



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:32 PM UTC

PDB ID : 6DLI / pdb_00006dli
Title : Crystal structure of glutamate racemase from *Thermus thermophilus* in complex with Beta-chloro-D-alanine
Authors : Cooling, G.T.; Vance, N.R.; Spies, M.A.
Deposited on : 2018-06-01
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

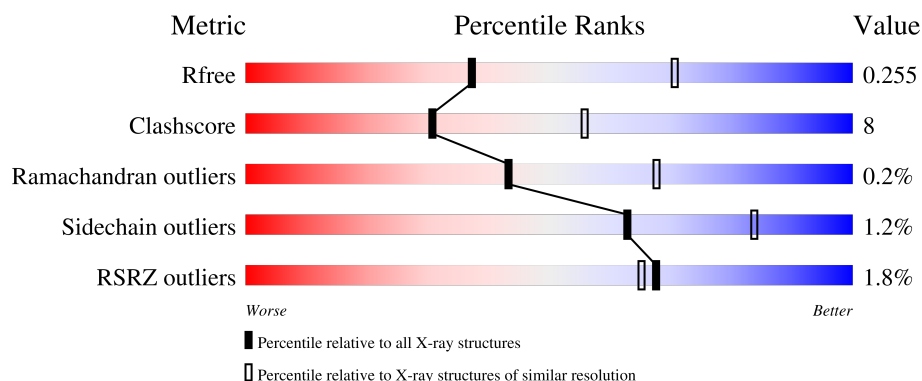
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	278	 3% 77% 14% 8%
1	B	278	 3% 78% 13% 8%
1	C	278	 % 76% 15% 8%
1	D	278	 % 76% 15% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7650 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 Glutamate racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1860	1204	315	337	4			
1	B	256	Total	C	N	O	S	0	0	0
			1888	1220	324	340	4			
1	C	256	Total	C	N	O	S	0	0	0
			1904	1229	325	346	4			
1	D	256	Total	C	N	O	S	0	0	0
			1902	1227	327	344	4			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q5SHT7
A	-19	GLY	-	expression tag	UNP Q5SHT7
A	-18	SER	-	expression tag	UNP Q5SHT7
A	-17	SER	-	expression tag	UNP Q5SHT7
A	-16	HIS	-	expression tag	UNP Q5SHT7
A	-15	HIS	-	expression tag	UNP Q5SHT7
A	-14	HIS	-	expression tag	UNP Q5SHT7
A	-13	HIS	-	expression tag	UNP Q5SHT7
A	-12	HIS	-	expression tag	UNP Q5SHT7
A	-11	HIS	-	expression tag	UNP Q5SHT7
A	-10	SER	-	expression tag	UNP Q5SHT7
A	-9	SER	-	expression tag	UNP Q5SHT7
A	-8	GLY	-	expression tag	UNP Q5SHT7
A	-7	LEU	-	expression tag	UNP Q5SHT7
A	-6	VAL	-	expression tag	UNP Q5SHT7
A	-5	PRO	-	expression tag	UNP Q5SHT7
A	-4	ARG	-	expression tag	UNP Q5SHT7
A	-3	GLY	-	expression tag	UNP Q5SHT7
A	-2	SER	-	expression tag	UNP Q5SHT7
A	-1	HIS	-	expression tag	UNP Q5SHT7
A	0	MET	-	expression tag	UNP Q5SHT7

