



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:17 AM UTC

PDB ID : 1POI / pdb_00001poi
Title : CRYSTAL STRUCTURE OF GLUTACONATE COENZYME A-TRANSFERASE FROM ACIDAMINOCOCCUS FERMENTANS TO 2.55 ANGSTOMS RESOLUTION
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Deposited on : 1997-01-24
Resolution : 2.50 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
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

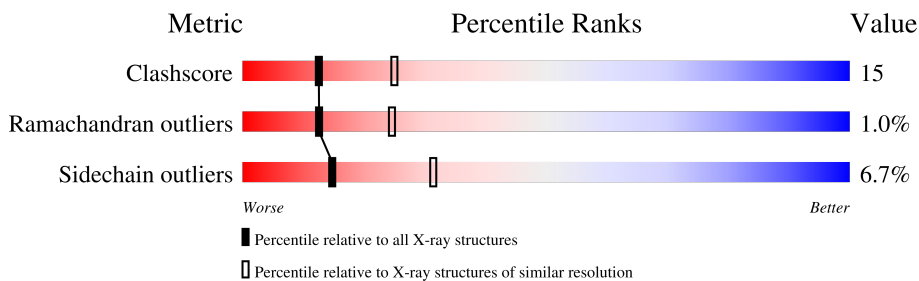
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	317	
1	C	317	
2	B	260	
2	D	260	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9433 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 GLUTACONATE COENZYME A-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2490	1594	413	470	13			
1	C	317	Total	C	N	O	S	0	0	0
			2490	1594	413	470	13			

- Molecule 2 is a protein called GLUTACONATE COENZYME A-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	0	0
			2007	1273	344	379	11			
2	D	260	Total	C	N	O	S	4	0	0
			2007	1273	344	379	11			

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cu	0	0
			1	1		

- Molecule 4 is water.

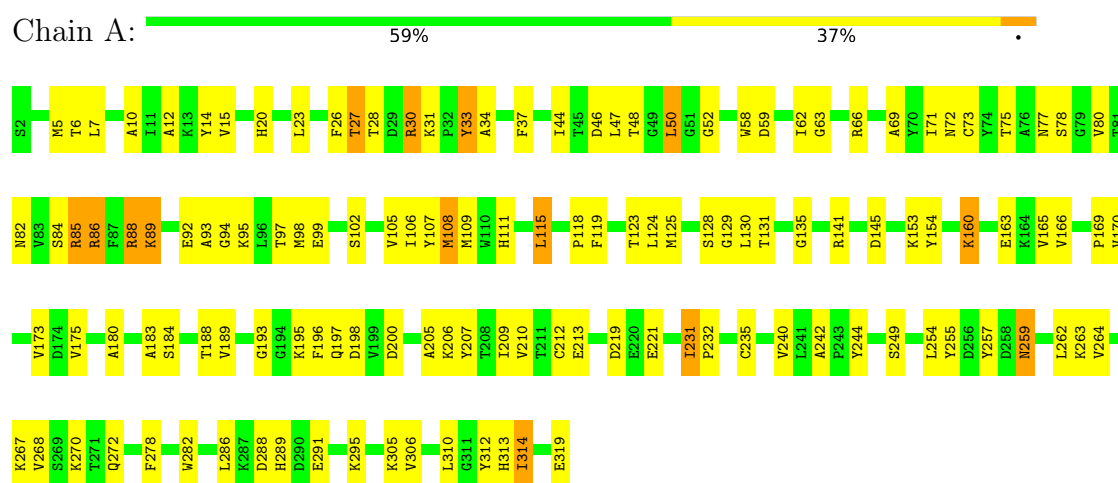
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		
4	B	91	Total	O	0	0
			91	91		
4	C	116	Total	O	0	0
			116	116		
4	D	80	Total	O	0	0
			80	80		

3 Residue-property plots

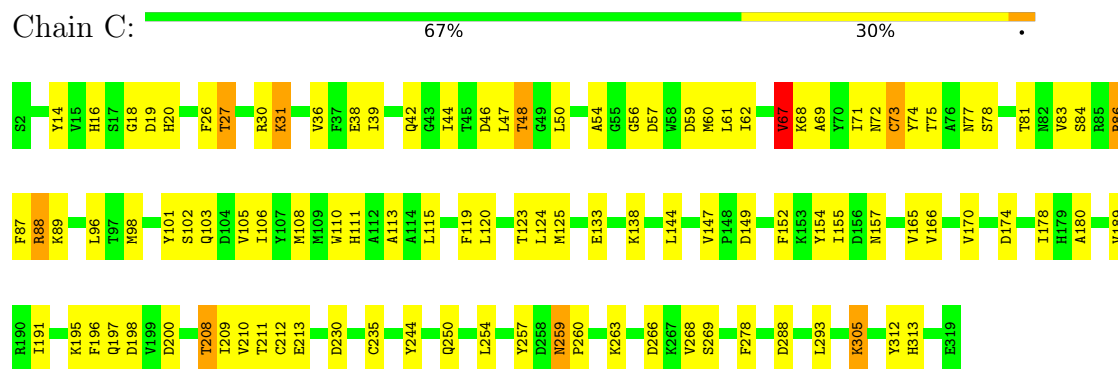
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

