



Full wwPDB X-ray Structure Validation Report i

Aug 19, 2023 – 07:47 PM EDT

PDB ID : 2GZM
Title : Crystal Structure of the Glutamate Racemase from Bacillus anthracis
Authors : May, M.; Santarsiero, B.D.; Johnson, M.E.; Mesecar, A.D.
Deposited on : 2006-05-11
Resolution : 1.99 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

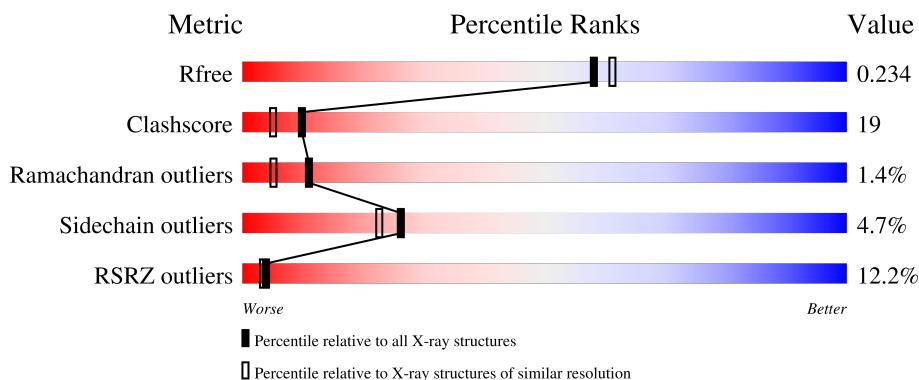
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

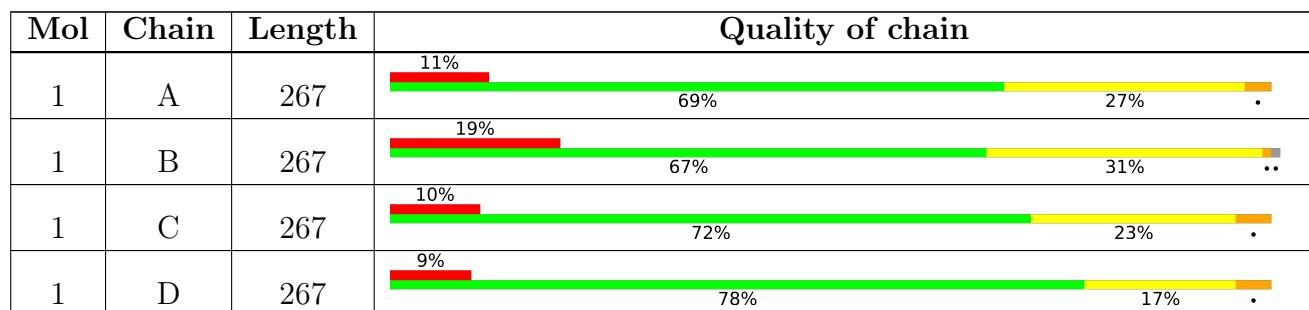
The reported resolution of this entry is 1.99 Å.

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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.



2 Entry composition [\(i\)](#)

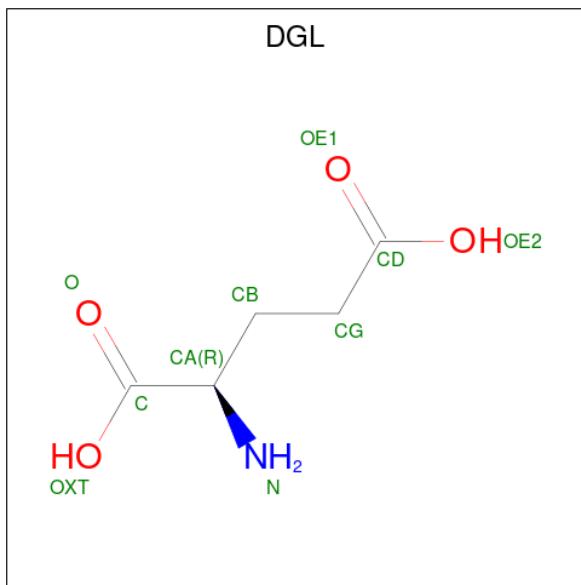
There are 3 unique types of molecules in this entry. The entry contains 8887 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	266	Total 2099	C 1335	N 359	O 394	S 11	0	3	0
1	B	265	Total 2070	C 1317	N 352	O 389	S 12	0	1	0
1	C	266	Total 2082	C 1323	N 356	O 392	S 11	0	1	0
1	D	266	Total 2102	C 1335	N 362	O 394	S 11	0	3	0

- Molecule 2 is D-GLUTAMIC ACID (three-letter code: DGL) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 10	C 5	N 1	O 4	0	0
2	B	1	Total 10	C 5	N 1	O 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 10 5 1 4	0	0
2	D	1	Total C N O 10 5 1 4	0	0

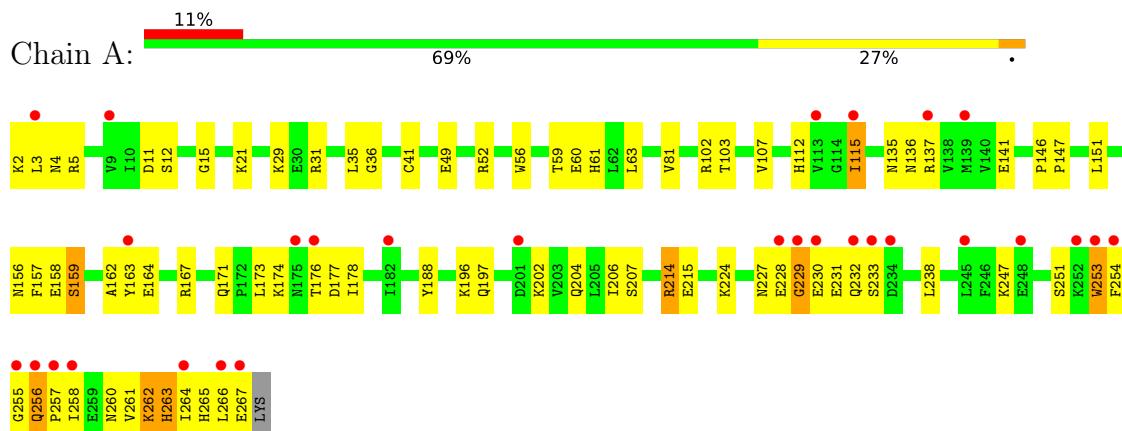
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	130	Total O 130 130	0	0
3	B	95	Total O 95 95	0	0
3	C	130	Total O 130 130	0	0
3	D	139	Total O 139 139	0	0

