



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:22 pm BST

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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

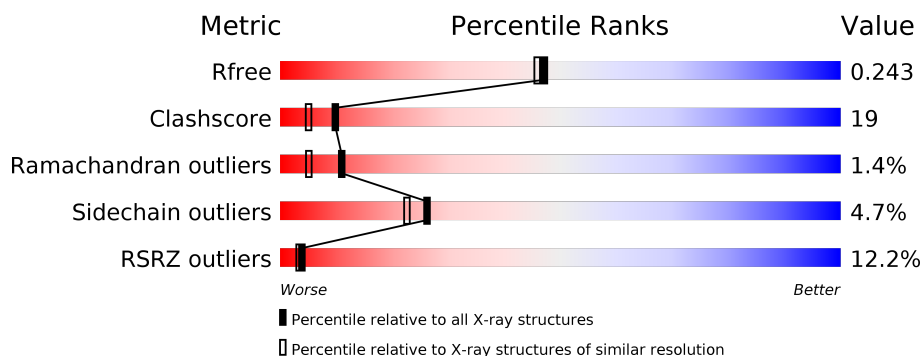
1 Overall quality at a glance

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 on 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	<div> <div>11%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	B	267	<div> <div>19%</div> <div>67%</div> <div>31%</div> <div>..</div> </div>
1	C	267	<div> <div>10%</div> <div>72%</div> <div>23%</div> <div>.</div> </div>
1	D	267	<div> <div>9%</div> <div>78%</div> <div>17%</div> <div>.</div> </div>

2 Entry composition [i](#)

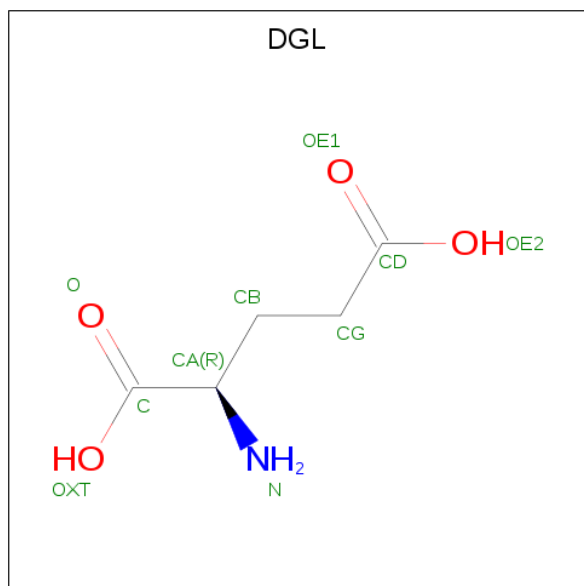
There are 3 unique types of molecules in this entry. The entry contains 8887 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

Chain A:

11% 69% 27%

Node	Category
K2	Yellow
L3	Yellow
N4	Yellow
R5	Yellow
V9	Green
I10	Green
D11	Green
S12	Yellow
G15	Yellow
K21	Yellow
K29	Yellow
E30	Green
R31	Yellow
L35	Yellow
G36	Yellow
C41	Yellow
E49	Yellow
R52	Yellow
W56	Yellow
T59	Yellow
E60	Yellow
H61	Yellow
L62	Yellow
L63	Yellow
V81	Yellow
R102	Yellow
T103	Yellow
V107	Yellow
H112	Yellow
V113	Green
G114	Yellow
I115	Green
N135	Yellow
N136	Yellow
R137	Yellow
V138	Green
M139	Green
V140	Green
E141	Yellow
P146	Yellow
P147	Yellow
L151	Yellow
N156	Yellow
F157	Yellow
E158	Yellow
S159	Yellow
A162	Green
E163	Yellow
Y164	Yellow
R167	Yellow
Q171	Yellow
P172	Yellow
L173	Yellow
K174	Yellow
N175	Green
T176	Yellow
D177	Yellow
I178	Yellow
I182	Green
Y188	Yellow
K196	Yellow
Q197	Yellow
D201	Green
K202	Yellow
V203	Yellow
Q204	Yellow
L205	Yellow
L206	Yellow
S207	Yellow
R214	Yellow
E215	Yellow
K224	Yellow
N227	Yellow
E228	Yellow
G229	Yellow
E230	Yellow
E231	Yellow
Q232	Yellow
S233	Yellow
G234	Green
L238	Yellow
L245	Green
P246	Yellow
K247	Yellow
E248	Yellow
S251	Yellow
K252	Yellow
K253	Yellow
K254	Yellow
G255	Yellow
Q256	Yellow
P257	Yellow
I258	Yellow
E259	Green
N260	Green
V261	Green
K262	Green
H263	Green
I264	Green
H265	Green
L266	Green
E267	Green
LVS	Grey

Chain B:

