:72:LEU:HD21	1:D:76:MET:HE1	1.90	0.54
1:C:319:ASN:C	1:C:319:ASN:HD22	2.16	0.53
1:A:133:GLN:HG3	5:A:1640:HOH:O	2.09	0.53
1:B:315:SER:OG	1:B:317:SER:HB2	2.09	0.53
1:B:354:LEU:C	1:B:354:LEU:HD23	2.34	0.53
1:D:388:TYR:CZ	1:D:390:ALA:HB3	2.44	0.53
1:B:94:GLN:HE22	1:B:350:GLY:H	1.57	0.53
1:A:88:ILE:CD1	1:A:128:LEU:HD11	2.38	0.53
1:D:160:GLY:H	1:D:163:ASN:ND2	2.06	0.53
1:B:134:ILE:O	1:B:138:GLU:HG3	2.08	0.53
1:C:94:GLN:HE22	1:C:350:GLY:N	2.07	0.53
1:B:67:ASN:HA	1:B:344:GLN:O	2.08	0.53
1:C:75:ASN:HD22	1:D:355:ASN:HD21	1.56	0.53
1:D:130:ARG:HD3	1:D:133:GLN:NE2	2.24	0.53
1:C:253:ARG:HD3	1:C:259:TYR:CE2	2.44	0.52
1:C:192:GLY:HA3	1:C:285:GLU:OE2	2.09	0.52
1:D:160:GLY:N	1:D:163:ASN:HD22	2.07	0.52
1:B:94:GLN:HE21	1:B:351:PHE:H	1.56	0.52
1:B:160:GLY:N	1:B:163:ASN:HD22	2.07	0.52
1:C:33:GLU:CD	1:C:33:GLU:H	2.17	0.52
1:A:243:GLU:HG3	5:A:1172:HOH:O	2.08	0.52
1:D:191:SER:HB3	1:D:194:LEU:HG	1.92	0.52
1:A:393:HIS:HB2	1:B:93:TRP:CH2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ALA:HB3	1:D:277:PRO:HD3	1.91	0.52
1:B:191:SER:HB3	1:B:194:LEU:HG	1.91	0.51
1:C:94:GLN:HE22	1:C:350:GLY:H	1.58	0.51
1:C:276:ALA:HA	1:C:282:ILE:HD11	1.92	0.51
1:A:108:ASP:HB3	1:A:191:SER:HB2	1.91	0.51
1:A:191:SER:OG	4:A:471:SIN:H21	2.11	0.51
1:B:130:ARG:NH1	1:B:133:GLN:HE22	2.08	0.51
1:A:381:PHE:CD1	1:A:391:THR:HG21	2.46	0.51
1:C:397:VAL:HG13	1:D:107:PRO:HA	1.93	0.51
1:D:67:ASN:HA	1:D:344:GLN:O	2.10	0.51
1:D:94:GLN:HE21	1:D:351:PHE:H	1.58	0.51
1:D:155:GLU:O	1:D:182:GLU:HG2	2.11	0.51
1:B:90:LEU:HD23	1:B:121:VAL:HG22	1.93	0.51
1:D:24:LYS:HE3	1:D:25:ASP:OD2	2.11	0.51
1:D:144:GLU:H	1:D:144:GLU:CD	2.16	0.51
1:D:93:TRP:CD1	1:D:108:ASP:HB2	2.45	0.51
1:D:94:GLN:HE22	1:D:350:GLY:H	1.58	0.51
1:D:191:SER:OG	4:D:474:SIN:H21	2.10	0.51
1:D:248:PHE:CD1	1:D:267:PRO:HG3	2.46	0.51
1:B:93:TRP:CD1	1:B:108:ASP:HB2	2.47	0.50
1:C:191:SER:HB3	1:C:194:LEU:HG	1.92	0.50
1:A:55:VAL:O	1:A:59:GLN:HG3	2.12	0.50
1:B:191:SER:OG	4:B:472:SIN:H21	2.12	0.50
1:D:333:GLN:CA	1:D:344:GLN:HE22	2.23	0.50
1:A:24:LYS:HE3	1:A:25:ASP:OD2	2.11	0.50
1:A:90:LEU:HD22	1:A:124:ILE:HD12	1.94	0.50
1:B:253:ARG:HD3	1:B:259:TYR:CE2	2.47	0.50
1:B:200:ILE:HD11	1:B:205:HIS:HB2	1.93	0.50
