



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:25 PM UTC

PDB ID : 2GZM / pdb_00002gzm
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 ⓘ 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

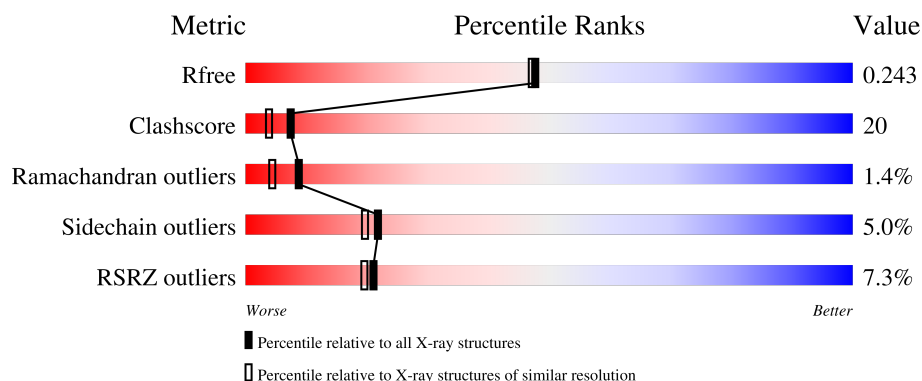
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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.

Mol	Chain	Length	Quality of chain
1	A	267	 6% 66% 29% 5%
1	B	267	 9% 63% 33% ..
1	C	267	 6% 67% 28% .
1	D	267	 8% 75% 19% 5% .

2 Entry composition [i](#)

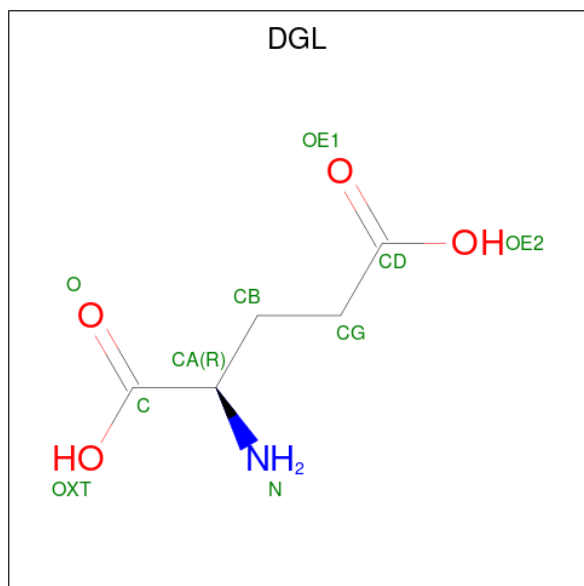
There are 3 unique types of molecules in this entry. The entry contains 8887 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: C₅H₉NO₄).



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

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

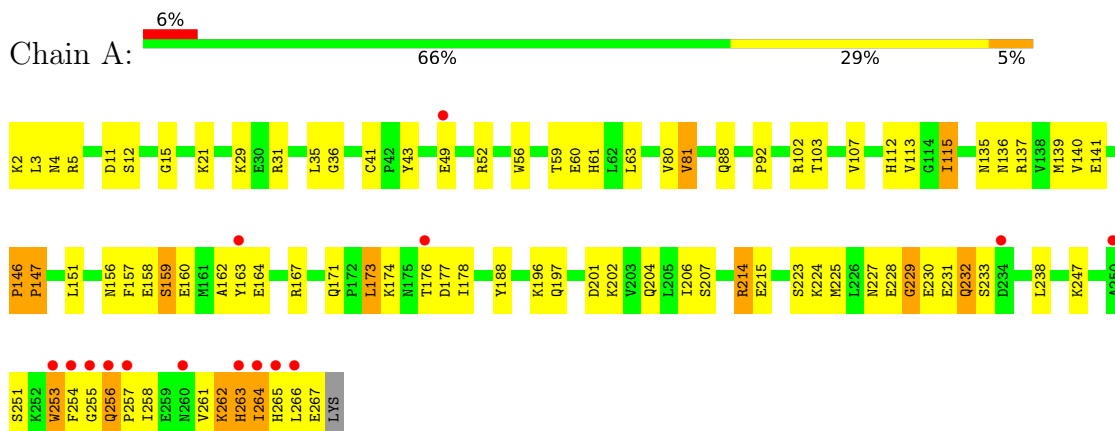
- Molecule 3 is water.