3 Residue-property plots

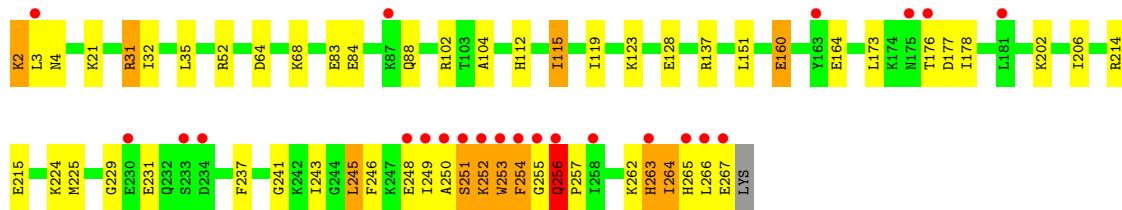
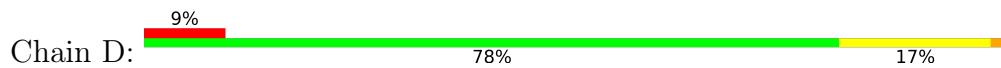
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Glutamate racemase



H265
L266
E267
LYS

- Molecule 1: Glutamate racemase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.35 Å 90.52 Å 116.80 Å 90.00° 100.02° 90.00°	Depositor
Resolution (Å)	20.00 – 1.99 19.76 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-1.99) 98.5 (19.76-1.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.32 (at 1.99 Å)	Xtriage
Refinement program	CNS	Depositor
R , R_{free}	0.203 , 0.241 0.197 , 0.234	Depositor DCC
R_{free} test set	3930 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 65.7	EDS
L-test for twinning ²	$< L > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8887	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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: DGL

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	0.44	0/2135	0.67	0/2891
1	B	0.41	0/2106	0.65	0/2853
1	C	0.45	0/2118	0.67	0/2869
1	D	0.49	0/2138	0.70	1/2894 (0.0%)
All	All	0.45	0/8497	0.67	1/11507 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	245	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

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	2099	0	2155	89	0
1	B	2070	0	2123	95	0
1	C	2082	0	2133	78	0
1	D	2102	0	2157	88	0
2	A	10	0	7	0	0
2	B	10	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	7	0	0
2	D	10	0	7	0	0
3	A	130	0	0	7	0
3	B	95	0	0	5	0
3	C	130	0	0	4	0
3	D	139	0	0	10	0
All	All	8887	0	8596	327	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 19.