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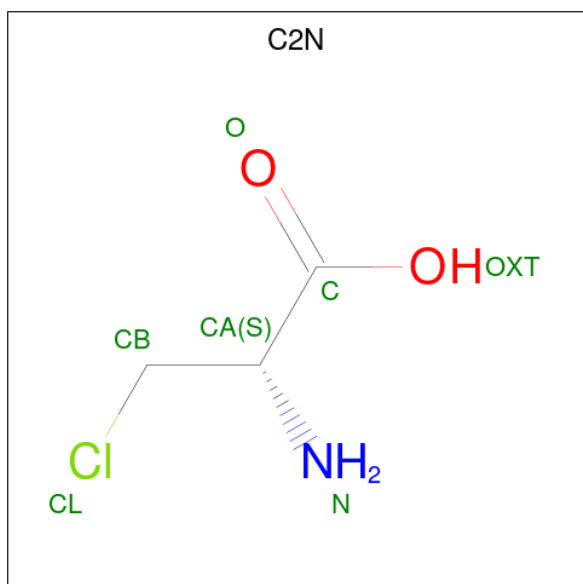
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	expression tag	UNP Q5SHT7
B	-20	MET	-	expression tag	UNP Q5SHT7
B	-19	GLY	-	expression tag	UNP Q5SHT7
B	-18	SER	-	expression tag	UNP Q5SHT7
B	-17	SER	-	expression tag	UNP Q5SHT7
B	-16	HIS	-	expression tag	UNP Q5SHT7
B	-15	HIS	-	expression tag	UNP Q5SHT7
B	-14	HIS	-	expression tag	UNP Q5SHT7
B	-13	HIS	-	expression tag	UNP Q5SHT7
B	-12	HIS	-	expression tag	UNP Q5SHT7
B	-11	HIS	-	expression tag	UNP Q5SHT7
B	-10	SER	-	expression tag	UNP Q5SHT7
B	-9	SER	-	expression tag	UNP Q5SHT7
B	-8	GLY	-	expression tag	UNP Q5SHT7
B	-7	LEU	-	expression tag	UNP Q5SHT7
B	-6	VAL	-	expression tag	UNP Q5SHT7
B	-5	PRO	-	expression tag	UNP Q5SHT7
B	-4	ARG	-	expression tag	UNP Q5SHT7
B	-3	GLY	-	expression tag	UNP Q5SHT7
B	-2	SER	-	expression tag	UNP Q5SHT7
B	-1	HIS	-	expression tag	UNP Q5SHT7
B	0	MET	-	expression tag	UNP Q5SHT7
B	1	VAL	-	expression tag	UNP Q5SHT7
C	-20	MET	-	expression tag	UNP Q5SHT7
C	-19	GLY	-	expression tag	UNP Q5SHT7
C	-18	SER	-	expression tag	UNP Q5SHT7
C	-17	SER	-	expression tag	UNP Q5SHT7
C	-16	HIS	-	expression tag	UNP Q5SHT7
C	-15	HIS	-	expression tag	UNP Q5SHT7
C	-14	HIS	-	expression tag	UNP Q5SHT7
C	-13	HIS	-	expression tag	UNP Q5SHT7
C	-12	HIS	-	expression tag	UNP Q5SHT7
C	-11	HIS	-	expression tag	UNP Q5SHT7
C	-10	SER	-	expression tag	UNP Q5SHT7
C	-9	SER	-	expression tag	UNP Q5SHT7
C	-8	GLY	-	expression tag	UNP Q5SHT7
C	-7	LEU	-	expression tag	UNP Q5SHT7
C	-6	VAL	-	expression tag	UNP Q5SHT7
C	-5	PRO	-	expression tag	UNP Q5SHT7
C	-4	ARG	-	expression tag	UNP Q5SHT7
C	-3	GLY	-	expression tag	UNP Q5SHT7
C	-2	SER	-	expression tag	UNP Q5SHT7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP Q5SHT7
C	0	MET	-	expression tag	UNP Q5SHT7
C	1	VAL	-	expression tag	UNP Q5SHT7
D	-20	MET	-	expression tag	UNP Q5SHT7
D	-19	GLY	-	expression tag	UNP Q5SHT7
D	-18	SER	-	expression tag	UNP Q5SHT7
D	-17	SER	-	expression tag	UNP Q5SHT7
D	-16	HIS	-	expression tag	UNP Q5SHT7
D	-15	HIS	-	expression tag	UNP Q5SHT7
D	-14	HIS	-	expression tag	UNP Q5SHT7
D	-13	HIS	-	expression tag	UNP Q5SHT7
D	-12	HIS	-	expression tag	UNP Q5SHT7
D	-11	HIS	-	expression tag	UNP Q5SHT7
D	-10	SER	-	expression tag	UNP Q5SHT7
D	-9	SER	-	expression tag	UNP Q5SHT7
D	-8	GLY	-	expression tag	UNP Q5SHT7
D	-7	LEU	-	expression tag	UNP Q5SHT7
D	-6	VAL	-	expression tag	UNP Q5SHT7
D	-5	PRO	-	expression tag	UNP Q5SHT7
D	-4	ARG	-	expression tag	UNP Q5SHT7
D	-3	GLY	-	expression tag	UNP Q5SHT7
D	-2	SER	-	expression tag	UNP Q5SHT7
D	-1	HIS	-	expression tag	UNP Q5SHT7
D	0	MET	-	expression tag	UNP Q5SHT7
D	1	VAL	-	expression tag	UNP Q5SHT7