19% 67% 31%

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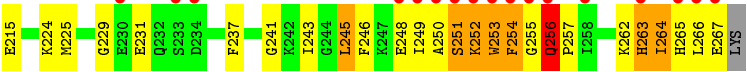
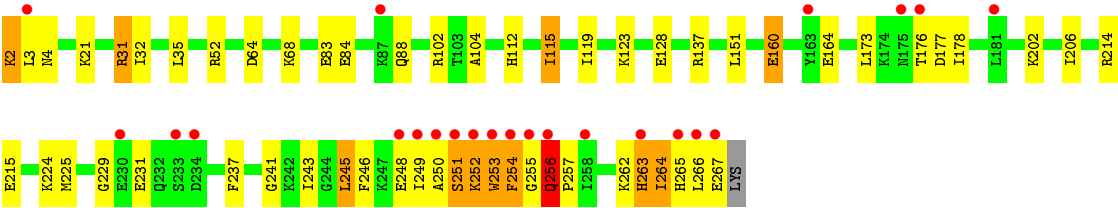
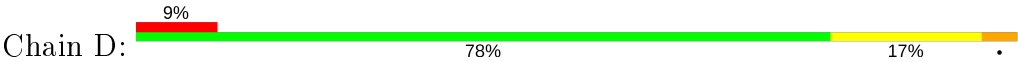
Chain B: A horizontal bar chart showing the distribution of amino acid types. The bar is divided into three segments: 19% (red), 67% (green), and 31% (yellow). A small grey segment is at the far right. A legend on the right shows a red dot for 'top' and a grey dot for 'bottom'.

Chain C:

Category	Percentage
Green	72%
Yellow	23%
Orange	5%



● 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 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
$\langle I/\sigma(I) \rangle$ 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 , 65.7	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 [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(°)	Ideal(°)
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:HG2	1:D:202:LYS:O	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:HH11	1:A:214[A]:ARG:HG2	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:N	1:D:256:GLN:HE21	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:256:GLN:CB	1:D:257:PRO:CA	2.70	0.62
1:D:241:GLY:O	1:D:262[A]:LYS:HD3	2.00	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:CD	1:A:49:GLU:H	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:CG	1:A:214[A]:ARG:HH11	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:C	1:A:253:TRP:CD1	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:228:GLU:O	1:A:229:GLY:O	2.26	0.54
1:A:214[A]:ARG:NH2	1:B:102:ARG:HB3	2.12	0.54
1:B:157:PHE:CZ	1:B:252:LYS:HD3	2.42	0.54
1:B:46:ARG:NH1	1:B:50:GLU:OE1	2.38	0.54
1:C:176:THR:HG22	1:C:178:ILE:HG23	1.90	0.54
1:C:2:LYS:N	1:C:2:LYS:HD2	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:HD13	1:C:115:ILE:C	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:C	1:C:35:LEU:HD12	2.33	0.49
1:A:56:TRP:O	1:A:60:GLU:HG2	2.12	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:B:48:ARG:HH12	1:B:80:VAL:HG22	1.74	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:HG2	1:C:214:ARG:NH1	2.29	0.47
1:D:253:TRP:H	1:D:253:TRP:HD1	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:B:115:ILE:HD13	1:B:116:ILE:N	2.29	0.47
1:A:188:TYR:N	1:A:188:TYR:CD1	2.81	0.47
1:B:250:ALA:HB3	3:B:597:HOH:O	2.15	0.47
1:D:263:HIS:CD2	1:D:263:HIS:C	2.88	0.47
1:C:86:GLN:HG2	1:C:93:VAL:HB	1.96	0.47
1:A:253:TRP:HD1	1:A:253:TRP:C	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:HG3	1:C:137[A]:ARG:HH11	1.79	0.46
1:A:263:HIS:C	1:A:263:HIS:ND1	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:119:ILE:O	1:B:123:LYS:HG3	2.15	0.45
1:B:40:ARG:NH1	1:B:54:PHE:CD1	2.85	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:HH11	1:B:48:ARG:HG2	1.80	0.45
1:C:188:TYR:N	1:C:188:TYR:CD1	2.84	0.45
1:C:58:MET:CG	1:C:265:HIS:HE1	2.21	0.45
1:A:21:LYS:NZ	1:A:254:PHE:CE2	2.77	0.45
1:C:102:ARG:HG2	1:D:214[A]:ARG:HD2	1.99	0.45
1:C:83:GLU:HG3	3:C:569:HOH:O	2.17	0.45
1:A:177:ASP:CG	1:A:177:ASP:O	2.55	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:A:103:THR:HG22	1:A:206:ILE:HD12	1.98	0.45
1:C:177:ASP:O	1:C:177:ASP:CG	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:HA	1:A:202:LYS:HE2	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:214:ARG:CZ	3:B:581:HOH:O	2.67	0.43
1:B:48:ARG:NH1	1:B:48:ARG:HG2	2.32	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:235:HIS:O	1:B:259:GLU:CG	2.62	0.43
1:B:11:ASP:O	1:B:58[A]:MET:CE	2.66	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:158:GLU:O	1:A:163:TYR:CE1	2.70	0.42
1:A:102:ARG:C	1:B:214:ARG:NH1	2.73	0.42
1:B:34:TYR:HB3	1:B:237:PHE:CD1	2.54	0.42
1:A:264[B]:ILE:HG23	1:D:128:GLU:OE2	2.20	0.42
1:A:52:ARG:HA	1:A:81:VAL:HG11	2.02	0.42
1:B:242:LYS:O	1:B:245:LEU:HB2	2.19	0.42
1:B:57:GLU:HG2	1:B:266:LEU:O	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:C:151:LEU:HD21	1:C:162:ALA:HA	2.03	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

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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:112:HIS:ND1	1:D:177:ASP:OD1	2.26	0.40
1:D:2:LYS:HD3	1:D:3:LEU:H	1.81	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:251:SER:O	1:D:252:LYS:CG	2.69	0.40
1:D:31:ARG:HD3	1:D:32:ILE:N	2.36	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 ⓘ

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

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

Mol	Chain	Res	Type
1	A	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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.53	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, 77	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^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.