All (327) 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:256:GLN:HB3	1:D:257:PRO:HA	1.12	1.08
1:C:102:ARG:HD2	1:D:214[A]:ARG:NH1	1.69	1.08
1:D:256:GLN:HB3	1:D:257:PRO:CA	1.86	1.03
1:D:252:LYS:HG3	1:D:253:TRP:HD1	1.23	1.02
1:A:31:ARG:HG2	1:A:232:GLN:HG3	1.45	0.96
1:C:256:GLN:HB3	1:C:257:PRO:HA	1.43	0.96
1:A:256:GLN:HB3	1:A:257:PRO:HA	1.45	0.95
1:A:214[A]:ARG:HH21	1:B:102:ARG:HB3	1.30	0.94
1:B:2:LYS:HD2	1:B:3:LEU:H	1.33	0.93
1:B:264:ILE:HG22	1:B:265:HIS:H	1.33	0.93
1:D:245:LEU:HD12	1:D:246:PHE:N	1.85	0.92
1:C:214:ARG:NH1	1:D:102[A]:ARG:HD2	1.86	0.90
1:B:243:ILE:HD11	1:B:262:LYS:H	1.33	0.90
1:D:252:LYS:HG3	1:D:253:TRP:CD1	2.08	0.88
1:D:102[B]:ARG:NH1	3:D:536:HOH:O	2.06	0.88
1:D:248:GLU:HA	1:D:251:SER:HB3	1.56	0.88
1:D:245:LEU:HD12	1:D:246:PHE:H	1.39	0.87
1:C:135:ASN:OD1	1:C:137[A]:ARG:HG2	1.76	0.86
1:D:243:ILE:HD11	1:D:262[A]:LYS:N	1.90	0.86
1:D:243:ILE:HD11	1:D:262[B]:LYS:N	1.90	0.86
1:A:261:VAL:HG22	1:D:123:LYS:HG2	1.58	0.86
1:B:256:GLN:HB3	1:B:257:PRO:HA	1.59	0.84
1:A:112:HIS:CE1	1:A:176:THR:HG23	2.13	0.84
1:A:262[A]:LYS:HD3	1:A:263:HIS:N	1.93	0.83
1:C:258:ILE:HG13	1:C:259:GLU:H	1.43	0.82
1:D:245:LEU:HD13	1:D:249:ILE:HD12	1.61	0.82
1:D:256:GLN:CB	1:D:257:PRO:HA	2.04	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LYS:HE3	1:B:258:ILE:HA	1.62	0.81
1:B:180:THR:HG23	1:B:206:ILE:HD11	1.60	0.80
1:C:58:MET:HG2	1:C:265:HIS:HE1	1.45	0.80
1:D:2:LYS:HD3	1:D:4:ASN:H	1.48	0.78
1:A:163:TYR:HB3	3:A:602:HOH:O	1.82	0.77
1:A:156:ASN:O	1:A:162:ALA:HB2	1.85	0.77
1:B:180:THR:CG2	1:B:206:ILE:HD11	2.14	0.76
1:A:214[A]:ARG:HE	1:B:102:ARG:HG2	1.50	0.76
1:A:2:LYS:O	1:A:5:ARG:HD3	1.84	0.76
1:D:202:LYS:O	1:D:202:LYS:HG2	1.86	0.75
1:C:256:GLN:HB3	1:C:257:PRO:CA	2.17	0.75
1:B:119:ILE:HD11	1:B:123:LYS:HD2	1.69	0.74
1:C:14:VAL:HG11	1:C:249:ILE:HG21	1.70	0.74
1:A:251:SER:HA	1:A:255:GLY:HA2	1.70	0.73
1:A:251:SER:HA	1:A:255:GLY:CA	2.18	0.73
1:C:155:GLY:HA3	1:C:252:LYS:HE3	1.70	0.73
1:B:54:PHE:O	1:B:58[A]:MET:HG3	1.88	0.73
1:D:256:GLN:HE21	1:D:256:GLN:H	1.36	0.73
1:A:256:GLN:HB3	1:A:257:PRO:CA	2.18	0.73
1:B:57:GLU:HB3	1:B:265:HIS:CE1	2.23	0.72
1:A:176:THR:CG2	1:A:178:ILE:HG23	2.20	0.71
1:A:171:GLN:HE22	1:A:174:LYS:HD2	1.55	0.71
1:A:103:THR:N	1:B:214:ARG:HH12	1.89	0.70
1:B:128:GLU:HG3	3:B:533:HOH:O	1.90	0.70
1:B:48:ARG:NH1	1:B:80:VAL:HG22	2.07	0.69
1:C:102:ARG:HD2	1:D:214[A]:ARG:CZ	2.21	0.69
1:B:235:HIS:O	1:B:259:GLU:HG2	1.92	0.69
1:D:2:LYS:HD3	1:D:3:LEU:N	2.06	0.69
1:B:206:ILE:HD12	1:B:206:ILE:N	2.08	0.69
1:A:103:THR:N	1:B:214:ARG:NH1	2.40	0.68
1:A:214[A]:ARG:HG2	1:A:214[A]:ARG:HH11	1.58	0.68
1:D:251:SER:HA	1:D:255:GLY:HA2	1.75	0.68
1:D:245:LEU:HD13	1:D:249:ILE:CD1	2.24	0.68
1:A:31:ARG:HG2	1:A:232:GLN:CG	2.23	0.67
1:D:243:ILE:HD11	1:D:262[A]:LYS:H	1.58	0.67
1:B:7:ILE:HD11	1:B:220:LEU:HD11	1.76	0.67
1:C:14:VAL:HG13	1:C:253:TRP:CH2	2.29	0.67
1:C:229:GLY:O	1:C:230:GLU:HB2	1.94	0.66
1:A:266:LEU:O	1:A:267:GLU:HB2	1.94	0.66
1:C:258:ILE:HG13	1:C:259:GLU:N	2.10	0.65
1:B:264:ILE:HG22	1:B:265:HIS:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLU:HG2	3:A:596:HOH:O	1.96	0.65
1:A:176:THR:HG22	1:A:178:ILE:HG23	1.78	0.65
1:C:155:GLY:HA3	1:C:252:LYS:CE	2.27	0.64
1:C:251:SER:HA	1:C:255:GLY:HA2	1.79	0.64
1:B:2:LYS:CD	1:B:3:LEU:H	2.08	0.64
1:A:262[B]:LYS:HD3	1:A:263:HIS:N	2.12	0.64
1:A:102:ARG:NH1	3:A:565:HOH:O	2.29	0.64
1:B:243:ILE:HG13	1:B:262:LYS:HB2	1.78	0.64
1:D:119:ILE:HG13	1:D:123:LYS:HD3	1.80	0.64
1:D:256:GLN:HE21	1:D:256:GLN:N	1.96	0.63
1:C:52:ARG:HG3	1:C:81:VAL:HG12	1.79	0.63
1:A:102:ARG:NH2	1:A:215:GLU:OE2	2.28	0.63
1:C:106:LYS:HE3	1:D:214[B]:ARG:HD2	1.79	0.63
1:D:214[B]:ARG:NH2	3:D:561:HOH:O	2.31	0.63