1:C:276:ALA:HB3	1:C:277:PRO:HD3	1.94	0.50
1:A:363:TYR:O	1:A:367:GLN:HG2	2.12	0.49
1:C:51:ARG:HH12	1:C:145:ASN:ND2	2.08	0.49
1:A:105:THR:CG2	1:B:397:VAL:HG23	2.42	0.49
1:B:94:GLN:HE22	1:B:350:GLY:N	2.10	0.49
1:B:130:ARG:HA	1:B:133:GLN:NE2	2.28	0.49
1:A:155:GLU:O	1:A:182:GLU:HG2	2.12	0.49
1:D:382:ALA:O	1:D:385:GLU:HG2	2.13	0.49
1:A:333:GLN:CA	1:A:344:GLN:HE22	2.25	0.49
1:B:292:GLU:HG2	5:B:1746:HOH:O	2.11	0.49
1:A:130:ARG:NH1	1:A:133:GLN:HE22	2.10	0.49
1:A:397:VAL:HG13	1:B:107:PRO:HA	1.95	0.49
1:C:67:ASN:HA	1:C:344:GLN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:TRP:CD1	1:C:108:ASP:HB2	2.46	0.49
1:A:320:TRP:H	1:B:377:GLN:HE22	1.61	0.49
1:D:130:ARG:HH11	1:D:133:GLN:HE22	1.61	0.49
1:C:289:PRO:HD3	1:C:318:PHE:CG	2.48	0.49
1:D:319:ASN:C	1:D:319:ASN:HD22	2.21	0.49
1:B:9:SER:H	1:B:12:GLN:NE2	2.10	0.48
1:A:333:GLN:HA	1:A:344:GLN:HE22	1.77	0.48
1:C:130:ARG:HA	1:C:133:GLN:NE2	2.28	0.48
1:C:333:GLN:CA	1:C:344:GLN:HE22	2.26	0.48
1:B:276:ALA:HA	1:B:282:ILE:HD11	1.94	0.48
1:C:320:TRP:CZ2	1:D:370:MET:HE2	2.49	0.48
1:D:50:ARG:HG3	1:D:50:ARG:HH11	1.79	0.48
1:D:276:ALA:HA	1:D:282:ILE:HD11	1.95	0.48
1:B:253:ARG:HD3	1:B:259:TYR:CD2	2.48	0.48
1:C:93:TRP:CH2	1:D:393:HIS:HB2	2.48	0.48
1:D:325:ASP:O	1:D:329:ILE:HG13	2.13	0.48
1:D:363:TYR:O	1:D:367:GLN:HG2	2.14	0.48
1:A:93:TRP:CD1	1:A:108:ASP:HB2	2.49	0.48
1:C:50:ARG:HG3	1:C:50:ARG:HH11	1.78	0.48
1:A:105:THR:HG23	1:B:397:VAL:HG23	1.95	0.48
1:C:88:ILE:CD1	1:C:128:LEU:HD11	2.44	0.48
1:D:94:GLN:HE22	1:D:350:GLY:N	2.11	0.48
1:A:77:ALA:HB1	1:A:88:ILE:CD1	2.44	0.48
1:D:115:ASN:C	1:D:118:PRO:HD2	2.39	0.48
1:B:24:LYS:HE3	1:B:25:ASP:OD2	2.14	0.47
1:C:264:GLY:O	1:C:267:PRO:HD2	2.13	0.47
1:D:100:ASN:ND2	1:D:102:SER:H	2.10	0.47
1:A:253:ARG:HD3	1:A:259:TYR:CD2	2.49	0.47
1:A:255:ARG:HG3	5:A:1639:HOH:O	2.14	0.47
1:C:160:GLY:N	1:C:163:ASN:HD22	2.12	0.47
1:C:354:LEU:HD23	1:C:354:LEU:C	2.39	0.47
1:C:378:GLU:HG3	5:C:1307:HOH:O	2.14	0.47
1:D:55:VAL:O	1:D:59:GLN:HG3	2.15	0.47
1:D:123:ARG:HB2	5:D:1731:HOH:O	2.15	0.47
1:D:315:SER:HA	1:D:316:PRO:HD3	1.77	0.47
1:C:253:ARG:HD3	1:C:259:TYR:CD2	2.50	0.47
1:D:9:SER:OG	1:D:12:GLN:HG3	2.15	0.47