- Molecule 2 is 3-chloro-D-alanine (CCD ID: C2N) (formula: $C_3H_6ClNO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			7	3	1	1	2		
2	B	1	Total	C	Cl	N	O	0	0
			7	3	1	1	2		
2	C	1	Total	C	Cl	N	O	0	0
			7	3	1	1	2		
2	D	1	Total	C	Cl	N	O	0	0
			7	3	1	1	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

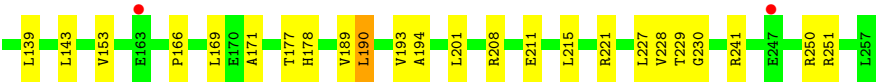
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	20	Total	O	0	0
			20	20		
4	C	19	Total	O	0	0
			19	19		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	O	0	0
			3	3		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.89Å 95.61Å 179.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.05 – 2.70 60.05 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (60.05-2.70) 99.6 (60.05-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.209 , 0.244 0.220 , 0.255	Depositor DCC
R_{free} test set	1871 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtrriage
Anisotropy	0.456	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7650	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0554e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, C2N

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	0/1902	0.95	2/2606 (0.1%)
1	B	0.87	2/1930 (0.1%)	1.02	2/2638 (0.1%)
1	C	0.92	0/1946	1.05	4/2657 (0.2%)
1	D	0.79	0/1944	0.97	1/2655 (0.0%)
All	All	0.83	2/7722 (0.0%)	1.00	9/10556 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	PRO	C-O	-5.44	1.17	1.24
1	B	141	VAL	C-O	-5.33	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	ALA	CA-C-N	11.16	133.79	119.84
1	C	165	ALA	C-N-CA	11.16	133.79	119.84
1	B	89	ASP	N-CA-C	6.23	120.96	113.23
1	C	82	ALA	N-CA-C	5.68	121.24	113.97
1	A	89	ASP	N-CA-C	5.35	119.66	113.18
1	A	25	ARG	CB-CG-CD	-5.34	99.01	111.30
1	B	221	ARG	N-CA-C	-5.34	100.53	109.24
1	C	220	GLY	N-CA-C	5.20	120.93	112.61
1	D	54	ARG	CB-CG-CD	5.16	123.16	111.30

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	1860	0	1833	29	0
1	B	1888	0	1887	30	0
1	C	1904	0	1910	34	0
1	D	1902	0	1906	40	0
2	A	7	0	3	2	0
2	B	7	0	3	0	0
2	C	7	0	3	1	0
2	D	7	0	3	1	0
3	A	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	8	0	0	0	0
4	B	20	0	0	1	0
4	C	19	0	0	2	0
4	D	3	0	0	0	0
All	All	7650	0	7572	126	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 8.