1:A:35:LEU:HD21	1:A:265:HIS:HE1	1.63	0.63
1:D:176:THR:HG22	1:D:177:ASP:H	1.64	0.63
1:B:102:ARG:NH1	1:B:215:GLU:OE2	2.32	0.62
1:C:155:GLY:CA	1:C:252:LYS:HE3	2.29	0.62
1:C:251:SER:HA	1:C:255:GLY:CA	2.28	0.62
1:A:171:GLN:NE2	1:A:174:LYS:HD2	2.13	0.62
1:D:245:LEU:HD22	1:D:249:ILE:HD11	1.81	0.62
1:A:157:PHE:CD1	1:A:158:GLU:HG3	2.35	0.62
1:D:202:LYS:HB3	3:D:615:HOH:O	1.99	0.62
1:D:241:GLY:O	1:D:262[A]:LYS:HD3	2.00	0.62
1:D:256:GLN:CB	1:D:257:PRO:CA	2.70	0.62
1:B:39:ALA:HB2	1:B:240:THR:O	1.99	0.62
1:D:243:ILE:HD11	1:D:262[B]:LYS:H	1.59	0.61
1:B:48:ARG:HH22	1:B:124:SER:HB2	1.64	0.61
1:C:246:PHE:CD2	1:C:260:ASN:ND2	2.68	0.61
1:D:176:THR:HG22	1:D:177:ASP:N	2.15	0.61
1:B:247:LYS:HE2	1:B:258:ILE:HG23	1.83	0.61
1:C:135:ASN:OD1	1:C:137[B]:ARG:HG2	2.01	0.61
1:B:2:LYS:HD3	1:B:3:LEU:HG	1.83	0.61
1:D:35:LEU:HD13	1:D:263:HIS:CE1	2.36	0.61
1:B:14:VAL:HG11	1:B:249:ILE:HG21	1.83	0.60
1:C:15:GLY:HA2	1:C:253:TRP:CH2	2.36	0.60
1:A:49:GLU:H	1:A:49:GLU:CD	2.05	0.60
1:B:252:LYS:C	1:B:253:TRP:HD1	2.05	0.60
1:A:264[A]:ILE:HD13	1:D:128:GLU:OE1	2.02	0.60
1:A:2:LYS:HG3	1:A:3:LEU:H	1.66	0.60
1:A:264[A]:ILE:HG21	1:D:128:GLU:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:MET:HG2	1:C:265:HIS:CE1	2.32	0.59
1:C:112:HIS:CE1	1:C:176:THR:HG23	2.37	0.59
1:C:256:GLN:CB	1:C:257:PRO:HA	2.26	0.59
1:B:245:LEU:O	1:B:249:ILE:HG13	2.03	0.59
1:B:259:GLU:O	1:B:259:GLU:HG3	2.02	0.59
1:D:245:LEU:O	1:D:248:GLU:N	2.34	0.59
1:B:14:VAL:HG21	1:B:249:ILE:HG22	1.85	0.58
1:B:57:GLU:HB3	1:B:265:HIS:HE1	1.66	0.58
1:B:2:LYS:HD2	1:B:3:LEU:N	2.13	0.58
1:A:15:GLY:HA2	1:A:253:TRP:HH2	1.68	0.58
1:A:112:HIS:CE1	1:A:176:THR:CG2	2.85	0.58
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.69	0.57
1:B:257:PRO:HG2	1:B:259:GLU:H	1.69	0.57
1:A:247:LYS:HE3	1:A:257:PRO:O	2.04	0.57
1:A:214[A]:ARG:HH11	1:A:214[A]:ARG:CG	2.17	0.57
1:C:141:GLU:HG3	1:C:176:THR:HG21	1.86	0.57
1:A:196:LYS:HD2	3:A:570:HOH:O	2.03	0.57
1:C:35:LEU:HD12	1:C:36:GLY:N	2.19	0.57
1:B:50:GLU:HB3	1:B:54:PHE:CE2	2.40	0.56
1:C:254:PHE:HD1	1:C:255:GLY:H	1.53	0.56
1:B:55:THR:HG21	1:B:81:VAL:HG21	1.88	0.56
1:B:243:ILE:CD1	1:B:262:LYS:H	2.12	0.56
1:A:176:THR:HG21	1:A:178:ILE:HG23	1.86	0.56
1:C:231:GLU:HG2	3:D:623:HOH:O	2.05	0.56
1:B:14:VAL:HG21	1:B:249:ILE:CG2	2.35	0.56
1:D:243:ILE:CD1	3:D:567:HOH:O	2.53	0.56
1:C:176:THR:CG2	1:C:178:ILE:HG23	2.35	0.56
1:A:253:TRP:CD1	1:A:253:TRP:C	2.79	0.56
1:B:57:GLU:C	1:B:265:HIS:HE1	2.09	0.56
1:B:157:PHE:CD1	1:B:158:GLU:HG3	2.41	0.56
1:D:2:LYS:CD	1:D:4:ASN:H	2.18	0.56
1:A:214[A]:ARG:NE	1:B:102:ARG:HG2	2.19	0.55
1:A:214[A]:ARG:HD3	1:B:106:LYS:HD2	1.88	0.55
1:A:256:GLN:CB	1:A:257:PRO:HA	2.29	0.55
1:B:115:ILE:HD13	1:B:115:ILE:C	2.27	0.55
1:C:56:TRP:NE1	1:C:84:GLU:OE2	2.34	0.55
1:A:147:PRO:O	1:A:151:LEU:HD13	2.06	0.55
1:B:245:LEU:HB3	1:B:249:ILE:HD11	1.89	0.55
1:D:104:ALA:HA	1:D:206:ILE:CD1	2.36	0.55
1:B:164:GLU:O	1:B:168:GLU:HG3	2.07	0.55
1:B:258:ILE:HG22	1:B:258:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLU:O	1:A:163:TYR:HE1	1.90	0.54
1:A:29:LYS:HG2	1:A:231:GLU:HG2	1.88	0.54
1:A:264[B]:ILE:HG21	1:D:128:GLU:OE1	2.07	0.54
1:A:214[A]:ARG:NH2	1:B:102:ARG:HB3	2.12	0.54
1:A:228:GLU:O	1:A:229:GLY:O	2.26	0.54
1:B:46:ARG:NH1	1:B:50:GLU:OE1	2.38	0.54
1:B:157:PHE:CZ	1:B:252:LYS:HD3	2.42	0.54
1:C:176:THR:HG22	1:C:178:ILE:HG23	1.90	0.54
1:C:2:LYS:HD2	1:C:2:LYS:N	2.23	0.53
1:D:257:PRO:HB2	3:D:628:HOH:O	2.08	0.53
1:A:107:VAL:HG21	1:A:204:GLN:HG2	1.89	0.53
1:B:112:HIS:NE2	1:B:176:THR:HB	2.24	0.53
1:D:253:TRP:CD1	1:D:253:TRP:N	2.75	0.53
1:A:262[A]:LYS:HD3	1:A:262[A]:LYS:C	2.29	0.52
1:B:135:ASN:O	1:B:138:VAL:HG12	2.10	0.52