1:D:51:ARG:HH12	1:D:145:ASN:ND2	2.12	0.47
1:C:200:ILE:HD11	1:C:205:HIS:HB2	1.97	0.46
1:A:253:ARG:HD3	1:A:259:TYR:CE2	2.50	0.46
1:B:130:ARG:HH11	1:B:133:GLN:NE2	2.10	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:SER:HG	1:B:317:SER:HB2	1.80	0.46
1:D:289:PRO:HD3	1:D:318:PHE:CG	2.50	0.46
1:C:232:GLU:HG3	1:C:284:MET:HE2	1.98	0.46
1:C:283:TRP:HB2	1:C:311:ALA:HB3	1.98	0.46
1:D:64:GLU:O	1:D:65:TRP:HB3	2.14	0.46
1:D:370:MET:O	1:D:374:VAL:HG23	2.15	0.46
1:B:276:ALA:HB3	1:B:277:PRO:HD3	1.97	0.46
1:D:264:GLY:O	1:D:267:PRO:HD2	2.15	0.46
1:B:160:GLY:H	1:B:163:ASN:ND2	2.12	0.45
1:C:140:ASP:OD1	1:C:142:SER:HB3	2.15	0.45
1:D:90:LEU:HD23	1:D:121:VAL:HG22	1.98	0.45
1:A:26:VAL:HG13	5:A:1969:HOH:O	2.16	0.45
1:A:276:ALA:HA	1:A:282:ILE:HD11	1.99	0.45
1:C:205:HIS:HD2	5:C:1194:HOH:O	1.99	0.45
1:B:397:VAL:HG22	1:B:397:VAL:O	2.17	0.45
1:C:144:GLU:CD	1:C:145:ASN:H	2.25	0.45
1:D:200:ILE:HD11	1:D:205:HIS:HB2	1.99	0.45
1:C:422:THR:O	1:C:426:GLN:HB2	2.17	0.45
1:A:93:TRP:CH2	1:B:393:HIS:HB2	2.52	0.44
1:C:155:GLU:O	1:C:182:GLU:HG2	2.17	0.44
1:D:253:ARG:HD3	1:D:259:TYR:CE2	2.52	0.44
1:B:16:GLU:HB3	5:B:1519:HOH:O	2.17	0.44
1:B:50:ARG:HG3	1:B:50:ARG:HH11	1.82	0.44
1:A:264:GLY:C	1:A:267:PRO:HD2	2.43	0.44
1:C:363:TYR:O	1:C:367:GLN:HG2	2.17	0.44
1:B:140:ASP:OD1	1:B:142:SER:HB3	2.17	0.44
1:D:333:GLN:CB	1:D:344:GLN:HE22	2.31	0.44
1:A:134:ILE:O	1:A:138:GLU:HG3	2.17	0.44
1:D:199:LEU:HD11	1:D:231:ALA:HA	2.00	0.44
1:C:115:ASN:C	1:C:118:PRO:HD2	2.43	0.44
1:C:315:SER:HA	1:C:316:PRO:HD3	1.79	0.44
1:C:321:LYS:HD3	1:D:378:GLU:CD	2.43	0.44
1:C:160:GLY:H	1:C:163:ASN:ND2	2.15	0.43
1:C:248:PHE:CD1	1:C:267:PRO:HG3	2.52	0.43
1:B:51:ARG:HH12	1:B:145:ASN:HD21	1.66	0.43
1:B:284:MET:HE2	1:B:286:THR:HG22	2.00	0.43
1:B:295:ARG:O	1:B:299:GLU:HG3	2.17	0.43
1:C:153:ASP:HA	1:C:180:HIS:CE1	2.53	0.43
1:C:329:ILE:HG21	1:D:374:VAL:HG21	2.00	0.43
1:B:115:ASN:C	1:B:118:PRO:HD2	2.44	0.43
1:C:381:PHE:CE1	1:C:391:THR:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ARG:HA	1:D:133:GLN:NE2	2.32	0.43
1:B:6:THR:HA	1:B:7:PRO:HD3	1.91	0.43
1:D:189:LYS:C	1:D:189:LYS:HD3	2.44	0.43
1:D:200:ILE:HD12	1:D:200:ILE:O	2.19	0.43
1:D:253:ARG:HD3	1:D:259:TYR:CD2	2.53	0.43
