



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:34 PM GMT

PDB ID : 1POI
Title : CRYSTAL STRUCTURE OF GLUTACONATE COENZYME A-TRANSFERASE FROM ACIDAMINOCOCCUS FERMENTANS TO 2.55 ANGSTOMS RESOLUTION
Authors : Jacob, U.; Mack, M.; Clausen, T.; Huber, R.; Buckel, W.; Messerschmidt, A.
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

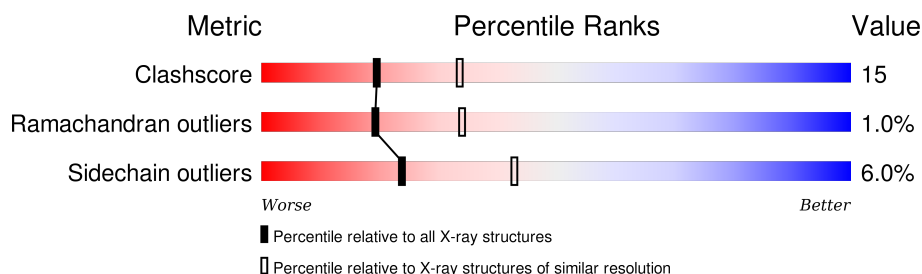
1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	317	 66% 31% •
1	C	317	 70% 28% •
2	B	260	 63% 32% 5%
2	D	260	 68% 30% •

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 (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is water.

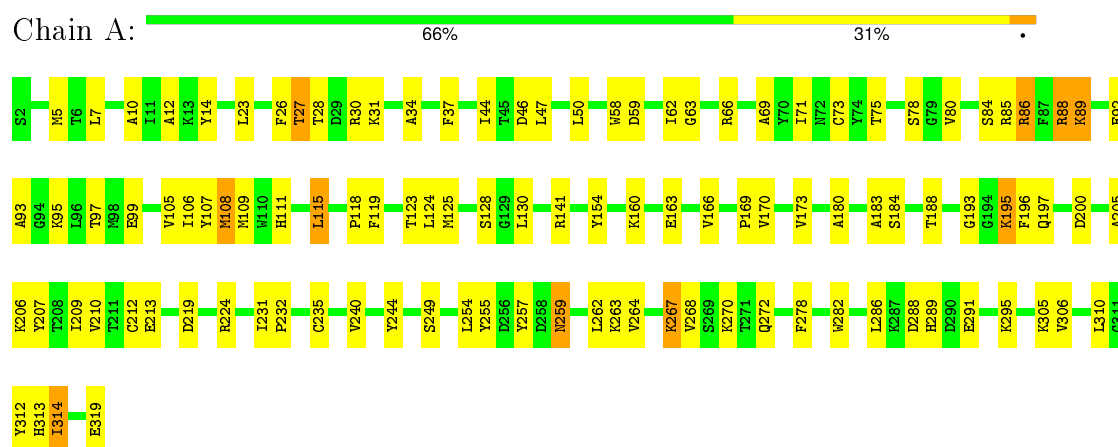
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		
4	B	91	Total	O	0	0
			91	91		
4	C	116	Total	O	0	0
			116	116		
4	D	80	Total	O	0	0
			80	80		

3 Residue-property plots

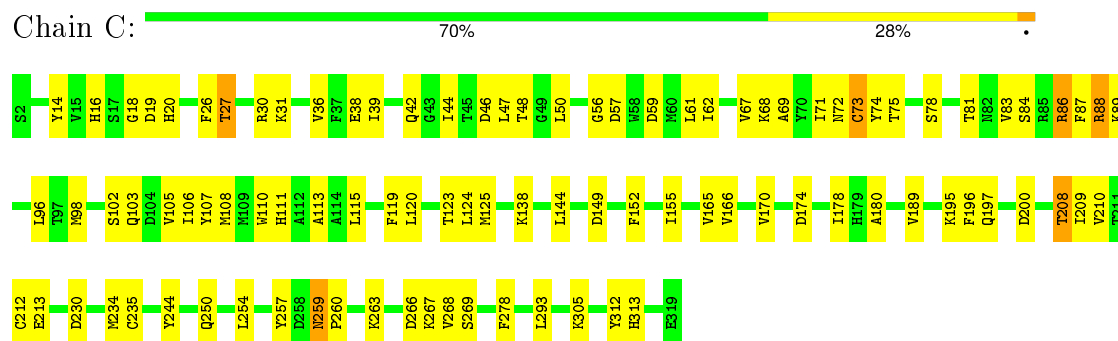
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