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

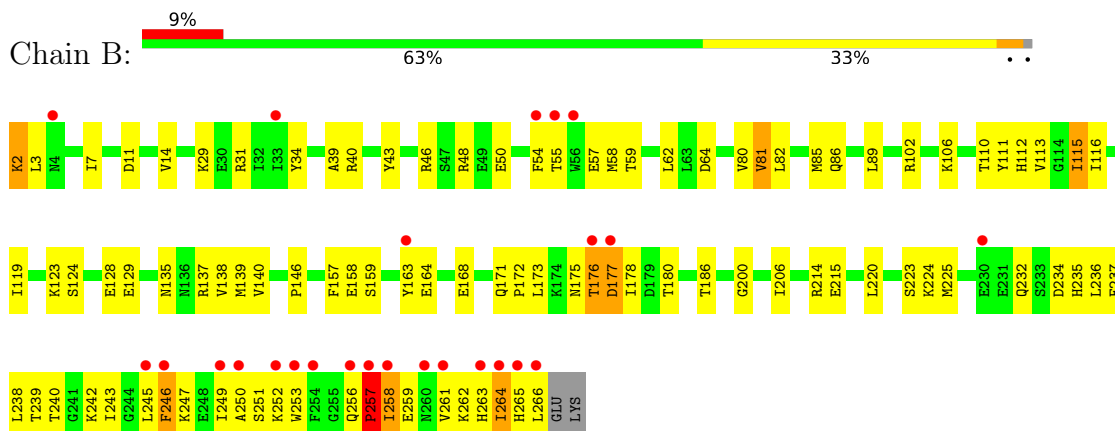
3 Residue-property plots [i](#)

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.