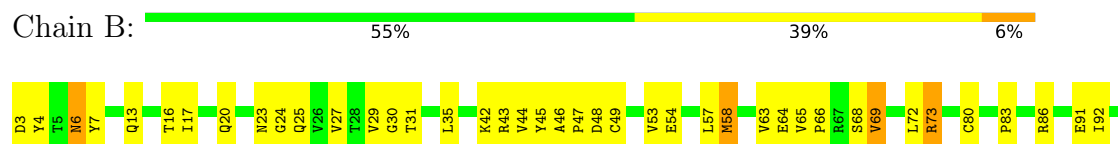
• Molecule 1: GLUTACONATE COENZYME A-TRANSFERASE

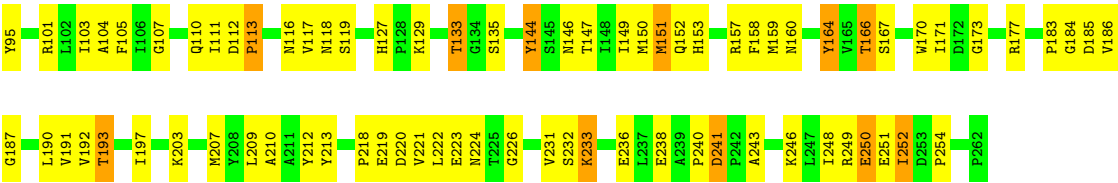


• Molecule 1: GLUTACONATE COENZYME A-TRANSFERASE

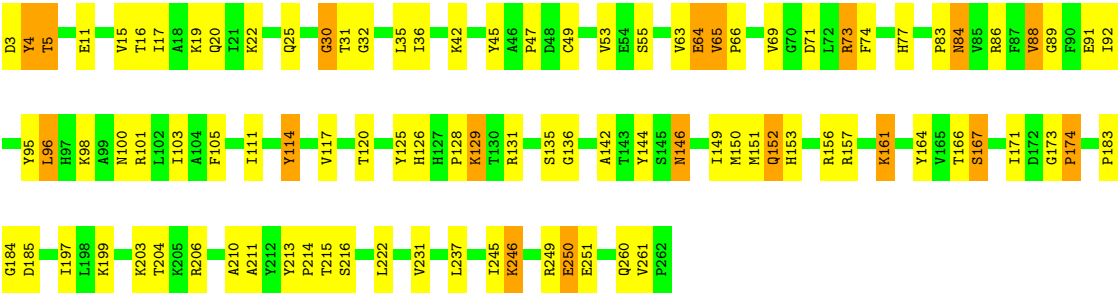


• Molecule 2: GLUTACONATE COENZYME A-TRANSFERASE





● Molecule 2: GLUTACONATE COENZYME A-TRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	145.12Å 152.27Å 130.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9433	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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:
CU