1:C:104:ALA:HA	1:C:206:ILE:HD11	1.92	0.52
1:B:258:ILE:HD12	1:B:258:ILE:N	2.25	0.51
1:C:102:ARG:HD2	1:D:214[A]:ARG:HH11	1.67	0.51
1:D:245:LEU:HA	1:D:248:GLU:HG2	1.93	0.51
1:C:243:ILE:HG22	1:C:247:LYS:HE2	1.91	0.51
1:A:157:PHE:CE1	1:A:158:GLU:HG3	2.46	0.51
1:B:34:TYR:HE2	1:B:246:PHE:HZ	1.59	0.51
1:C:15:GLY:HA2	1:C:253:TRP:HH2	1.76	0.51
1:C:266:LEU:O	1:C:267:GLU:HB2	2.11	0.50
1:D:119:ILE:CG1	1:D:123:LYS:HD3	2.41	0.50
1:D:251:SER:O	1:D:252:LYS:CB	2.59	0.50
1:C:115:ILE:C	1:C:115:ILE:HD13	2.31	0.50
1:D:266:LEU:O	1:D:267:GLU:HB3	2.11	0.50
1:B:177:ASP:HA	3:B:591:HOH:O	2.11	0.50
1:D:68:LYS:O	1:D:225:MET:HE1	2.11	0.50
1:C:163:TYR:O	1:C:167:ARG:HB2	2.11	0.50
1:A:167:ARG:NH2	3:A:602:HOH:O	2.45	0.50
1:C:256:GLN:HE22	1:C:258:ILE:HG23	1.77	0.50
1:A:61:HIS:HE1	3:A:567:HOH:O	1.93	0.49
1:A:251:SER:HA	1:A:255:GLY:N	2.27	0.49
1:D:102[B]:ARG:NH2	1:D:215:GLU:OE2	2.31	0.49
1:D:245:LEU:CD1	1:D:246:PHE:N	2.69	0.49
1:A:254:PHE:CD2	1:A:255:GLY:N	2.81	0.49
1:B:82:LEU:O	1:B:86:GLN:HG3	2.13	0.49
1:C:14:VAL:HG11	1:C:249:ILE:CG2	2.41	0.49
1:B:245:LEU:HB3	1:B:249:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:HD12	1:C:35:LEU:C	2.33	0.49
1:A:56:TRP:O	1:A:60:GLU:HG2	2.12	0.48
1:B:48:ARG:HH12	1:B:80:VAL:HG22	1.74	0.48
1:B:251:SER:C	1:B:253:TRP:H	2.14	0.48
1:B:256:GLN:HB3	1:B:257:PRO:CA	2.37	0.48
1:C:262:LYS:HE3	1:C:263:HIS:O	2.13	0.48
1:D:248:GLU:C	1:D:250:ALA:N	2.66	0.48
1:B:157:PHE:HZ	1:B:252:LYS:HD3	1.78	0.48
1:C:104:ALA:HA	1:C:206:ILE:CD1	2.43	0.48
1:C:262:LYS:HD3	1:C:262:LYS:C	2.34	0.48
1:D:112:HIS:O	1:D:178:ILE:HA	2.14	0.48
1:D:251:SER:O	1:D:252:LYS:HG2	2.12	0.48
1:A:176:THR:HG22	1:A:177:ASP:N	2.28	0.48
1:C:66:ASN:HA	3:C:574:HOH:O	2.13	0.48
1:C:214:ARG:NH1	1:C:214:ARG:HG2	2.29	0.47
1:D:253:TRP:HD1	1:D:253:TRP:H	1.57	0.47
1:C:162:ALA:O	1:C:166:VAL:HG23	2.15	0.47
1:B:112:HIS:HD1	1:B:139:MET:HB3	1.78	0.47
1:D:35:LEU:HD21	1:D:265:HIS:HE1	1.79	0.47
1:A:159:SER:O	1:A:163:TYR:HD1	1.97	0.47
1:D:249:ILE:HD13	3:D:635:HOH:O	2.14	0.47
1:A:188:TYR:CD1	1:A:188:TYR:N	2.81	0.47
1:B:115:ILE:HD13	1:B:116:ILE:N	2.29	0.47
1:B:250:ALA:HB3	3:B:597:HOH:O	2.15	0.47
1:D:263:HIS:C	1:D:263:HIS:CD2	2.88	0.47
1:C:86:GLN:HG2	1:C:93:VAL:HB	1.96	0.47
1:A:253:TRP:C	1:A:253:TRP:HD1	2.18	0.47
1:B:119:ILE:CD1	1:B:123:LYS:HD2	2.43	0.46
1:A:224:LYS:HD3	3:A:620:HOH:O	2.14	0.46
1:A:136:ASN:OD1	1:B:29:LYS:HE2	2.16	0.46
1:B:11:ASP:O	1:B:58[A]:MET:HE3	2.13	0.46
1:C:137[A]:ARG:HH11	1:C:137[A]:ARG:HG3	1.79	0.46
1:A:263:HIS:ND1	1:A:263:HIS:C	2.69	0.46
1:D:245:LEU:O	1:D:249:ILE:N	2.38	0.46
1:D:119:ILE:CD1	1:D:123:LYS:HD3	2.46	0.46
1:C:171:GLN:N	1:C:172:PRO:CD	2.80	0.46
1:B:40:ARG:NH1	1:B:54:PHE:CD1	2.85	0.45
1:B:119:ILE:O	1:B:123:LYS:HG3	2.15	0.45
1:D:237:PHE:CD2	1:D:257:PRO:HG3	2.51	0.45
1:B:256:GLN:CB	1:B:257:PRO:HA	2.37	0.45
1:C:211:GLU:OE1	1:D:214[B]:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LYS:HG2	1:D:254:PHE:CE1	2.51	0.45
1:B:48:ARG:HG2	1:B:48:ARG:HH11	1.80	0.45
1:C:58:MET:CG	1:C:265:HIS:HE1	2.21	0.45
1:C:188:TYR:CD1	1:C:188:TYR:N	2.84	0.45
1:A:21:LYS:NZ	1:A:254:PHE:CE2	2.77	0.45
1:C:83:GLU:HG3	3:C:569:HOH:O	2.17	0.45
1:C:102:ARG:HG2	1:D:214[A]:ARG:HD2	1.99	0.45
1:A:35:LEU:HD12	1:A:36:GLY:N	2.32	0.45
1:A:177:ASP:O	1:A:177:ASP:CG	2.55	0.45
1:B:250:ALA:HA	1:B:253:TRP:HB2	1.99	0.45
1:D:52:ARG:NH1	1:D:84:GLU:OE1	2.44	0.45
1:A:238:LEU:HB3	1:A:263:HIS:CD2	2.51	0.45
1:A:103:THR:HG22	1:A:206:ILE:HD12	1.98	0.45
1:C:177:ASP:CG	1:C:177:ASP:O	2.54	0.45
1:C:214:ARG:NH2	1:D:102[A]:ARG:HB3	2.32	0.45
1:C:228:GLU:O	1:C:229:GLY:O	2.35	0.45
1:C:156:ASN:O	1:C:162:ALA:HB2	2.17	0.45
1:D:104:ALA:HA	1:D:206:ILE:HD11	1.99	0.45