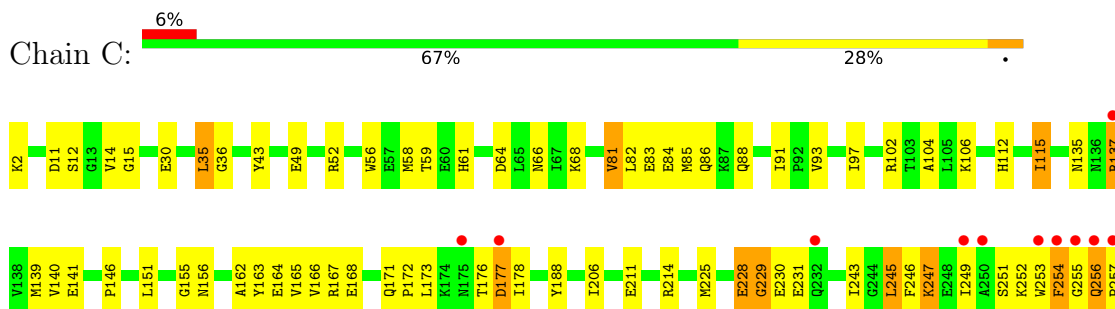
• Molecule 1: Glutamate racemase

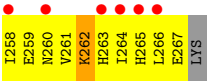


• Molecule 1: Glutamate racemase

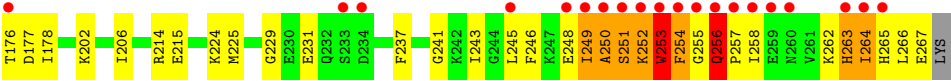


• Molecule 1: Glutamate racemase





● Molecule 1: Glutamate racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.35Å 90.52Å 116.80Å 90.00° 100.02° 90.00°	Depositor
Resolution (Å)	20.00 – 1.99 20.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-1.99) 98.4 (20.00-1.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.241 0.206 , 0.243	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 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.55	0/2135	1.01	10/2891 (0.3%)
1	B	0.51	0/2106	1.01	9/2853 (0.3%)
1	C	0.57	0/2118	0.99	10/2869 (0.3%)
1	D	0.61	0/2138	1.03	12/2894 (0.4%)
All	All	0.56	0/8497	1.01	41/11507 (0.4%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	VAL	N-CA-C	11.45	123.89	112.90
1	D	253	TRP	N-CA-C	-10.14	100.22	111.07
1	D	81	VAL	N-CA-C	9.74	122.25	112.90
1	B	81	VAL	N-CA-C	9.34	121.86	112.90
1	B	146	PRO	N-CA-C	8.79	121.43	110.70
1	D	249	ILE	N-CA-C	-8.76	101.61	113.00
1	C	146	PRO	N-CA-C	8.76	121.39	110.70
1	D	146	PRO	N-CA-C	8.15	120.64	110.70
1	A	80	VAL	N-CA-C	8.13	118.49	111.90
1	A	146	PRO	N-CA-C	7.96	120.42	110.70
1	B	258	ILE	N-CA-C	-7.15	105.38	112.17
1	B	178	ILE	N-CA-C	-6.97	102.33	110.21
1	A	140	VAL	N-CA-C	6.90	117.81	107.80
1	B	43	TYR	N-CA-C	-6.86	105.06	113.50
1	D	258	ILE	N-CA-C	-6.72	106.94	113.53
1	D	88	GLN	N-CA-C	6.63	119.85	111.69
1	B	113	VAL	N-CA-C	6.59	118.09	108.53
1	B	140	VAL	N-CA-C	6.32	116.97	107.80
1	C	140	VAL	N-CA-C	6.32	117.02	108.17
1	A	81	VAL	N-CA-C	6.20	119.11	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	TYR	N-CA-C	-6.04	106.04	113.41
1	C	88	GLN	N-CA-C	6.02	120.69	113.23
1	C	97	ILE	N-CA-C	5.73	115.92	110.53
1	C	81	VAL	CB-CA-C	-5.67	104.17	111.20
1	A	43	TYR	N-CA-C	-5.64	106.23	113.23
1	A	147	PRO	N-CA-C	5.61	120.94	114.03
1	A	201	ASP	N-CA-C	5.59	118.14	111.71
1	C	82	LEU	N-CA-C	5.57	117.82	111.02
1	D	250	ALA	N-CA-C	-5.54	104.06	112.04
1	A	113	VAL	N-CA-C	5.47	116.45	108.53
1	D	80	VAL	N-CA-C	5.42	116.82	111.67
1	D	7	ILE	N-CA-C	-5.32	100.76	108.36
1	B	186	THR	N-CA-C	5.30	117.05	111.28
1	B	177	ASP	N-CA-C	5.27	117.73	108.56
1	C	91	ILE	CA-C-N	-5.21	114.58	119.85
1	C	91	ILE	C-N-CA	-5.21	114.58	119.85
1	A	232	GLN	N-CA-C	5.16	116.75	110.41
1	D	140	VAL	N-CA-C	5.09	115.18	107.80
1	D	81	VAL	CB-CA-C	-5.07	104.91	111.20
1	A	88	GLN	N-CA-C	5.05	118.60	112.23
1	D	134	ILE	CB-CA-C	-5.02	105.62	111.94

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	2099	0	2155	91	0
1	B	2070	0	2123	103	0
1	C	2082	0	2133	83	0
1	D	2102	0	2157	93	0
2	A	10	0	7	0	0
2	B	10	0	7	0	0
2	C	10	0	7	0	0
2	D	10	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	130	0	0	7	0
3	B	95	0	0	6	0
3	C	130	0	0	4	0
3	D	139	0	0	10	0
All	All	8887	0	8596	347	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 20.