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	0.72	0/2550	1.14	24/3458 (0.7%)
1	C	0.70	0/2550	1.09	13/3458 (0.4%)
2	B	0.65	0/2053	1.22	28/2786 (1.0%)
2	D	0.62	0/2053	1.16	26/2786 (0.9%)
All	All	0.68	0/9206	1.15	91/12488 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	252	ILE	N-CA-C	9.27	119.13	110.42
2	B	135	SER	N-CA-C	8.44	120.25	111.14
1	A	198	ASP	N-CA-C	8.31	121.39	111.33
2	D	65	VAL	N-CA-C	8.01	117.69	108.96
1	A	72	ASN	N-CA-C	7.99	122.42	109.40
2	B	49	CYS	N-CA-C	-7.57	99.31	110.52
1	C	305	LYS	N-CA-C	7.55	121.44	110.42
2	D	129	LYS	N-CA-C	-7.46	102.08	112.45
2	D	45	TYR	N-CA-C	7.38	119.41	111.36
1	C	54	ALA	N-CA-C	7.19	120.27	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	49	CYS	N-CA-C	-7.13	99.08	110.14
2	B	58	MET	N-CA-C	6.84	120.39	109.24
2	B	177	ARG	N-CA-C	6.80	118.35	111.07
1	C	101	TYR	N-CA-C	-6.78	99.10	109.41
2	D	184	GLY	N-CA-C	6.71	121.37	112.77
1	C	211	THR	N-CA-C	-6.36	99.27	109.96
2	D	167	SER	CA-C-N	6.24	126.19	119.76
2	D	167	SER	C-N-CA	6.24	126.19	119.76
1	C	77	ASN	N-CA-C	-6.23	100.26	109.11
1	A	129	GLY	N-CA-C	-6.19	107.86	114.67
2	D	4	TYR	N-CA-C	6.11	119.32	109.79
2	D	213	TYR	CA-C-N	6.07	125.75	119.56
2	D	213	TYR	C-N-CA	6.07	125.75	119.56
1	A	221	GLU	N-CA-C	6.00	117.49	111.07
2	B	63	VAL	N-CA-C	-5.98	96.90	109.34
2	B	116	ASN	N-CA-C	-5.94	101.49	110.28
1	A	30	ARG	N-CA-C	5.93	119.58	111.39
1	A	33	TYR	N-CA-C	5.89	117.50	111.14
1	A	189	VAL	N-CA-C	5.88	116.34	108.11
1	A	242	ALA	CA-C-N	5.78	126.07	119.83
1	A	242	ALA	C-N-CA	5.78	126.07	119.83
1	C	288	ASP	N-CA-C	5.78	115.87	108.24
2	B	72	LEU	N-CA-C	-5.77	105.50	112.54
1	C	198	ASP	N-CA-C	5.71	118.23	111.33
2	B	144	TYR	N-CA-C	5.70	120.93	113.30
1	A	98	MET	N-CA-C	5.68	118.47	108.75
2	D	146	ASN	N-CA-C	-5.66	101.47	109.96
1	C	133	GLU	N-CA-C	5.63	118.28	108.76
2	D	65	VAL	CA-C-N	5.61	125.37	119.76
2	D	65	VAL	C-N-CA	5.61	125.37	119.76
1	A	20	HIS	N-CA-C	-5.60	98.62	108.20
2	D	64	GLU	N-CA-C	-5.60	100.57	109.59
1	C	67	VAL	CB-CA-C	-5.59	105.19	111.23
1	A	94	GLY	N-CA-C	-5.58	107.06	115.32
1	C	67	VAL	N-CA-C	5.57	116.39	107.98
1	A	231	ILE	CA-C-N	5.56	126.04	120.14
1	A	231	ILE	C-N-CA	5.56	126.04	120.14
2	D	250	GLU	N-CA-C	5.55	120.04	113.16
2	B	65	VAL	CA-C-N	5.54	126.02	120.14
2	B	65	VAL	C-N-CA	5.54	126.02	120.14
2	B	167	SER	CA-C-N	5.54	127.05	120.23
2	B	167	SER	C-N-CA	5.54	127.05	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	184	GLY	N-CA-C	5.49	120.73	113.37
2	B	151	MET	N-CA-C	5.49	117.74	109.23
2	D	135	SER	N-CA-C	5.48	117.70	111.02
2	D	144	TYR	N-CA-C	5.41	121.07	113.02
2	B	104	ALA	N-CA-C	5.38	118.01	109.50
2	D	5	THR	N-CA-C	5.38	119.33	112.34
1	A	52	GLY	N-CA-C	-5.37	102.87	112.22
1	A	77	ASN	N-CA-C	-5.37	100.86	109.39
2	B	45	TYR	N-CA-C	5.33	116.77	111.07
1	C	154	TYR	N-CA-C	-5.31	101.04	109.59
1	A	48	THR	N-CA-C	-5.30	101.31	109.52
2	B	220	ASP	N-CA-C	-5.25	105.45	111.07
1	C	157	ASN	N-CA-C	-5.24	101.66	109.42
2	B	241	ASP	CA-C-N	5.24	125.55	119.47
2	B	241	ASP	C-N-CA	5.24	125.55	119.47
2	B	147	THR	N-CA-C	5.22	117.80	109.81
2	B	149	ILE	N-CA-C	5.21	115.60	107.99
2	B	127	HIS	CA-C-N	5.20	125.61	119.99
2	B	127	HIS	C-N-CA	5.20	125.61	119.99
2	D	30	GLY	N-CA-C	-5.20	100.86	113.18
2	D	173	GLY	CA-C-N	5.19	126.33	119.84
2	D	173	GLY	C-N-CA	5.19	126.33	119.84
1	A	85	ARG	N-CA-C	5.16	117.69	111.40
1	A	131	THR	N-CA-C	-5.15	107.65	114.04
2	B	31	THR	N-CA-C	-5.13	99.86	110.80
2	D	88	VAL	N-CA-C	-5.13	105.32	110.30
1	A	102	SER	N-CA-C	-5.12	103.28	110.50
1	A	145	ASP	N-CA-C	-5.11	102.12	110.20
1	A	160	LYS	CA-C-N	5.10	125.10	119.89
1	A	160	LYS	C-N-CA	5.10	125.10	119.89
2	D	98	LYS	N-CA-C	-5.10	104.38	111.52
2	D	246	LYS	N-CA-C	-5.10	104.99	111.11
2	B	146	ASN	N-CA-C	-5.09	101.66	109.76
2	B	173	GLY	CA-C-N	5.08	125.32	119.83
2	B	173	GLY	C-N-CA	5.08	125.32	119.83
1	C	191	ILE	N-CA-C	-5.08	100.33	107.75
1	A	82	ASN	N-CA-C	5.08	116.50	111.07
2	D	74	PHE	N-CA-C	-5.01	104.89	111.96
2	D	136	GLY	N-CA-C	-5.01	101.31	113.18

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	164	TYR	Sidechain
2	D	114	TYR	Sidechain

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	2490	0	2449	78	0
1	C	2490	0	2449	71	0
2	B	2007	0	1987	73	0
2	D	2007	0	1987	67	0
3	A	1	0	0	0	0
4	A	151	0	0	10	0
4	B	91	0	0	5	0
4	C	116	0	0	1	0
4	D	80	0	0	3	0
All	All	9433	0	8872	273	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 15.