1:B:31:ARG:HG2	1:B:232:GLN:HG3	1.99	0.44
1:B:85:MET:O	1:B:89:LEU:HG	2.17	0.44
1:B:159:SER:O	1:B:163:TYR:HD1	2.00	0.44
1:B:252:LYS:C	1:B:253:TRP:CD1	2.89	0.44
1:D:21:LYS:NZ	1:D:21:LYS:HB3	2.31	0.44
1:A:202:LYS:HE2	1:A:202:LYS:HA	1.99	0.44
1:D:31:ARG:NH1	3:D:594:HOH:O	2.50	0.44
1:C:261:VAL:HG12	1:C:262:LYS:N	2.33	0.44
1:B:223:SER:O	1:B:225:MET:HG3	2.17	0.44
1:D:248:GLU:HA	1:D:251:SER:CB	2.38	0.44
1:D:254:PHE:O	1:D:256:GLN:O	2.36	0.44
1:D:256:GLN:N	1:D:256:GLN:NE2	2.65	0.44
1:A:176:THR:CG2	1:A:177:ASP:N	2.81	0.44
1:C:164:GLU:HB3	3:C:631:HOH:O	2.18	0.43
1:A:253:TRP:HD1	1:A:254:PHE:N	2.15	0.43
1:B:59:THR:HG21	1:B:85:MET:HE3	2.00	0.43
1:B:48:ARG:NH1	1:B:48:ARG:HG2	2.32	0.43
1:B:214:ARG:CZ	3:B:581:HOH:O	2.67	0.43
1:D:264:ILE:HG13	1:D:265:HIS:N	2.33	0.43
1:A:146:PRO:HB2	1:A:147:PRO:HD3	2.00	0.43
1:B:11:ASP:O	1:B:58[A]:MET:CE	2.66	0.43
1:B:235:HIS:O	1:B:259:GLU:CG	2.62	0.43
1:D:252:LYS:CG	1:D:253:TRP:CD1	2.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ASN:HA	1:A:227:ASN:ND2	2.33	0.43
1:A:59:THR:O	1:A:63:LEU:HG	2.19	0.43
1:D:21:LYS:HG2	1:D:254:PHE:CZ	2.53	0.43
1:A:256:GLN:HE22	1:A:258:ILE:CG1	2.32	0.43
1:B:48:ARG:NH2	1:B:124:SER:HB2	2.32	0.43
1:A:135:ASN:OD1	1:A:137:ARG:HB3	2.19	0.43
1:B:110:THR:O	1:B:111:TYR:HB2	2.19	0.43
1:A:141:GLU:HG3	1:A:176:THR:HG21	2.01	0.42
1:B:14:VAL:HG11	1:B:249:ILE:CG2	2.48	0.42
1:A:264[A]:ILE:HG23	1:D:128:GLU:OE2	2.20	0.42
1:B:171:GLN:N	1:B:172:PRO:CD	2.82	0.42
1:B:256:GLN:CB	1:B:257:PRO:CA	2.97	0.42
1:D:251:SER:O	1:D:252:LYS:HB3	2.19	0.42
1:A:102:ARG:C	1:B:214:ARG:NH1	2.73	0.42
1:A:158:GLU:O	1:A:163:TYR:CE1	2.70	0.42
1:B:34:TYR:HB3	1:B:237:PHE:CD1	2.54	0.42
1:A:52:ARG:HA	1:A:81:VAL:HG11	2.02	0.42
1:A:264[B]:ILE:HG23	1:D:128:GLU:OE2	2.20	0.42
1:B:57:GLU:HG2	1:B:266:LEU:O	2.19	0.42
1:B:242:LYS:O	1:B:245:LEU:HB2	2.19	0.42
1:C:245:LEU:O	1:C:249:ILE:HG13	2.20	0.42
1:C:15:GLY:HA2	1:C:253:TRP:CZ3	2.54	0.42
1:C:61:HIS:HD2	3:C:597:HOH:O	2.02	0.42
1:D:224:LYS:HE2	3:D:639:HOH:O	2.19	0.42
1:C:165:VAL:HA	1:C:168:GLU:HG2	2.02	0.42
1:A:173:LEU:O	1:A:174:LYS:C	2.58	0.41
1:A:214[A]:ARG:CG	1:A:214[A]:ARG:NH1	2.76	0.41
1:D:243:ILE:HD11	3:D:567:HOH:O	2.16	0.41
1:A:115:ILE:C	1:A:115:ILE:HD13	2.41	0.41
1:B:236:LEU:HD21	1:B:238:LEU:HD21	2.01	0.41
1:D:160:GLU:O	1:D:164:GLU:HG3	2.20	0.41
1:C:49:GLU:OE1	1:C:49:GLU:HA	2.19	0.41
1:C:176:THR:HG22	1:C:177:ASP:N	2.36	0.41
1:D:253:TRP:HD1	1:D:253:TRP:N	2.16	0.41
1:C:139:MET:HE2	1:C:141:GLU:OE2	2.20	0.41
1:A:112:HIS:ND1	1:A:177:ASP:OD1	2.36	0.41
1:A:254:PHE:CG	1:A:255:GLY:N	2.87	0.41
1:A:12:SER:O	1:A:41:CYS:HB2	2.21	0.41
1:B:261:VAL:HG23	1:B:261:VAL:O	2.21	0.41
1:B:262:LYS:HD2	1:B:263:HIS:H	1.86	0.41
1:C:151:LEU:HD21	1:C:162:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:SER:HA	1:C:255:GLY:N	2.35	0.41
1:C:155:GLY:HA3	1:C:252:LYS:HE2	2.03	0.41
1:C:243:ILE:O	1:C:247:LYS:HD3	2.21	0.40
1:D:2:LYS:HD3	1:D:3:LEU:H	1.81	0.40
1:D:112:HIS:ND1	1:D:177:ASP:OD1	2.26	0.40
1:C:176:THR:HG21	1:C:178:ILE:HG23	2.02	0.40
1:C:243:Ile:HG13	1:C:262:LYS:HB2	2.03	0.40
1:D:31:ARG:HD3	1:D:32:ILE:N	2.36	0.40
1:D:251:SER:O	1:D:252:LYS:CG	2.69	0.40
1:B:224:LYS:NZ	3:B:555:HOH:O	2.52	0.40
1:C:11:ASP:CG	1:C:12:SER:N	2.75	0.40
1:D:115:Ile:C	1:D:115:ILE:HD13	2.42	0.40
1:A:11:ASP:CG	1:A:12:SER:N	2.74	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	267/267 (100%)	253 (95%)	9 (3%)	5 (2%)	8 3
1	B	264/267 (99%)	240 (91%)	21 (8%)	3 (1%)	14 8
1	C	265/267 (99%)	255 (96%)	8 (3%)	2 (1%)	19 13
1	D	267/267 (100%)	259 (97%)	3 (1%)	5 (2%)	8 3
All	All	1063/1068 (100%)	1007 (95%)	41 (4%)	15 (1%)	11 5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	B	175	ASN