All (347) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:112:HIS:HE1	1:B:139:MET:HE2	1.57	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:223:SER:OG	1:A:225:MET:HE3	1.92	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:112:HIS:CE1	1:A:139:MET:HE3	2.32	0.65
1:B:11:ASP:O	1:B:58[A]:MET:HE1	1.96	0.65
1:D:253:TRP:CD1	1:D:253:TRP:H	2.14	0.65
1:A:49:GLU:H	1:A:49:GLU:CD	2.05	0.65
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:B:252:LYS:C	1:B:253:TRP:HD1	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:TRP:CD1	1:A:253:TRP:C	2.79	0.60
1:B:57:GLU:C	1:B:265:HIS:HE1	2.09	0.60
1:B:115:ILE:HD13	1:B:115:ILE:C	2.27	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
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:A:262[A]:LYS:HD3	1:A:262[A]:LYS:C	2.29	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: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:C:56:TRP:NE1	1:C:84:GLU:OE2	2.34	0.55
1:C:115:ILE:C	1:C:115:ILE:HD13	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:251:SER:C	1:B:253:TRP:H	2.14	0.54
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:C:35:LEU:HD12	1:C:35:LEU:C	2.33	0.53
1:B:112:HIS:NE2	1:B:176:THR:HB	2.24	0.53
1:C:262:LYS:HD3	1:C:262:LYS:C	2.34	0.53
1:D:253:TRP:CD1	1:D:253:TRP:N	2.75	0.53
1:D:248:GLU:C	1:D:250:ALA:N	2.66	0.52
1:B:112:HIS:CE1	1:B:139:MET:HE2	2.43	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:D:263:HIS:C	1:D:263:HIS:CD2	2.88	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:A:92:PRO:HG3	1:A:225:MET:HE1	1.92	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:C:112:HIS:NE2	1:C:139:MET:HE2	2.26	0.50
1:C:163:TYR:O	1:C:167:ARG:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:HIS:ND1	1:A:263:HIS:C	2.69	0.50
1:A:167:ARG:NH2	3:A:602:HOH:O	2.45	0.50
1:A:177:ASP:O	1:A:177:ASP:CG	2.55	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:C:177:ASP:CG	1:C:177:ASP:O	2.54	0.49
1:D:102[B]:ARG:NH2	1:D:215:GLU:OE2	2.31	0.49
1:B:252:LYS:C	1:B:253:TRP:CD1	2.89	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:A:253:TRP:C	1:A:253:TRP:HD1	2.18	0.49
1:B:245:LEU:HB3	1:B:249:ILE:CD1	2.42	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: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:B:59:THR:HG21	1:B:85:MET:HE3	1.94	0.48
1:D:248:GLU:O	1:D:251:SER:OG	2.30	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: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:102:ARG:C	1:B:214:ARG:NH1	2.73	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:C:86:GLN:HG2	1:C:93:VAL:HB	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:C	1:A:115:ILE:HD13	2.41	0.46
1:A:173:LEU:O	1:A:174:LYS:C	2.58	0.46
1:A:136:ASN:OD1	1:B:29:LYS:HE2	2.16	0.46
1:C:137[A]:ARG:HH11	1:C:137[A]:ARG:HG3	1.79	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
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:C:59:THR:OG1	1:C:85:MET:HE1	2.16	0.45
1:A:35:LEU:HD12	1:A:36:GLY:N	2.32	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:C:11:ASP:CG	1:C:12:SER:N	2.75	0.45
1:A:11:ASP:CG	1:A:12:SER:N	2.74	0.45
1:A:103:THR:HG22	1:A:206:ILE:HD12	1.98	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:D:115:ILE:HD13	1:D:115:ILE:C	2.42	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: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:139:MET:HE2	1:C:141:GLU:OE2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:GLU:HA	1:D:251:SER:CB	2.38	0.44
1:B:200:GLY:C	3:B:547:HOH:O	2.60	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: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:234:ASP:CG	1:B:234:ASP:O	2.61	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
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:C:262:LYS:HE3	1:C:263:HIS:C	2.44	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:D:68:LYS:HB2	1:D:225:MET:HE3	2.00	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: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:C:30:GLU:OE1	1:C:68:LYS:NZ	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:VAL:HA	1:C:168:GLU:HG2	2.02	0.42
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:D:245:LEU:O	1:D:246:PHE:C	2.62	0.41
1:D:248:GLU:C	1:D:250:ALA:H	2.24	0.41
1:B:11:ASP:C	1:B:58[A]:MET:HE1	2.45	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:B:62:LEU:C	1:B:64:ASP:N	2.78	0.41
1:D:253:TRP:HD1	1:D:253:TRP:N	2.16	0.41
1:A:112:HIS:ND1	1:A:177:ASP:OD1	2.36	0.41
1:A:12:SER:O	1:A:41:CYS:HB2	2.21	0.41
1:B:245:LEU:O	1:B:246:PHE:C	2.64	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
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:144:ALA:C	1:D:146:PRO:HD3	2.46	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:176:THR:HG22	1:C:177:ASP:N	2.36	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:B:245:LEU:C	1:B:249:ILE:HG13	2.46	0.40
1:C:68:LYS:HB2	1:C:225:MET:HE3	2.04	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%)	6	3
1	B	264/267 (99%)	240 (91%)	21 (8%)	3 (1%)	11	7
1	C	265/267 (99%)	255 (96%)	8 (3%)	2 (1%)	16	11
1	D	267/267 (100%)	259 (97%)	3 (1%)	5 (2%)	6	3
All	All	1063/1068 (100%)	1007 (95%)	41 (4%)	15 (1%)	9	4