All (273) 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)
2:B:191:VAL:HG21	2:B:207:MET:HE2	1.42	1.01
2:B:83:PRO:HD2	2:B:86:ARG:HG3	1.55	0.86
2:B:3:ASP:HB2	2:B:246:LYS:HA	1.54	0.86
2:D:152:GLN:HA	2:D:152:GLN:NE2	1.95	0.82
2:D:152:GLN:HA	2:D:152:GLN:HE21	1.45	0.81
1:A:111:HIS:HE1	1:C:111:HIS:CE1	2.01	0.78
1:A:111:HIS:HE1	1:C:111:HIS:HE1	1.32	0.76
2:D:84:ASN:HD22	2:D:84:ASN:H	1.34	0.76
2:B:13:GLN:O	2:B:16:THR:HG22	1.87	0.75
1:C:196:PHE:HA	2:D:84:ASN:HD21	1.52	0.74
1:A:118:PRO:HG3	1:C:123:THR:HG23	1.67	0.74
2:B:29:VAL:O	2:B:53:VAL:HG12	1.88	0.74
1:C:268:VAL:HG11	1:C:278:PHE:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:GLY:O	2:D:36:ILE:HG12	1.91	0.71
1:A:111:HIS:CE1	1:C:111:HIS:HE1	2.09	0.70
2:B:29:VAL:HG12	2:B:105:PHE:CD1	2.29	0.67
2:B:119:SER:H	2:B:166:THR:HG21	1.60	0.67
1:A:12:ALA:HB2	4:A:416:HOH:O	1.95	0.66
2:D:17:ILE:HD11	2:D:150:MET:HE1	1.76	0.66
2:B:3:ASP:CB	2:B:246:LYS:HA	2.25	0.66
2:D:84:ASN:H	2:D:84:ASN:ND2	1.94	0.66
1:A:46:ASP:HB3	4:A:470:HOH:O	1.95	0.65
1:A:7:LEU:HB2	1:A:240:VAL:HG11	1.79	0.65
1:A:267:LYS:HA	1:A:270:LYS:HE3	1.77	0.65
1:C:119:PHE:HA	1:C:170:VAL:HG23	1.79	0.65
1:A:5:MET:HG3	1:A:10:ALA:HB2	1.79	0.64
1:C:14:TYR:HB2	1:C:209:ILE:HD11	1.79	0.64
2:D:206:ARG:HG2	2:D:206:ARG:HH11	1.63	0.63
1:C:59:ASP:OD1	1:C:84:SER:HB3	1.99	0.63
2:D:17:ILE:HG23	2:D:105:PHE:CZ	2.34	0.63
2:B:107:GLY:O	2:B:117:VAL:HG11	1.98	0.63
1:A:44:ILE:O	1:A:66:ARG:HD2	1.99	0.62
1:C:208:THR:HG23	1:C:235:CYS:O	1.98	0.62
2:D:22:LYS:O	2:D:25:GLN:HG2	1.98	0.62
1:A:206:LYS:HE3	1:A:207:TYR:CE2	2.35	0.62
2:B:119:SER:H	2:B:166:THR:CG2	2.12	0.62
2:B:191:VAL:HG21	2:B:207:MET:CE	2.25	0.62
2:B:192:VAL:HG22	2:B:197:ILE:HG22	1.81	0.62
1:C:87:PHE:HE1	1:C:98:MET:SD	2.23	0.61
1:C:213:GLU:HG3	1:C:254:LEU:CD1	2.31	0.61
2:B:4:TYR:HE1	2:B:6:ASN:HB3	1.64	0.60
1:A:173:VAL:O	1:A:205:ALA:HA	2.02	0.60
2:D:31:THR:HA	2:D:35:LEU:HD22	1.82	0.60
1:A:305:LYS:O	1:A:313:HIS:HD2	1.82	0.60
2:B:4:TYR:HD1	2:B:6:ASN:H	1.48	0.60
2:D:42:LYS:O	2:D:47:PRO:HA	2.01	0.60
2:B:190:LEU:HD11	2:B:197:ILE:HB	1.84	0.60
1:A:268:VAL:HG11	1:A:278:PHE:HB2	1.83	0.59
1:A:259:ASN:O	1:A:263:LYS:HG3	2.03	0.58
1:C:26:PHE:HE1	2:D:69:VAL:HG23	1.67	0.58
1:C:20:HIS:HA	1:C:48:THR:O	2.03	0.58
1:A:27:THR:O	1:A:31:LYS:HD3	2.04	0.58
1:A:128:SER:OG	1:A:130:LEU:HB2	2.03	0.58
2:B:35:LEU:HD21	2:B:66:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ARG:HD3	1:A:270:LYS:HG2	1.85	0.57
2:B:23:ASN:HA	2:B:46:ALA:HB1	1.86	0.57
1:C:50:LEU:HA	1:C:71:ILE:HB	1.87	0.57
2:B:112:ASP:HB2	2:B:113:PRO:HD2	1.86	0.57
2:D:92:ILE:O	2:D:96:LEU:HD23	2.04	0.57
2:D:95:TYR:CZ	2:D:183:PRO:HB3	2.40	0.57
2:D:69:VAL:HG22	4:D:307:HOH:O	2.04	0.56
1:C:138:LYS:HE2	1:C:149:ASP:HB3	1.87	0.56
1:C:195:LYS:HE2	1:C:230:ASP:OD1	2.06	0.56
2:B:83:PRO:HD2	2:B:86:ARG:CG	2.33	0.55
2:D:11:GLU:OE1	2:D:245:ILE:HG23	2.04	0.55
1:C:195:LYS:HD2	1:C:195:LYS:N	2.21	0.55
2:D:17:ILE:HD11	2:D:150:MET:CE	2.37	0.55
2:D:63:VAL:HG23	2:D:77:HIS:CE1	2.42	0.55
1:A:310:LEU:HG	4:A:426:HOH:O	2.07	0.55