All (126) 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:D:75:CYS:SG	2:D:301:C2N:N	2.69	0.66
1:D:189:VAL:O	1:D:190:LEU:HD23	1.95	0.66
1:B:211:GLU:HG2	1:B:216:LEU:HD12	1.78	0.64
1:A:157:VAL:HG23	1:B:153:VAL:HG21	1.81	0.63
1:C:15:VAL:HG21	1:C:238:LEU:HG	1.82	0.62
1:C:241:ARG:C	1:C:242:LEU:HD23	2.25	0.61
1:A:75:CYS:SG	2:A:301:C2N:N	2.73	0.61
1:B:28:LEU:CD2	1:B:216:LEU:HD21	2.31	0.61
1:B:28:LEU:HD22	1:B:216:LEU:HD21	1.84	0.60
1:B:3:ASP:OD1	1:B:5:LYS:N	2.34	0.60
1:D:251:ARG:HH11	1:D:251:ARG:HG3	1.67	0.59
1:C:211:GLU:HB2	1:C:216:LEU:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:HB3	1:D:64:LEU:HD13	1.84	0.59
1:D:103:ARG:HG3	1:D:106:ARG:NH1	2.18	0.59
1:D:251:ARG:HG3	1:D:251:ARG:NH1	2.16	0.59
1:D:229:THR:O	1:D:251:ARG:NH1	2.35	0.58
1:C:127:ARG:HD2	1:C:128:TYR:CE1	2.39	0.57
1:C:99:GLU:OE2	1:C:103:ARG:HD3	2.05	0.56
1:C:101:ALA:HA	1:C:201:LEU:HD13	1.87	0.56
1:D:101:ALA:HA	1:D:201:LEU:HD13	1.86	0.56
1:C:99:GLU:OE1	1:C:103:ARG:NH1	2.39	0.55
1:B:28:LEU:HD22	1:B:216:LEU:CD2	2.38	0.54
1:A:16:GLY:O	1:A:177:THR:HB	2.07	0.54
1:B:141:VAL:HB	1:B:142:PRO:HD3	1.89	0.54
1:C:161:TYR:C	1:C:162:LEU:HD23	2.32	0.54
1:C:242:LEU:HD23	1:C:242:LEU:N	2.22	0.54
1:C:136:ALA:C	1:C:138:PRO:HD3	2.33	0.54
1:C:31:GLU:OE1	1:C:69:LYS:NZ	2.37	0.53
1:C:211:GLU:HB2	1:C:216:LEU:HD12	1.89	0.53
1:D:166:PRO:HB2	1:D:169:LEU:CD1	2.39	0.53
1:B:136:ALA:C	1:B:138:PRO:HD3	2.34	0.53
1:B:241:ARG:HG2	1:B:241:ARG:O	2.08	0.53
1:C:156:LEU:HD12	1:D:153:VAL:HG12	1.92	0.53
1:B:28:LEU:HB3	1:B:31:GLU:HG2	1.91	0.52
1:C:75:CYS:SG	2:C:301:C2N:N	2.83	0.52
1:C:162:LEU:HD23	1:C:162:LEU:N	2.24	0.52
1:D:208:ARG:O	1:D:211:GLU:HB3	2.10	0.51
1:D:133:TRP:CZ2	1:D:135:LYS:HB2	2.45	0.51
1:A:232:PRO:HG3	1:A:251:ARG:HB2	1.93	0.51
1:C:77:THR:HG23	1:C:118:ALA:HB3	1.93	0.50
1:B:141:VAL:CB	1:B:142:PRO:HD3	2.41	0.50
1:D:42:VAL:CG2	1:D:43:PRO:HA	2.41	0.50
1:C:2:LYS:N	4:C:402:HOH:O	2.45	0.49
1:D:166:PRO:O	1:D:169:LEU:HD13	2.12	0.49