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Mol	Chain	Res	Type
1	B	264	ILE
1	C	256	GLN
1	D	252	LYS
1	D	256	GLN
1	A	229	GLY
1	A	233	SER
1	B	257	PRO
1	C	229	GLY
1	D	229	GLY
1	D	231	GLU
1	D	251	SER
1	A	159	SER
1	A	230	GLU

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	235/233 (101%)	225 (96%)	10 (4%)	29 26
1	B	232/233 (100%)	224 (97%)	8 (3%)	37 36
1	C	233/233 (100%)	219 (94%)	14 (6%)	19 14
1	D	235/233 (101%)	220 (94%)	15 (6%)	17 13
All	All	935/932 (100%)	888 (95%)	47 (5%)	26 20

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ILE
1	A	197	GLN
1	A	207	SER
1	A	214[A]	ARG
1	A	214[B]	ARG
1	A	253	TRP
1	A	260	ASN
1	A	262[A]	LYS

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Mol	Chain	Res	Type
1	A	262[B]	LYS
1	A	263	HIS
1	B	2	LYS
1	B	115	ILE
1	B	129	GLU
1	B	137	ARG
1	B	173	LEU
1	B	239	THR
1	B	246	PHE
1	B	257	PRO
1	C	35	LEU
1	C	64	ASP
1	C	115	ILE
1	C	137[A]	ARG
1	C	137[B]	ARG
1	C	173	LEU
1	C	177	ASP
1	C	228	GLU
1	C	245	LEU
1	C	247	LYS
1	C	254	PHE
1	C	262	LYS
1	C	263	HIS
1	C	264	ILE
1	D	2	LYS
1	D	31	ARG
1	D	64	ASP
1	D	83	GLU
1	D	88	GLN
1	D	115	ILE
1	D	137	ARG
1	D	151	LEU
1	D	160	GLU
1	D	173	LEU
1	D	253	TRP
1	D	254	PHE
1	D	256	GLN
1	D	263	HIS
1	D	264	ILE

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	66	ASN
1	A	75	ASN
1	A	171	GLN
1	A	256	GLN
1	A	260	ASN
1	A	265	HIS
1	B	98	HIS
1	B	171	GLN
1	B	256	GLN
1	B	263	HIS
1	B	265	HIS
1	C	75	ASN
1	C	265	HIS
1	D	75	ASN
1	D	175	ASN
1	D	256	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DGL	D	504	-	8,9,9	0.65	0	10,11,11	1.29	1 (10%)
2	DGL	C	503	-	8,9,9	0.62	0	10,11,11	1.30	1 (10%)
2	DGL	B	502	-	8,9,9	0.63	0	10,11,11	1.22	1 (10%)
2	DGL	A	501	-	8,9,9	0.56	0	10,11,11	1.25	1 (10%)

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
2	DGL	D	504	-	-	2/9/9/9	-
2	DGL	C	503	-	-	2/9/9/9	-
2	DGL	B	502	-	-	2/9/9/9	-
2	DGL	A	501	-	-	2/9/9/9	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	DGL	CG-CB-CA	-3.13	106.54	113.84
2	B	502	DGL	CG-CB-CA	-2.75	107.43	113.84
2	A	501	DGL	CG-CB-CA	-2.57	107.85	113.84
2	D	504	DGL	CG-CB-CA	-2.39	108.27	113.84