1:B:363:TYR:O	1:B:367:GLN:HG2	2.18	0.43
1:D:157:GLY:O	1:D:158:PHE:HB2	2.19	0.43
1:A:72:LEU:HD21	1:A:76:MET:HE1	2.00	0.43
1:C:72:LEU:HD21	1:C:76:MET:HE1	2.00	0.43
1:C:33:GLU:CD	1:C:33:GLU:N	2.76	0.43
1:C:90:LEU:HD22	1:C:124:ILE:HD12	2.01	0.43
1:C:200:ILE:C	1:C:200:ILE:HD12	2.44	0.42
1:A:97:GLY:HA2	1:B:397:VAL:HG21	2.00	0.42
1:C:242:ASP:O	1:C:246:GLN:HG3	2.18	0.42
1:A:140:ASP:OD1	1:A:142:SER:HB3	2.19	0.42
1:D:88:ILE:CD1	1:D:128:LEU:HD11	2.49	0.42
1:A:70:GLY:HA2	1:A:89:TYR:O	2.18	0.42
1:A:319:ASN:C	1:A:319:ASN:ND2	2.77	0.42
1:C:393:HIS:HB2	1:D:93:TRP:CH2	2.55	0.42
1:A:94:GLN:HE21	1:A:351:PHE:H	1.64	0.42
1:B:33:GLU:H	1:B:33:GLU:CD	2.28	0.42
1:C:234:ALA:O	1:C:263:ASN:HB3	2.20	0.42
1:C:10:ALA:HB1	1:C:33:GLU:OE2	2.19	0.42
1:C:140:ASP:OD1	1:C:140:ASP:C	2.62	0.42
1:C:189:LYS:HD3	1:C:189:LYS:C	2.44	0.42
1:A:315:SER:OG	1:A:317:SER:HB2	2.19	0.42
1:A:382:ALA:O	1:A:385:GLU:HG2	2.20	0.42
1:B:157:GLY:HA3	1:B:164:VAL:HG22	2.02	0.42
1:C:333:GLN:CB	1:C:344:GLN:HE22	2.33	0.42
5:C:1662:HOH:O	1:D:123:ARG:HG2	2.19	0.42
1:D:130:ARG:NH1	1:D:133:GLN:HE22	2.18	0.42
1:A:130:ARG:HH11	1:A:133:GLN:NE2	2.16	0.42
1:B:130:ARG:HD3	1:B:133:GLN:HE22	1.85	0.42
1:C:144:GLU:CG	1:C:145:ASN:N	2.83	0.42
1:D:144:GLU:CD	1:D:144:GLU:N	2.78	0.42
1:A:9:SER:H	1:A:12:GLN:NE2	2.18	0.42
1:D:134:ILE:O	1:D:138:GLU:HG3	2.20	0.42
1:B:345:PHE:CD1	1:B:345:PHE:N	2.88	0.41
1:C:378:GLU:CD	1:D:321:LYS:HD3	2.45	0.41
1:D:200:ILE:HD12	1:D:200:ILE:C	2.44	0.41
1:A:89:TYR:OH	1:A:180:HIS:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:PHE:CD1	1:B:391:THR:HG21	2.55	0.41
1:C:130:ARG:HD3	1:C:133:GLN:NE2	2.34	0.41
1:D:11:GLU:CD	1:D:11:GLU:H	2.28	0.41
1:D:387:GLY:O	1:D:389:THR:HG23	2.21	0.41
1:B:333:GLN:CA	1:B:344:GLN:HE22	2.31	0.41
1:C:95:VAL:HG13	1:C:99:ALA:O	2.21	0.41
1:C:283:TRP:CD1	1:C:283:TRP:C	2.98	0.41
1:A:283:TRP:CD1	1:A:283:TRP:C	2.98	0.41
1:A:381:PHE:CE1	1:A:391:THR:HG21	2.56	0.41
1:D:117:VAL:HB	1:D:118:PRO:HD3	2.02	0.41
1:A:23:TRP:HE3	1:A:26:VAL:HG21	1.86	0.41
1:A:192:GLY:HA3	1:A:285:GLU:OE2	2.21	0.41
1:B:315:SER:HA	1:B:316:PRO:HD3	1.81	0.41
1:A:255:ARG:HH11	1:A:255:ARG:HG2	1.86	0.41
1:B:200:ILE:HD13	1:B:204:GLN:HB3	2.02	0.41