1:C:151:ASP:OD2	1:C:152:PRO:HD2	2.13	0.49
1:B:28:LEU:HB3	1:B:31:GLU:CG	2.43	0.49
1:A:179:TYR:N	1:A:180:PRO:CD	2.77	0.48
1:D:74:ALA:O	1:D:177:THR:CG2	2.61	0.48
1:A:101:ALA:HA	1:A:201:LEU:HD13	1.96	0.48
1:C:151:ASP:CG	1:C:152:PRO:HD2	2.38	0.48
1:D:189:VAL:O	1:D:189:VAL:HG12	2.14	0.48
1:B:3:ASP:OD1	1:B:3:ASP:C	2.57	0.47
1:D:230:GLY:C	1:D:251:ARG:NH2	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LEU:HD23	1:D:143:LEU:HA	1.52	0.47
1:B:151:ASP:OD1	1:B:153:VAL:N	2.36	0.47
1:C:99:GLU:CD	1:C:103:ARG:HH11	2.22	0.47
1:B:84:PRO:HG3	1:B:127:ARG:NH2	2.30	0.47
1:C:147:GLY:HA2	1:C:149:TRP:CZ3	2.49	0.46
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.45	0.46
1:D:251:ARG:HH11	1:D:251:ARG:CG	2.28	0.46
1:A:197:ASP:OD1	1:A:199:ALA:N	2.49	0.46
1:A:206:VAL:O	1:A:210:LEU:HG	2.14	0.46
1:D:36:PHE:HA	1:D:227:LEU:O	2.15	0.46
1:D:37:GLY:O	1:D:228:VAL:HA	2.16	0.45
1:D:215:LEU:HD23	1:D:215:LEU:HA	1.79	0.45
1:D:227:LEU:HD23	1:D:250:ARG:HG2	1.98	0.45
1:A:95:PHE:CG	1:A:206:VAL:HG22	2.52	0.45
1:B:12:ASP:CG	1:B:13:SER:N	2.75	0.44
1:B:179:TYR:N	1:B:180:PRO:CD	2.79	0.44
1:C:123:GLY:C	1:C:126:PRO:HD2	2.41	0.44
1:A:226:HIS:O	1:A:249:VAL:HA	2.17	0.44
1:B:49:LEU:HD21	1:B:122:SER:HB2	2.00	0.44
1:B:137:CYS:N	1:B:138:PRO:HD3	2.32	0.44
1:D:7:PRO:HB3	1:D:32:GLU:HG2	1.98	0.44
1:A:113:LEU:O	1:A:134:ALA:HA	2.17	0.44
1:D:74:ALA:O	1:D:177:THR:HG21	2.17	0.44
1:D:241:ARG:HE	1:D:241:ARG:HB2	1.50	0.43
1:A:51:MET:HA	1:A:54:ARG:NH1	2.33	0.43
1:B:77:THR:HG23	1:B:118:ALA:HB3	2.00	0.43
1:C:37:GLY:O	1:C:228:VAL:HA	2.18	0.43
1:A:112:GLY:C	1:A:172:LEU:HD12	2.43	0.43
1:D:171:ALA:HA	1:D:194:ALA:O	2.18	0.43
1:B:141:VAL:N	1:B:142:PRO:CD	2.80	0.43
1:C:166:PRO:HB2	1:C:169:LEU:HG	2.01	0.43
1:A:157:VAL:CG2	1:B:153:VAL:HG21	2.48	0.43
1:C:54:ARG:NH1	4:C:403:HOH:O	2.52	0.43
1:B:58:GLU:HG2	1:B:257:LEU:HB3	2.01	0.42
1:B:113:LEU:O	1:B:134:ALA:HA	2.17	0.42
1:C:179:TYR:N	1:C:180:PRO:CD	2.82	0.42