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502	DGL	OE2-CD-CG-CB
2	B	502	DGL	OE1-CD-CG-CB
2	C	503	DGL	OE2-CD-CG-CB
2	C	503	DGL	OE1-CD-CG-CB
2	A	501	DGL	OE2-CD-CG-CB
2	D	504	DGL	OE1-CD-CG-CB
2	D	504	DGL	OE2-CD-CG-CB
2	A	501	DGL	OE1-CD-CG-CB

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)

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	266/267 (99%)	0.53	29 (10%) 5 5	21, 34, 65, 81	0
1	B	265/267 (99%)	0.99	50 (18%) 1 1	25, 43, 91, 102	0
1	C	266/267 (99%)	0.52	28 (10%) 6 5	19, 33, 68, 87	0
1	D	266/267 (99%)	0.44	23 (8%) 10 9	20, 30, 63, 76	0
All	All	1063/1068 (99%)	0.62	130 (12%) 4 3	19, 35, 70, 102	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	ILE	10.7
1	B	266	LEU	10.1
1	B	264	ILE	7.1
1	C	266	LEU	7.0
1	D	249	ILE	6.7
1	C	255	GLY	6.6
1	B	249	ILE	6.6
1	C	175	ASN	6.4
1	C	256	GLN	6.3
1	B	255	GLY	5.9
1	A	255	GLY	5.8
1	B	176	THR	5.7
1	A	256	GLN	5.6
1	B	257	PRO	5.5
1	D	3	LEU	5.4
1	D	175	ASN	5.3
1	C	267	GLU	5.2
1	B	265	HIS	5.2
1	B	254	PHE	5.1
1	C	254	PHE	5.0
1	D	254	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	266	LEU	4.8
1	B	175	ASN	4.7
1	A	234	ASP	4.7
1	B	4	ASN	4.7
1	B	234	ASP	4.6
1	A	175	ASN	4.6
1	A	254	PHE	4.5
1	A	245	LEU	4.4
1	D	251	SER	4.3
1	B	163	TYR	4.1
1	D	248	GLU	4.0
1	B	256	GLN	4.0
1	C	248	GLU	4.0
1	B	230	GLU	4.0
1	A	228	GLU	3.9
1	D	256	GLN	3.8
1	A	233	SER	3.7
1	C	230	GLU	3.7
1	D	255	GLY	3.7
1	D	252	LYS	3.7
1	C	176	THR	3.6
1	B	253	TRP	3.6
1	D	234	ASP	3.6
1	B	177	ASP	3.5
1	C	258	ILE	3.5
1	B	2	LYS	3.5
1	D	266	LEU	3.5
1	C	4	ASN	3.4
1	B	248	GLU	3.4
1	B	242	LYS	3.4
1	A	258	ILE	3.4
1	C	253	TRP	3.4
1	C	257	PRO	3.3
1	B	10	ILE	3.3
1	D	258	ILE	3.3
1	B	3	LEU	3.3
1	B	229	GLY	3.3
1	B	64	ASP	3.3
1	D	233	SER	3.2
1	D	176	THR	3.2
1	C	249	ILE	3.2
1	A	267	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	230	GLU	3.2
1	A	163	TYR	3.1
1	A	253	TRP	3.1
1	A	176	THR	3.1
1	A	137	ARG	3.0
1	D	163	TYR	2.9
1	B	228	GLU	2.9
1	B	87	LYS	2.9
1	C	245	LEU	2.8
1	A	252	LYS	2.8
1	D	267	GLU	2.8
1	B	233	SER	2.7
1	B	252	LYS	2.7
1	B	245	LEU	2.7
1	D	250	ALA	2.7
1	A	264[A]	ILE	2.7
1	A	182	ILE	2.6
1	C	9	VAL	2.6
1	C	233	SER	2.6
1	B	88	GLN	2.6
1	B	263	HIS	2.6
1	A	3	LEU	2.6
1	B	160	GLU	2.5
1	B	33	ILE	2.5
1	B	250	ALA	2.5
1	A	113	VAL	2.5
1	B	35	LEU	2.5
1	B	116	ILE	2.5
1	B	261	VAL	2.5
1	A	232	GLN	2.4
1	C	242	LYS	2.4
1	D	253	TRP	2.4
1	D	230	GLU	2.4
1	B	62	LEU	2.3
1	B	39	ALA	2.3
1	A	229	GLY	2.3
1	A	257	PRO	2.3
1	B	201	ASP	2.3
1	C	201	ASP	2.3
1	C	265	HIS	2.3
1	B	181	LEU	2.3
1	D	87	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	251	SER	2.3
1	B	136	ASN	2.3
1	B	260	ASN	2.3
1	B	139	MET	2.3
1	D	181	LEU	2.2
1	C	251	SER	2.2
1	B	197	GLN	2.2
1	B	246	PHE	2.2
1	A	139	MET	2.2
1	C	171	GLN	2.2
1	B	109	ASN	2.2
1	C	64	ASP	2.1
1	A	9	VAL	2.1
1	A	115	ILE	2.1
1	C	234	ASP	2.1
1	C	3	LEU	2.1
1	C	2	LYS	2.1
1	D	265	HIS	2.1
1	C	113	VAL	2.1
1	A	201	ASP	2.1
1	A	248	GLU	2.0
1	B	90	PRO	2.0
1	B	224	LYS	2.0
1	C	35	LEU	2.0
1	D	263	HIS	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 monosaccharides 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(Å ²)	Q<0.9
2	DGL	B	502	10/10	0.91	0.12	31,33,39,39	0
2	DGL	C	503	10/10	0.96	0.11	22,24,25,25	0
2	DGL	D	504	10/10	0.97	0.12	20,22,25,27	0
2	DGL	A	501	10/10	0.98	0.10	19,23,24,24	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.