1:B:234:ALA:O	1:B:263:ASN:HB3	2.21	0.41
1:A:107:PRO:HA	1:B:397:VAL:HG13	2.01	0.41
1:A:333:GLN:HB3	1:A:344:GLN:HE22	1.84	0.41
1:B:70:GLY:HA2	1:B:89:TYR:O	2.20	0.41
1:B:117:VAL:HB	1:B:118:PRO:HD3	2.01	0.41
1:C:241:VAL:HG13	1:C:242:ASP:N	2.36	0.41
1:C:393:HIS:HB3	1:D:351:PHE:CE2	2.56	0.41
1:C:404:ARG:HD3	5:C:1943:HOH:O	2.20	0.41
1:A:345:PHE:CD1	1:A:345:PHE:N	2.89	0.41
1:B:77:ALA:HB1	1:B:88:ILE:CD1	2.50	0.41
1:B:104:HIS:HE1	5:D:1395:HOH:O	2.03	0.41
1:B:226:ILE:HG12	1:B:281:LEU:HB2	2.03	0.41
1:C:144:GLU:HG2	1:C:145:ASN:N	2.36	0.40
1:C:200:ILE:HD13	1:C:204:GLN:HB3	2.03	0.40
1:C:382:ALA:O	1:C:385:GLU:HG2	2.21	0.40
1:D:144:GLU:CD	1:D:145:ASN:H	2.30	0.40
1:D:269:ILE:CG2	1:D:273:LYS:HE3	2.51	0.40
1:B:189:LYS:HD3	1:B:189:LYS:C	2.46	0.40
1:B:370:MET:O	1:B:374:VAL:HG23	2.21	0.40
1:A:205:HIS:HD2	5:A:1258:HOH:O	2.04	0.40
1:A:248:PHE:CD1	1:A:267:PRO:HG3	2.56	0.40
1:C:245:ASP:HB3	5:C:1456:HOH:O	2.21	0.40
1:C:255:ARG:HH11	1:C:255:ARG:HG2	1.85	0.40
1:A:7:PRO:HB3	1:A:43:VAL:HG23	2.04	0.40
1:A:181:TRP:CD1	1:A:181:TRP:N	2.89	0.40
1:B:20:ASN:HA	1:B:21:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HD22	1:B:124:ILE:HD12	2.04	0.40
1:C:381:PHE:O	1:C:384:GLU:HG3	2.22	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	425/429 (99%)	416 (98%)	9 (2%)	0	100	100
1	B	425/429 (99%)	413 (97%)	12 (3%)	0	100	100
1	C	425/429 (99%)	413 (97%)	12 (3%)	0	100	100
1	D	425/429 (99%)	413 (97%)	12 (3%)	0	100	100
All	All	1700/1716 (99%)	1655 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	337/339 (99%)	333 (99%)	4 (1%)	63	74
1	B	337/339 (99%)	333 (99%)	4 (1%)	63	74
1	C	337/339 (99%)	332 (98%)	5 (2%)	57	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	337/339 (99%)	333 (99%)	4 (1%)	63	74
All	All	1348/1356 (99%)	1331 (99%)	17 (1%)	61	72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	90	LEU
1	A	292	GLU
1	A	319	ASN
1	B	72	LEU
1	B	90	LEU
1	B	292	GLU
1	B	319	ASN
1	C	72	LEU
1	C	90	LEU
1	C	292	GLU
1	C	319	ASN
1	C	369	GLN
1	D	72	LEU
1	D	90	LEU
1	D	284	MET
1	D	292	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	59	GLN
1	A	75	ASN
1	A	79	GLN
1	A	94	GLN
1	A	100	ASN
1	A	104	HIS
1	A	133	GLN
1	A	145	ASN