1:C:83:LEU:HD23	1:C:83:LEU:HA	1.82	0.42
1:D:169:LEU:N	1:D:169:LEU:HD12	2.34	0.42
1:B:232:PRO:HG3	1:B:251:ARG:HB2	2.00	0.42
1:D:123:GLY:C	1:D:126:PRO:HD2	2.44	0.42
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:VAL:HG21	1:B:238:LEU:HG	2.01	0.42
1:A:37:GLY:O	1:A:228:VAL:HA	2.20	0.42
1:A:197:ASP:OD1	1:A:197:ASP:C	2.63	0.42
1:C:168:ASP:OD1	1:C:168:ASP:N	2.33	0.42
1:C:211:GLU:HB2	1:C:216:LEU:HD11	2.01	0.42
1:D:42:VAL:HG22	1:D:43:PRO:HA	2.01	0.42
1:D:54:ARG:HH11	1:D:54:ARG:CB	2.32	0.42
1:D:189:VAL:O	1:D:189:VAL:CG1	2.67	0.42
1:A:109:ARG:CB	1:A:170:GLU:OE2	2.68	0.42
1:C:176:CYS:HB3	1:C:179:TYR:CG	2.55	0.42
1:D:27:LEU:C	1:D:29:PRO:HD3	2.45	0.41
1:A:52:VAL:O	1:A:55:PHE:HB2	2.19	0.41
1:A:75:CYS:SG	2:A:301:C2N:CA	3.08	0.41
1:D:16:GLY:HA3	1:D:178:HIS:CE1	2.56	0.41
1:D:166:PRO:HB2	1:D:169:LEU:HD13	2.02	0.41
1:A:211:GLU:HB2	1:A:216:LEU:HD11	2.02	0.41
1:B:99:GLU:CG	1:B:128:TYR:CE2	3.03	0.41
1:C:156:LEU:HD12	1:D:153:VAL:CG1	2.50	0.41
1:A:127:ARG:HD2	1:A:128:TYR:CE2	2.55	0.41
1:C:112:GLY:O	1:C:172:LEU:HD12	2.21	0.41
1:B:251:ARG:NE	4:B:402:HOH:O	2.53	0.41
1:A:40:ALA:O	1:B:47:LYS:HE3	2.21	0.41
1:D:190:LEU:HD23	1:D:190:LEU:HA	1.89	0.41
1:D:221:ARG:NH1	1:D:221:ARG:HG3	2.36	0.41
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.96	0.40
1:C:127:ARG:O	1:C:127:ARG:HG2	2.20	0.40
1:C:156:LEU:HB2	1:D:153:VAL:CG1	2.52	0.40
1:D:42:VAL:HG22	1:D:43:PRO:CA	2.52	0.40
1:A:211:GLU:HA	1:A:216:LEU:HG	2.04	0.40
1:A:254:LEU:O	1:A:257:LEU:HB2	2.21	0.40
1:A:127:ARG:HH21	1:A:127:ARG:HD3	1.70	0.40
1:A:228:VAL:O	1:A:251:ARG:HA	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	254/278 (91%)	250 (98%)	4 (2%)	0	100	100
1	B	254/278 (91%)	248 (98%)	5 (2%)	1 (0%)	30	54
1	C	254/278 (91%)	250 (98%)	3 (1%)	1 (0%)	30	54
1	D	254/278 (91%)	250 (98%)	4 (2%)	0	100	100
All	All	1016/1112 (91%)	998 (98%)	16 (2%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	PRO
1	B	218	PRO