2:D:35:LEU:HG	4:D:335:HOH:O	2.05	0.55
1:C:27:THR:O	1:C:31:LYS:HD3	2.06	0.54
2:B:43:ARG:NH1	2:B:252:ILE:HG13	2.23	0.54
1:A:105:VAL:HG21	1:A:125:MET:SD	2.47	0.54
2:B:209:LEU:HD22	2:B:231:VAL:HG12	1.88	0.54
1:C:88:ARG:HG3	1:C:89:LYS:N	2.23	0.54
2:D:15:VAL:O	2:D:19:LYS:HG3	2.08	0.54
1:A:23:LEU:HD12	1:A:58:TRP:NE1	2.22	0.54
2:B:25:GLN:HB2	2:B:101:ARG:O	2.08	0.54
1:A:46:ASP:CB	4:A:470:HOH:O	2.56	0.54
1:A:63:GLY:HA3	1:A:86:ARG:HG3	1.90	0.54
2:D:17:ILE:HG23	2:D:105:PHE:CE2	2.43	0.54
1:A:169:PRO:HA	4:A:375:HOH:O	2.06	0.53
1:C:73:CYS:HB3	1:C:106:ILE:HG13	1.90	0.53
2:D:103:ILE:HD12	2:D:146:ASN:O	2.08	0.53
1:A:268:VAL:HG11	1:A:278:PHE:CB	2.39	0.53
1:C:195:LYS:HE2	1:C:230:ASP:CG	2.33	0.53
1:A:305:LYS:O	1:A:313:HIS:CD2	2.62	0.53
1:C:87:PHE:CE1	1:C:98:MET:SD	3.01	0.53
2:D:3:ASP:N	2:D:249:ARG:HD2	2.24	0.53
1:A:289:HIS:HE1	4:A:378:HOH:O	1.91	0.52
2:D:206:ARG:HG2	2:D:206:ARG:NH1	2.23	0.52
2:B:95:TYR:CZ	2:B:183:PRO:HB3	2.45	0.52
2:D:3:ASP:N	2:D:249:ARG:HH11	2.06	0.52
2:D:152:GLN:HB2	2:D:157:ARG:HE	1.75	0.52
2:B:110:GLN:NE2	2:B:159:MET:SD	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ASN:HB2	2:B:164:TYR:O	2.10	0.52
2:D:88:VAL:O	2:D:91:GLU:HG2	2.10	0.52
1:A:50:LEU:HA	1:A:71:ILE:HB	1.92	0.52
2:D:114:TYR:OH	2:D:206:ARG:HD2	2.09	0.52
2:D:161:LYS:NZ	2:D:161:LYS:HB3	2.24	0.52
1:A:272:GLN:HB2	4:A:467:HOH:O	2.09	0.52
1:C:152:PHE:CD2	1:C:166:VAL:HG13	2.45	0.52
1:A:264:VAL:O	1:A:267:LYS:HG3	2.09	0.51
1:C:36:VAL:HG13	1:C:61:LEU:HD21	1.91	0.51
2:B:42:LYS:O	2:B:47:PRO:HA	2.10	0.51
2:B:209:LEU:HB3	2:B:231:VAL:HA	1.93	0.51
2:B:4:TYR:CE1	2:B:6:ASN:HB3	2.44	0.51
2:B:27:VAL:HG12	2:B:29:VAL:HG13	1.92	0.51
1:C:38:GLU:O	1:C:42:GLN:HG3	2.11	0.51
2:D:3:ASP:OD1	2:D:246:LYS:HB2	2.09	0.51
2:D:31:THR:HG22	2:D:35:LEU:HD22	1.92	0.51
1:A:5:MET:CG	1:A:10:ALA:HB2	2.40	0.51
1:C:69:ALA:HB2	1:C:144:LEU:HD13	1.93	0.51
1:A:115:LEU:O	2:D:89:GLY:HA2	2.10	0.51
1:A:193:GLY:O	1:A:195:LYS:HE3	2.11	0.51
2:B:6:ASN:O	2:B:249:ARG:NH2	2.43	0.51
1:C:86:ARG:NH1	1:C:269:SER:O	2.42	0.51
1:C:26:PHE:CE1	2:D:69:VAL:HG23	2.45	0.51
1:C:48:THR:HB	1:C:69:ALA:HB3	1.92	0.51
2:B:92:ILE:HG12	2:B:144:TYR:CD2	2.46	0.51
2:B:24:GLY:HA2	2:B:48:ASP:O	2.10	0.50
1:C:72:ASN:CG	1:C:73:CYS:N	2.69	0.50
2:B:3:ASP:HB2	2:B:246:LYS:CA	2.34	0.50
2:B:58:MET:HB2	2:B:80:CYS:HB3	1.94	0.50
1:A:26:PHE:HB2	1:A:196:PHE:CD1	2.46	0.50
1:C:110:TRP:O	1:C:113:ALA:HB3	2.12	0.50
2:D:25:GLN:HB2	2:D:101:ARG:O	2.11	0.50
1:A:30:ARG:NH1	4:A:343:HOH:O	2.45	0.50
1:A:80:VAL:HG11	1:A:262:LEU:O	2.11	0.50
2:D:63:VAL:CG2	2:D:77:HIS:CE1	2.95	0.50
1:A:93:ALA:HB3	1:A:95:LYS:HG3	1.94	0.49
2:D:16:THR:O	2:D:20:GLN:HG2	2.12	0.49
2:B:92:ILE:HG12	2:B:144:TYR:CE2	2.47	0.49
2:D:222:LEU:HD11	2:D:231:VAL:HG21	1.93	0.49
1:C:178:ILE:HG13	1:C:210:VAL:HG22	1.94	0.49
2:D:156:ARG:HG2	2:D:156:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:HIS:O	2:B:224:ASN:HB3	2.12	0.49
2:D:83:PRO:HG2	4:D:267:HOH:O	2.13	0.49
2:B:238:GLU:HG3	4:B:323:HOH:O	2.11	0.49