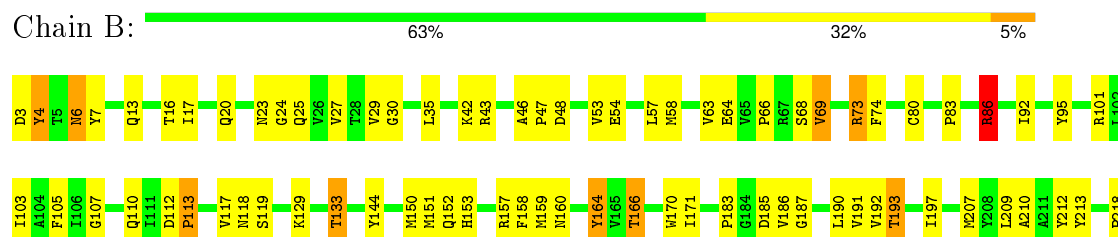
• Molecule 1: GLUTACONATE COENZYME A-TRANSFERASE

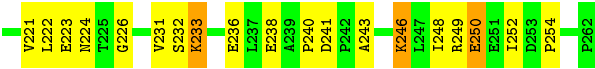


• Molecule 1: GLUTACONATE COENZYME A-TRANSFERASE

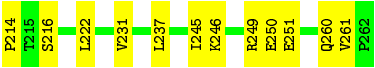
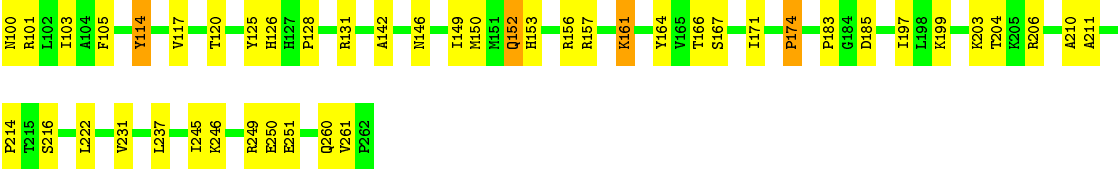
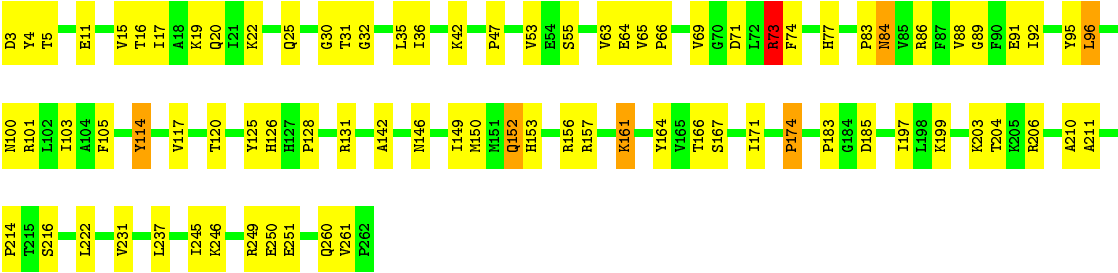


• Molecule 2: GLUTACONATE COENZYME A-TRANSFERASE





● Molecule 2: GLUTACONATE COENZYME A-TRANSFERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.55	0/2550	0.79	0/3458
1	C	0.56	0/2550	0.77	0/3458
2	B	0.49	0/2053	0.80	2/2786 (0.1%)
2	D	0.49	0/2053	0.76	1/2786 (0.0%)
All	All	0.53	0/9206	0.78	3/12488 (0.0%)

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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	86	ARG	NE-CZ-NH2	-6.36	117.12	120.30
2	B	63	VAL	N-CA-C	-5.22	96.90	111.00
2	D	73	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	164	TYR	Sidechain