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	177/214 (83%)	175 (99%)	2 (1%)	65	85
1	B	183/214 (86%)	180 (98%)	3 (2%)	55	80
1	C	187/214 (87%)	186 (100%)	1 (0%)	81	92
1	D	186/214 (87%)	183 (98%)	3 (2%)	55	80
All	All	733/856 (86%)	724 (99%)	9 (1%)	63	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	LEU
1	A	162	LEU
1	B	58	GLU
1	B	151	ASP

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Mol	Chain	Res	Type
1	B	242	LEU
1	C	162	LEU
1	D	139	LEU
1	D	190	LEU
1	D	193	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	HIS
1	B	76	ASN
1	B	117	GLN
1	C	76	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

7 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
3	GOL	D	302	-	5,5,5	1.02	0	5,5,5	0.77	0
2	C2N	D	301	-	4,6,6	1.32	1 (25%)	1,7,7	2.58	1 (100%)
3	GOL	A	302	-	5,5,5	0.57	0	5,5,5	0.89	0
2	C2N	A	301	-	4,6,6	1.41	1 (25%)	1,7,7	2.58	1 (100%)
2	C2N	C	301	-	4,6,6	1.79	1 (25%)	1,7,7	3.33	1 (100%)
2	C2N	B	301	-	4,6,6	1.92	1 (25%)	1,7,7	3.74	1 (100%)
3	GOL	C	302	-	5,5,5	0.26	0	5,5,5	0.32	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	GOL	D	302	-	-	4/4/4/4	-
2	C2N	D	301	-	-	1/5/6/6	-
3	GOL	A	302	-	-	1/4/4/4	-
2	C2N	A	301	-	-	1/5/6/6	-
2	C2N	C	301	-	-	1/5/6/6	-
2	C2N	B	301	-	-	1/5/6/6	-
3	GOL	C	302	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	C2N	OXT-C	-3.19	1.20	1.30
2	C	301	C2N	OXT-C	-3.08	1.20	1.30
2	A	301	C2N	OXT-C	-2.56	1.22	1.30
2	D	301	C2N	OXT-C	-2.51	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	C2N	OXT-C-O	-3.74	115.59	124.08
2	C	301	C2N	OXT-C-O	-3.33	116.53	124.08
2	D	301	C2N	OXT-C-O	-2.58	118.22	124.08
2	A	301	C2N	OXT-C-O	-2.58	118.22	124.08

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	C2N	C-CA-CB-CL
2	B	301	C2N	C-CA-CB-CL
2	C	301	C2N	C-CA-CB-CL
2	D	301	C2N	C-CA-CB-CL
3	C	302	GOL	O1-C1-C2-C3
3	C	302	GOL	C1-C2-C3-O3
3	D	302	GOL	O1-C1-C2-O2
3	D	302	GOL	O1-C1-C2-C3
3	D	302	GOL	C1-C2-C3-O3
3	C	302	GOL	O2-C2-C3-O3
3	A	302	GOL	C1-C2-C3-O3
3	C	302	GOL	O1-C1-C2-O2
3	D	302	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	C2N	1	0
2	A	301	C2N	2	0
2	C	301	C2N	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/278 (92%)	0.05	7 (2%) 56 53	42, 62, 93, 106	0
1	B	256/278 (92%)	0.05	7 (2%) 56 53	39, 61, 90, 104	0
1	C	256/278 (92%)	0.06	2 (0%) 82 81	41, 63, 88, 102	0
1	D	256/278 (92%)	0.04	2 (0%) 82 81	43, 65, 89, 102	0
All	All	1024/1112 (92%)	0.05	18 (1%) 67 65	39, 62, 89, 106	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	VAL	4.7
1	A	188	ALA	3.6
1	A	193	VAL	3.5
1	A	162	LEU	3.2
1	A	2	LYS	3.0
1	A	128	TYR	2.6
1	C	149	TRP	2.6
1	B	186	ILE	2.4
1	C	154	ALA	2.4
1	B	163	GLU	2.4
1	B	14	GLY	2.3
1	B	195	LEU	2.3
1	D	163	GLU	2.3
1	D	247	GLU	2.2
1	B	2	LYS	2.1
1	A	74	ALA	2.1
1	B	220	GLY	2.1
1	A	163	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	302	6/6	0.63	0.25	77,83,89,93	0
3	GOL	A	302	6/6	0.68	0.13	90,94,98,100	0
3	GOL	D	302	6/6	0.79	0.18	66,76,91,93	0
2	C2N	D	301	7/7	0.84	0.14	62,68,71,79	0
2	C2N	C	301	7/7	0.87	0.13	56,58,66,77	0
2	C2N	A	301	7/7	0.88	0.12	55,57,63,79	0
2	C2N	B	301	7/7	0.91	0.11	53,53,54,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.