All (15) Ramachandran outliers are listed below:

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

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%)	222 (94%)	13 (6%)	19	17
1	B	232/233 (100%)	223 (96%)	9 (4%)	28	28
1	C	233/233 (100%)	220 (94%)	13 (6%)	19	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	235/233 (101%)	220 (94%)	15 (6%)	16	12
All	All	935/932 (100%)	885 (95%)	50 (5%)	22	18

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ILE
1	A	160	GLU
1	A	173	LEU
1	A	197	GLN
1	A	207	SER
1	A	214[A]	ARG
1	A	214[B]	ARG
1	A	253	TRP
1	A	262[A]	LYS
1	A	262[B]	LYS
1	A	263	HIS
1	A	264[A]	ILE
1	A	264[B]	ILE
1	B	2	LYS
1	B	115	ILE
1	B	129	GLU
1	B	137	ARG
1	B	173	LEU
1	B	176	THR
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	264	ILE
1	D	2	LYS

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Mol	Chain	Res	Type
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 (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	66	ASN
1	A	171	GLN
1	A	204	GLN
1	A	256	GLN
1	A	260	ASN
1	A	265	HIS
1	B	98	HIS
1	B	171	GLN
1	B	204	GLN
1	B	256	GLN
1	B	263	HIS
1	B	265	HIS
1	C	26	GLN
1	C	171	GLN
1	C	204	GLN
1	C	222	HIS
1	C	256	GLN
1	C	265	HIS
1	D	66	ASN
1	D	175	ASN
1	D	197	GLN
1	D	222	HIS
1	D	256	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	8,11,11	1.33	1 (12%)
2	DGL	A	501	-	8,9,9	0.56	0	8,11,11	1.27	1 (12%)
2	DGL	C	503	-	8,9,9	0.62	0	8,11,11	1.40	1 (12%)
2	DGL	B	502	-	8,9,9	0.63	0	8,11,11	1.32	1 (12%)