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Mol	Chain	Res	Type	Group
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	75	0
1	C	2490	0	2449	70	0
2	B	2007	0	1987	73	0
2	D	2007	0	1987	65	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	267	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 (267) 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: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:H	2:D:84:ASN:HD22	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
2:D:32:GLY:O	2:D:36:ILE:HG12	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:191:VAL:HG21	2:B:207:MET:CE	2.25	0.66
1:A:12:ALA:HB2	4:A:416:HOH:O	1.95	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
2:B:119:SER:H	2:B:166:THR:CG2	2.12	0.62
1:A:206:LYS:HE3	1:A:207:TYR:CE2	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:191:VAL:HG21	2:B:207:MET:HE2	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
2:B:191:VAL:HG21	2:B:207:MET:HE1	1.87	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
2:D:35:LEU:HG	4:D:335:HOH:O	2.05	0.55
1:A:310:LEU:HG	4:A:426:HOH:O	2.07	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
2:B:25:GLN:HB2	2:B:101:ARG:O	2.08	0.54
1:A:23:LEU:HD12	1:A:58:TRP:NE1	2.22	0.54
1:A:46:ASP:CB	4:A:470:HOH:O	2.56	0.54
2:D:17:ILE:HG23	2:D:105:PHE:CE2	2.43	0.54
1:A:63:GLY:HA3	1:A:86:ARG:HG3	1.90	0.54
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:169:PRO:HA	4:A:375:HOH:O	2.06	0.53
1:A:268:VAL:HG11	1:A:278:PHE:CB	2.39	0.53
1:C:87:PHE:CE1	1:C:98:MET:SD	3.01	0.53
1:A:305:LYS:O	1:A:313:HIS:CD2	2.62	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:D:152:GLN:HB2	2:D:157:ARG:HE	1.75	0.52
2:D:3:ASP:N	2:D:249:ARG:HH11	2.06	0.52
2:B:95:TYR:CZ	2:B:183:PRO:HB3	2.45	0.52
2:D:88:VAL:O	2:D:91:GLU:HG2	2.10	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
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:HB3	2:D:161:LYS:NZ	2.24	0.52
1:C:152:PHE:CD2	1:C:166:VAL:HG13	2.45	0.52
1:A:272:GLN:HB2	4:A:467:HOH:O	2.09	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:209:LEU:HB3	2:B:231:VAL:HA	1.93	0.51
2:B:42:LYS:O	2:B:47:PRO:HA	2.10	0.51
2:B:27:VAL:HG12	2:B:29:VAL:HG13	1.92	0.51
2:B:4:TYR:CE1	2:B:6:ASN:HB3	2.44	0.51
2:D:31:THR:HG22	2:D:35:LEU:HD22	1.92	0.51
2:D:3:ASP:OD1	2:D:246:LYS:HB2	2.09	0.51
1:C:38:GLU:O	1:C:42:GLN:HG3	2.11	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
2:B:6:ASN:O	2:B:249:ARG:NH2	2.43	0.51
1:A:193:GLY:O	1:A:195:LYS:HE3	2.11	0.51
1:C:86:ARG:NH1	1:C:269:SER:O	2.42	0.51
1:A:115:LEU:O	2:D:89:GLY:HA2	2.10	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
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
2:D:25:GLN:HB2	2:D:101:ARG:O	2.11	0.50
1:C:110:TRP:O	1:C:113:ALA:HB3	2.12	0.50
2:D:63:VAL:CG2	2:D:77:HIS:CE1	2.95	0.50
1:A:80:VAL:HG11	1:A:262:LEU:O	2.11	0.50
1:A:30:ARG:NH1	4:A:343:HOH:O	2.45	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:195:LYS:HE2	1:C:230:ASP:CG	2.33	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
1:C:102:SER:OG	1:C:105:VAL:HG23	2.13	0.48
2:B:241:ASP:OD2	2:B:243:ALA:HB3	2.13	0.48
2:D:120:THR:OG1	2:D:166:THR:HG22	2.13	0.48
1:A:89:LYS:O	1:A:89:LYS:HE3	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:C:48:THR:HA	1:C:69:ALA:O	2.14	0.48
1:A:119:PHE:HA	1:A:170:VAL:HG23	1.96	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:218:PRO:HB3	2:B:231:VAL:HB	1.96	0.47
2:B:151:MET:O	2:B:193:THR:HA	2.15	0.47
1:C:250:GLN:NE2	2:D:73:ARG:HH21	2.12	0.47
1:C:20:HIS:O	1:C:174:ASP:HB2	2.15	0.47
2:B:187:GLY:HA2	4:B:336:HOH:O	2.14	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:72:ASN:CG	1:C:73:CYS:N	2.69	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
2:D:30:GLY:O	2:D:35:LEU:HD13	2.16	0.45
1:A:14:TYR:HB2	1:A:209:ILE:HD11	1.98	0.45
2:B:250:GLU:O	2:B:254:PRO:HG3	2.17	0.45
1:C:108:MET:HE2	1:C:120:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:GLU:OE2	2:B:73:ARG:NH1	2.49	0.45
1:C:39:ILE:HG23	1:C:44:ILE:HB	1.99	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
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: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
2:B:3:ASP:OD2	2:B:246:LYS:HG3	2.16	0.44
1:A:59:ASP:OD1	1:A:84:SER:HB3	2.17	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
2:B:86:ARG:NH2	1:C:200:ASP:OD1	2.47	0.44
1:C:111:HIS:HD2	1:C:200:ASP:OD1	2.01	0.44
2:B:43:ARG:HH11	2:B:252:ILE:HG13	1.82	0.44
1:A:282:TRP:O	1:A:286:LEU:HD12	2.18	0.44
1:C:30:ARG:NH1	4:C:338:HOH:O	2.50	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
2:B:232:SER:O	2:B:233:LYS: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
2:D:157:ARG:HG2	2:D:157:ARG:HH11	1.83	0.43
1:C:180:ALA:O	1:C:212:CYS:HA	2.17	0.43
2:B:209:LEU:HD13	2:B:221:VAL:HG11	1.99	0.43
1:C:213:GLU:HG3	1:C:254:LEU:HD12	2.00	0.43
1:A:105:VAL:O	1:A:109:MET:HG3	2.17	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
1:C:26:PHE:HD2	1:C:107:TYR:HH	1.65	0.43
2:B:7:TYR:CD2	2:B:240:PRO:HD2	2.54	0.43
2:D:197:ILE:HG12	2:D:211:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:CYS:SG	1:C:103:GLN:HA	2.59	0.43
1:A:183:ALA:HA	1:A:188:THR:O	2.19	0.42
1:A:78:SER:HB2	2:B:68:SER:HB3	2.00	0.42
1:A:73:CYS:HB3	1:A:106:ILE:HG13	2.00	0.42
1:A:231:ILE:HA	1:A:232:PRO:HD3	1.79	0.42
1:C:75:THR:HG22	1:C:84:SER:CB	2.49	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: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:98:MET:CE	2:D:131:ARG:NH1	2.82	0.42
2:B:43:ARG:HD2	2:B:252:ILE:HD11	2.01	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:D:246:LYS:HE2	2:D:250:GLU:OE1	2.19	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
1:A:34:ALA:O	1:A:37:PHE:HB2	2.19	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
2:B:53:VAL:CG2	2:B:57:LEU:HB2	2.50	0.41
1:A:58:TRP:O	1:A:62:ILE:HG13	2.20	0.41
2:D:164:TYR:CE2	2:D:166:THR:HG22	2.56	0.41
2:D:64:GLU:OE2	2:D:73:ARG:HD3	2.20	0.41
2:D:199:LYS:HG3	2:D:210:ALA:CB	2.49	0.41
2:B:152:GLN:HB2	2:B:157:ARG:CD	2.50	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
2:B:53:VAL:HG23	2:B:57:LEU:HB2	2.01	0.41
2:D:35:LEU:HA	2:D:35:LEU:HD12	1.88	0.41
1:C:259:ASN:HD22	1:C:259:ASN:HA	1.52	0.41
1:A:28:THR:O	1:A:249:SER:HB2	2.21	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
2:B:3:ASP:HB3	2:B:250:GLU:OE1	2.21	0.41
2:D:246:LYS:HD3	2:D:246:LYS:C	2.42	0.41
2:D:120:THR:OG1	2:D:166:THR:CG2	2.69	0.41
1:C:46:ASP:HA	1:C:68:LYS:HB2	2.03	0.41
1:A:75:THR:O	2:B:133:THR:HG22	2.21	0.41
1:A:184:SER:HB2	1:A:219:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:83:PRO:HD2	2:D:86:ARG:CD	2.52	0.40
2:D:66:PRO:HB3	2:D:71:ASP:HB3	2.04	0.40
1:A:244:TYR:HA	1:A:255:TYR:CZ	2.57	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%)	46	68
1	C	315/317 (99%)	296 (94%)	16 (5%)	3 (1%)	19	34
2	B	258/260 (99%)	239 (93%)	15 (6%)	4 (2%)	12	21
2	D	258/260 (99%)	237 (92%)	18 (7%)	3 (1%)	16	29
All	All	1146/1154 (99%)	1066 (93%)	69 (6%)	11 (1%)	19	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	233	LYS
2	B	171	ILE
2	D	171	ILE
1	A	27	THR
2	B	54	GLU
2	D	5	THR
2	D	100	ASN