1:A:206:LYS:HE3	1:A:207:TYR:CZ	2.48	0.48
1:A:93:ALA:CB	1:A:95:LYS:HG3	2.44	0.48
1:C:16:HIS:O	1:C:19:ASP:HB2	2.14	0.48
2:B:241:ASP:OD2	2:B:243:ALA:HB3	2.13	0.48
1:C:102:SER:OG	1:C:105:VAL:HG23	2.13	0.48
2:D:120:THR:OG1	2:D:166:THR:HG22	2.13	0.48
1:A:89:LYS:HE3	1:A:89:LYS:O	2.14	0.48
1:C:81:THR:HG22	1:C:83:VAL:O	2.14	0.48
2:D:214:PRO:HG3	2:D:237:LEU:O	2.13	0.48
1:A:119:PHE:HA	1:A:170:VAL:HG23	1.96	0.48
1:C:48:THR:HA	1:C:69:ALA:O	2.14	0.48
1:A:160:LYS:O	1:A:163:GLU:HB3	2.14	0.47
1:A:111:HIS:CE1	1:C:111:HIS:CE1	2.89	0.47
2:D:142:ALA:HB2	2:D:167:SER:HB3	1.95	0.47
2:B:64:GLU:HA	4:B:273:HOH:O	2.14	0.47
1:A:23:LEU:HD12	1:A:58:TRP:CE2	2.49	0.47
2:B:151:MET:O	2:B:193:THR:HA	2.15	0.47
2:B:218:PRO:HB3	2:B:231:VAL:HB	1.96	0.47
1:C:250:GLN:NE2	2:D:73:ARG:HH21	2.12	0.47
2:B:187:GLY:HA2	4:B:336:HOH:O	2.14	0.47
1:C:20:HIS:O	1:C:174:ASP:HB2	2.15	0.47
2:B:16:THR:O	2:B:20:GLN:HG2	2.15	0.47
2:B:35:LEU:CD2	2:B:66:PRO:HD2	2.45	0.47
2:B:209:LEU:CD2	2:B:231:VAL:HG12	2.45	0.47
1:A:282:TRP:CZ3	1:A:295:LYS:HG2	2.50	0.47
1:C:263:LYS:O	1:C:266:ASP:HB3	2.15	0.47
2:B:27:VAL:HG22	2:B:103:ILE:CG2	2.46	0.46
2:B:212:TYR:CE1	2:B:236:GLU:HB2	2.50	0.46
1:C:110:TRP:CZ3	1:C:197:GLN:HG3	2.51	0.46
2:D:65:VAL:HA	2:D:66:PRO:HD3	1.79	0.46
2:B:248:ILE:HA	2:B:252:ILE:HB	1.96	0.46
2:D:149:ILE:H	2:D:149:ILE:HD12	1.81	0.46
1:C:108:MET:HE2	1:C:120:LEU:HD11	1.97	0.46
1:C:18:GLY:HA2	1:C:46:ASP:O	2.16	0.46
2:D:174:PRO:HG2	2:D:203:LYS:O	2.15	0.46
1:A:14:TYR:HB2	1:A:209:ILE:HD11	1.98	0.45
2:D:30:GLY:O	2:D:35:LEU:HD13	2.16	0.45
2:D:246:LYS:HD3	2:D:246:LYS:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:GLU:O	2:B:254:PRO:HG3	2.17	0.45
2:B:64:GLU:OE2	2:B:73:ARG:NH1	2.49	0.45
2:B:111:ILE:HG22	2:B:151:MET:HE2	1.97	0.45
1:C:39:ILE:HG23	1:C:44:ILE:HB	1.99	0.45
2:B:158:PHE:O	2:B:226:GLY:HA3	2.17	0.45
1:C:155:ILE:HG13	1:C:165:VAL:HG22	1.98	0.45
1:C:268:VAL:HG11	1:C:278:PHE:CB	2.44	0.45
2:D:117:VAL:HG21	2:D:149:ILE:HG21	1.99	0.45
1:A:107:TYR:CE1	1:A:197:GLN:HB3	2.52	0.45
2:B:17:ILE:HD11	2:B:150:MET:SD	2.56	0.45
1:A:312:TYR:HE1	1:A:314:ILE:HD13	1.81	0.45
2:D:125:TYR:O	2:D:128:PRO:HD3	2.17	0.45
1:A:69:ALA:HA	1:A:97:THR:HB	1.99	0.45
1:A:59:ASP:OD1	1:A:84:SER:HB3	2.17	0.44
2:B:3:ASP:OD2	2:B:246:LYS:HG3	2.16	0.44
2:B:223:GLU:HG3	4:B:318:HOH:O	2.17	0.44
1:C:305:LYS:O	1:C:313:HIS:CD2	2.70	0.44
2:B:13:GLN:HG2	2:B:213:TYR:OH	2.17	0.44
1:A:263:LYS:HB3	4:A:444:HOH:O	2.16	0.44
1:C:36:VAL:HG21	1:C:57:ASP:HB2	1.99	0.44
1:A:180:ALA:O	1:A:212:CYS:HA	2.18	0.44
1:A:108:MET:O	1:A:111:HIS:N	2.50	0.44
1:A:282:TRP:O	1:A:286:LEU:HD12	2.18	0.44
2:B:43:ARG:HH11	2:B:252:ILE:HG13	1.82	0.44
2:B:86:ARG:NH2	1:C:200:ASP:OD1	2.47	0.44
1:C:30:ARG:NH1	4:C:338:HOH:O	2.50	0.44
1:C:111:HIS:HD2	1:C:200:ASP:OD1	2.01	0.44
2:D:199:LYS:HG3	2:D:210:ALA:HB2	1.99	0.44
1:A:88:ARG:O	1:A:92:GLU:HB2	2.18	0.44
1:A:267:LYS:HE3	1:A:268:VAL:HG23	1.99	0.44
1:C:75:THR:HG22	1:C:84:SER:HB2	2.00	0.44
1:C:88:ARG:HG3	1:C:89:LYS:H	1.83	0.44
1:C:180:ALA:O	1:C:212:CYS:HA	2.17	0.43