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	A	501	-	-	2/9/9/9	-
2	DGL	C	503	-	-	2/9/9/9	-
2	DGL	B	502	-	-	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($^{\circ}$)	Ideal($^{\circ}$)
2	C	503	DGL	CG-CB-CA	-3.19	106.54	113.86
2	B	502	DGL	CG-CB-CA	-2.80	107.43	113.86
2	A	501	DGL	CG-CB-CA	-2.62	107.85	113.86
2	D	504	DGL	CG-CB-CA	-2.44	108.27	113.86

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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	266/267 (99%)	0.17	15 (5%)	30 29	13, 34, 65, 81	3 (1%)
1	B	265/267 (99%)	0.66	25 (9%)	14 13	24, 43, 91, 102	1 (0%)
1	C	266/267 (99%)	0.11	17 (6%)	25 24	19, 32, 68, 87	1 (0%)
1	D	266/267 (99%)	0.07	21 (7%)	18 17	10, 30, 63, 76	3 (1%)
All	All	1063/1068 (99%)	0.25	78 (7%)	21 19	10, 35, 70, 102	8 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	249	ILE	6.8
1	B	258	ILE	6.0
1	B	266	LEU	5.3
1	B	261	VAL	4.6
1	A	264[A]	ILE	4.4
1	B	253	TRP	4.2
1	B	265	HIS	4.2
1	D	254	PHE	4.1
1	B	264	ILE	4.0
1	A	255	GLY	3.8
1	C	255	GLY	3.7
1	C	258	ILE	3.7
1	D	250	ALA	3.6
1	D	258	ILE	3.6
1	A	254	PHE	3.6
1	B	249	ILE	3.5
1	B	245	LEU	3.5
1	B	176	THR	3.5
1	B	257	PRO	3.5
1	A	253	TRP	3.4
1	B	254	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	266	LEU	3.4
1	A	260	ASN	3.4
1	C	253	TRP	3.3
1	C	264	ILE	3.3
1	D	263	HIS	3.3
1	C	257	PRO	3.3
1	C	263	HIS	3.3
1	A	263	HIS	3.2
1	C	265	HIS	3.2
1	D	233	SER	3.2
1	D	265	HIS	3.2
1	A	256	GLN	3.1
1	D	253	TRP	3.1
1	B	263	HIS	3.1
1	A	266	LEU	3.0
1	D	175	ASN	3.0
1	C	137[A]	ARG	2.9
1	C	249	ILE	2.9
1	D	252	LYS	2.9
1	D	264	ILE	2.9
1	D	176	THR	2.9
1	C	254	PHE	2.8
1	B	246	PHE	2.8
1	B	33	ILE	2.8
1	D	255	GLY	2.7
1	D	245	LEU	2.7
1	B	252	LYS	2.7
1	A	234	ASP	2.7
1	B	4	ASN	2.6
1	D	251	SER	2.6
1	B	250	ALA	2.5
1	B	177	ASP	2.5
1	B	260	ASN	2.5
1	C	175	ASN	2.5
1	B	55	THR	2.5
1	B	163	TYR	2.5
1	A	257	PRO	2.5
1	C	250	ALA	2.4
1	B	56	TRP	2.4
1	D	248	GLU	2.4
1	A	250	ALA	2.4
1	C	256	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	256	GLN	2.3
1	A	163	TYR	2.3
1	C	260	ASN	2.3
1	A	49	GLU	2.2
1	B	54	PHE	2.2
1	D	259	GLU	2.2
1	C	232	GLN	2.2
1	D	256	GLN	2.2
1	A	265	HIS	2.2
1	D	234	ASP	2.1
1	D	257	PRO	2.1
1	C	177	ASP	2.1
1	B	230	GLU	2.0
1	A	176	THR	2.0
1	D	260	ASN	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(Å ²)	Q<0.9
2	DGL	B	502	10/10	0.87	0.10	31,33,39,39	0
2	DGL	C	503	10/10	0.96	0.06	22,24,25,25	0
2	DGL	A	501	10/10	0.97	0.04	19,23,24,24	0
2	DGL	D	504	10/10	0.97	0.05	20,22,25,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.