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Mol	Chain	Res	Type
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%)	250 (94%)	15 (6%)	25	46
1	C	265/265 (100%)	252 (95%)	13 (5%)	31	55
2	B	217/217 (100%)	202 (93%)	15 (7%)	19	35
2	D	217/217 (100%)	202 (93%)	15 (7%)	19	35
All	All	964/964 (100%)	906 (94%)	58 (6%)	24	43

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	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	195	LYS
1	A	224	ARG
1	A	257	TYR
1	A	259	ASN
1	A	267	LYS
1	A	306	VAL
1	A	314	ILE
1	A	319	GLU
2	B	4	TYR
2	B	6	ASN

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Mol	Chain	Res	Type
2	B	73	ARG
2	B	74	PHE
2	B	86	ARG
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	246	LYS
2	B	250	GLU
1	C	47	LEU
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	208	THR
1	C	234	MET
1	C	257	TYR
1	C	259	ASN
1	C	260	PRO
1	C	267	LYS
2	D	4	TYR
2	D	73	ARG
2	D	74	PHE
2	D	84	ASN
2	D	96	LEU
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	216	SER
2	D	251	GLU
2	D	260	GLN
2	D	261	VAL

Some 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	72	ASN
1	A	111	HIS
1	A	303	ASN
1	A	313	HIS
2	B	6	ASN
2	B	13	GLN
2	B	25	GLN
2	B	224	ASN
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

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.