2:D:157:ARG:HG2	2:D:157:ARG:HH11	1.83	0.43
2:B:209:LEU:HD13	2:B:221:VAL:HG11	1.99	0.43
1:A:105:VAL:O	1:A:109:MET:HG3	2.17	0.43
1:C:213:GLU:HG3	1:C:254:LEU:HD12	2.00	0.43
2:D:125:TYR:HD2	2:D:126:HIS:CD2	2.36	0.43
1:C:305:LYS:O	1:C:313:HIS:HD2	2.02	0.43
2:B:7:TYR:CD2	2:B:240:PRO:HD2	2.54	0.43
2:B:232:SER:O	2:B:233:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:CD	1:A:135:GLY:H	2.25	0.43
2:D:197:ILE:HG12	2:D:211:ALA:HB3	1.99	0.43
1:C:73:CYS:SG	1:C:103:GLN:HA	2.59	0.43
1:A:28:THR:C	1:A:249:SER:HB2	2.44	0.42
1:A:183:ALA:HA	1:A:188:THR:O	2.19	0.42
1:A:73:CYS:HB3	1:A:106:ILE:HG13	2.00	0.42
1:A:78:SER:HB2	2:B:68:SER:HB3	2.00	0.42
1:A:231:ILE:HA	1:A:232:PRO:HD3	1.79	0.42
1:A:99:GLU:HG2	1:A:141:ARG:NH2	2.35	0.42
1:C:62:ILE:CG1	1:C:67:VAL:HG21	2.48	0.42
1:C:75:THR:HG22	1:C:84:SER:CB	2.49	0.42
1:C:124:LEU:O	1:C:125:MET:HB2	2.20	0.42
1:A:213:GLU:HG3	1:A:254:LEU:CD1	2.48	0.42
1:C:60:MET:HE2	1:C:60:MET:HB3	1.91	0.42
1:A:124:LEU:O	1:A:125:MET:HB2	2.19	0.42
1:A:154:TYR:CE1	1:A:166:VAL:HG22	2.54	0.42
2:B:43:ARG:HD2	2:B:252:ILE:HD11	2.01	0.42
1:C:98:MET:CE	2:D:131:ARG:NH1	2.82	0.42
1:A:288:ASP:OD1	1:A:291:GLU:HG3	2.20	0.42
2:D:53:VAL:HG23	2:D:55:SER:H	1.85	0.42
2:D:246:LYS:HE2	2:D:250:GLU:OE1	2.19	0.42
1:A:34:ALA:O	1:A:37:PHE:HB2	2.19	0.42
1:C:59:ASP:CG	1:C:84:SER:HB3	2.44	0.42
1:C:244:TYR:HB2	1:C:293:LEU:HD21	2.01	0.42
2:B:197:ILE:HG13	2:B:210:ALA:HB3	2.01	0.41
1:C:62:ILE:HG12	1:C:67:VAL:HG21	2.02	0.41
1:A:58:TRP:O	1:A:62:ILE:HG13	2.20	0.41
2:B:53:VAL:CG2	2:B:57:LEU:HB2	2.50	0.41
2:B:152:GLN:HB2	2:B:157:ARG:CD	2.50	0.41
2:D:64:GLU:OE2	2:D:73:ARG:HD3	2.20	0.41
2:D:164:TYR:CE2	2:D:166:THR:HG22	2.56	0.41
2:D:199:LYS:HG3	2:D:210:ALA:CB	2.49	0.41
2:B:86:ARG:HH22	1:C:200:ASP:HA	1.84	0.41
2:B:170:TRP:CZ2	2:B:187:GLY:HA3	2.56	0.41
1:A:28:THR:O	1:A:249:SER:HB2	2.21	0.41
2:B:53:VAL:HG23	2:B:57:LEU:HB2	2.01	0.41
1:C:259:ASN:HD22	1:C:259:ASN:HA	1.52	0.41
2:D:35:LEU:HD12	2:D:35:LEU:HA	1.88	0.41
2:D:111:ILE:HG22	2:D:151:MET:HE2	2.03	0.41
1:C:312:TYR:CD2	2:D:73:ARG:HG3	2.56	0.41
2:B:222:LEU:HD22	4:B:313:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:THR:O	2:B:133:THR:HG22	2.21	0.41
2:B:3:ASP:HB3	2:B:250:GLU:OE1	2.21	0.41
1:C:46:ASP:HA	1:C:68:LYS:HB2	2.03	0.41
2:D:120:THR:OG1	2:D:166:THR:CG2	2.69	0.41
1:A:184:SER:HB2	1:A:219:ASP:OD1	2.21	0.41
1:A:33:TYR:O	1:A:34:ALA:C	2.64	0.40
1:C:189:VAL:HG21	1:C:210:VAL:HG21	2.02	0.40
1:A:111:HIS:HD2	1:A:200:ASP:OD1	2.04	0.40
1:A:210:VAL:HG13	1:A:210:VAL:O	2.22	0.40
2:B:30:GLY:HA2	2:B:69:VAL:CG1	2.51	0.40
1:A:244:TYR:HA	1:A:255:TYR:CZ	2.57	0.40
2:D:66:PRO:HB3	2:D:71:ASP:HB3	2.04	0.40
2:D:83:PRO:HD2	2:D:86:ARG:CD	2.52	0.40
1:A:235:CYS:HA	4:A:372:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/317 (99%)	294 (93%)	20 (6%)	1 (0%)	36	55
1	C	315/317 (99%)	296 (94%)	16 (5%)	3 (1%)	12	24
2	B	258/260 (99%)	239 (93%)	15 (6%)	4 (2%)	7	14
2	D	258/260 (99%)	237 (92%)	18 (7%)	3 (1%)	10	20
All	All	1146/1154 (99%)	1066 (93%)	69 (6%)	11 (1%)	12	24