1	A	163	ASN
1	A	180	HIS
1	A	308	GLN
1	A	319	ASN
1	A	344	GLN

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Mol	Chain	Res	Type
1	A	369	GLN
1	B	12	GLN
1	B	59	GLN
1	B	75	ASN
1	B	94	GLN
1	B	100	ASN
1	B	104	HIS
1	B	133	GLN
1	B	145	ASN
1	B	163	ASN
1	B	180	HIS
1	B	319	ASN
1	B	344	GLN
1	B	368	ASN
1	B	377	GLN
1	C	12	GLN
1	C	59	GLN
1	C	75	ASN
1	C	94	GLN
1	C	100	ASN
1	C	133	GLN
1	C	145	ASN
1	C	163	ASN
1	C	180	HIS
1	C	308	GLN
1	C	319	ASN
1	C	344	GLN
1	C	355	ASN
1	C	368	ASN
1	C	369	GLN
1	D	12	GLN
1	D	75	ASN
1	D	79	GLN
1	D	94	GLN
1	D	100	ASN
1	D	104	HIS
1	D	133	GLN
1	D	145	ASN
1	D	163	ASN
1	D	180	HIS
1	D	308	GLN
1	D	319	ASN

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Mol	Chain	Res	Type
1	D	344	GLN
1	D	369	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 ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
4	SIN	D	474	-	7,7,7	1.27	0	8,8,8	0.87	0
3	GLV	A	461	2	4,4,4	2.22	2 (50%)	3,4,4	1.34	0
3	GLV	B	462	2	4,4,4	2.32	2 (50%)	3,4,4	1.31	0
3	GLV	C	463	2	4,4,4	2.25	1 (25%)	3,4,4	1.39	0
4	SIN	C	473	-	7,7,7	1.28	0	8,8,8	0.85	0
4	SIN	A	471	-	7,7,7	1.33	0	8,8,8	0.88	0
3	GLV	D	464	2	4,4,4	2.33	1 (25%)	3,4,4	1.41	0
4	SIN	B	472	-	7,7,7	1.30	0	8,8,8	0.86	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
4	SIN	D	474	-	-	2/5/5/5	-
3	GLV	A	461	2	-	0/0/2/2	-
3	GLV	B	462	2	-	0/0/2/2	-
3	GLV	C	463	2	-	0/0/2/2	-
4	SIN	C	473	-	-	2/5/5/5	-
4	SIN	A	471	-	-	2/5/5/5	-
3	GLV	D	464	2	-	0/0/2/2	-
4	SIN	B	472	-	-	2/5/5/5	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	464	GLV	C1-C2	4.01	1.52	1.44
3	B	462	GLV	C1-C2	3.98	1.52	1.44
3	C	463	GLV	C1-C2	3.88	1.52	1.44
3	A	461	GLV	C1-C2	3.73	1.52	1.44
3	A	461	GLV	O3-C2	-2.08	1.25	1.30
3	B	462	GLV	O3-C2	-2.02	1.25	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	473	SIN	C2-C3-C4-O4
4	B	472	SIN	C2-C3-C4-O4
4	D	474	SIN	C2-C3-C4-O4
4	C	473	SIN	C2-C3-C4-O3
4	B	472	SIN	C2-C3-C4-O3
4	D	474	SIN	C2-C3-C4-O3
4	A	471	SIN	C2-C3-C4-O4
4	A	471	SIN	C2-C3-C4-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	474	SIN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	471	SIN	1	0
4	B	472	SIN	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.