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	233	LYS

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Mol	Chain	Res	Type
2	B	171	ILE
2	D	171	ILE
1	A	27	THR
2	B	54	GLU
2	D	5	THR
2	D	100	ASN
1	C	74	TYR
1	C	27	THR
2	B	69	VAL
1	C	56	GLY

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	265/265 (100%)	247 (93%)	18 (7%)	14	31
1	C	265/265 (100%)	250 (94%)	15 (6%)	18	39
2	B	217/217 (100%)	201 (93%)	16 (7%)	13	27
2	D	217/217 (100%)	201 (93%)	16 (7%)	13	27
All	All	964/964 (100%)	899 (93%)	65 (7%)	15	31

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

Mol	Chain	Res	Type
1	A	6	THR
1	A	15	VAL
1	A	47	LEU
1	A	50	LEU
1	A	86	ARG
1	A	88	ARG
1	A	89	LYS
1	A	108	MET
1	A	115	LEU
1	A	123	THR
1	A	153	LYS

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Mol	Chain	Res	Type
1	A	165	VAL
1	A	175	VAL
1	A	257	TYR
1	A	259	ASN
1	A	306	VAL
1	A	314	ILE
1	A	319	GLU
2	B	6	ASN
2	B	44	VAL
2	B	73	ARG
2	B	91	GLU
2	B	113	PRO
2	B	129	LYS
2	B	133	THR
2	B	160	ASN
2	B	166	THR
2	B	185	ASP
2	B	186	VAL
2	B	193	THR
2	B	203	LYS
2	B	219	GLU
2	B	250	GLU
2	B	251	GLU
1	C	31	LYS
1	C	47	LEU
1	C	48	THR
1	C	67	VAL
1	C	73	CYS
1	C	78	SER
1	C	86	ARG
1	C	88	ARG
1	C	96	LEU
1	C	115	LEU
1	C	147	VAL
1	C	208	THR
1	C	257	TYR
1	C	259	ASN
1	C	260	PRO
2	D	4	TYR
2	D	73	ARG
2	D	84	ASN
2	D	96	LEU

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Mol	Chain	Res	Type
2	D	129	LYS
2	D	152	GLN
2	D	153	HIS
2	D	161	LYS
2	D	174	PRO
2	D	185	ASP
2	D	204	THR
2	D	215	THR
2	D	216	SER
2	D	251	GLU
2	D	260	GLN
2	D	261	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	42	GLN
1	A	111	HIS
1	A	313	HIS
2	B	6	ASN
2	B	13	GLN
2	B	189	GLN
1	C	16	HIS
1	C	111	HIS
1	C	250	GLN
1	C	259	ASN
1	C	313	HIS
2	D	77	HIS
2	D	84	ASN
2	D	152	GLN
2	D	224	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.