



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:09 PM UTC

PDB ID : 5ELM / pdb_00005elm
Title : Crystal structure of L-aspartate/glutamate specific racemase in complex with L-glutamate
Authors : Ahn, J.W.; Chang, J.H.; Kim, K.J.
Deposited on : 2015-11-04
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

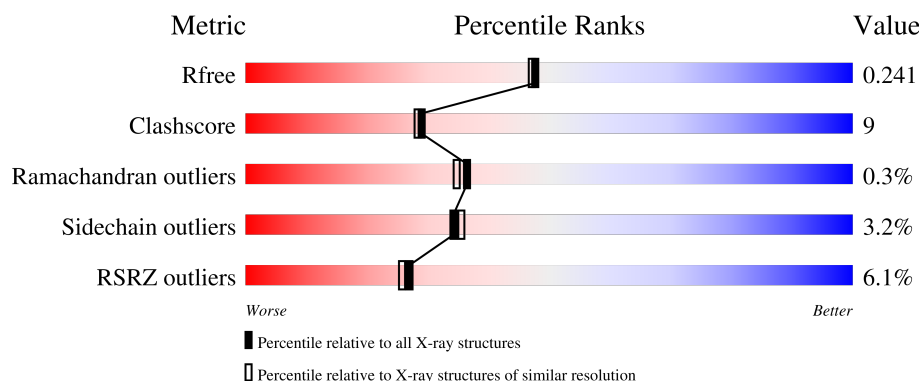
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	238	100% 91% 8%
1	B	238	10% 79% 19%
1	C	238	12% 76% 21%
1	D	238	84% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLU	C	301	-	-	X	-
3	GLU	D	301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7990 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 Asp/Glu_racemase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1821	1147	320	343	11			
1	B	235	Total	C	N	O	S	0	2	0
			1834	1157	323	343	11			
1	C	235	Total	C	N	O	S	0	1	0
			1832	1153	324	344	11			
1	D	235	Total	C	N	O	S	0	4	0
			1868	1173	337	347	11			

There are 36 discrepancies between the modelled and reference sequences:

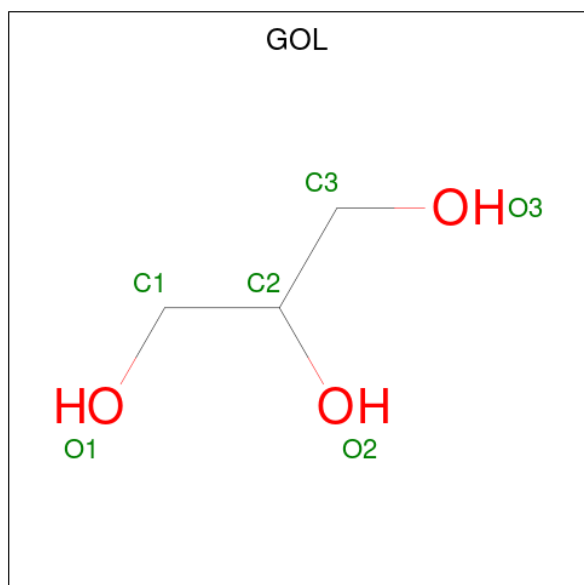
Chain	Residue	Modelled	Actual	Comment	Reference
A	197	SER	CYS	conflict	UNP C3SWD2
A	231	LEU	-	expression tag	UNP C3SWD2
A	232	GLU	-	expression tag	UNP C3SWD2
A	233	HIS	-	expression tag	UNP C3SWD2
A	234	HIS	-	expression tag	UNP C3SWD2
A	235	HIS	-	expression tag	UNP C3SWD2
A	236	HIS	-	expression tag	UNP C3SWD2
A	237	HIS	-	expression tag	UNP C3SWD2
A	238	HIS	-	expression tag	UNP C3SWD2
B	197	SER	CYS	conflict	UNP C3SWD2
B	231	LEU	-	expression tag	UNP C3SWD2
B	232	GLU	-	expression tag	UNP C3SWD2
B	233	HIS	-	expression tag	UNP C3SWD2
B	234	HIS	-	expression tag	UNP C3SWD2
B	235	HIS	-	expression tag	UNP C3SWD2
B	236	HIS	-	expression tag	UNP C3SWD2
B	237	HIS	-	expression tag	UNP C3SWD2
B	238	HIS	-	expression tag	UNP C3SWD2
C	197	SER	CYS	conflict	UNP C3SWD2
C	231	LEU	-	expression tag	UNP C3SWD2
C	232	GLU	-	expression tag	UNP C3SWD2

Continued on next page...

Continued from previous page...

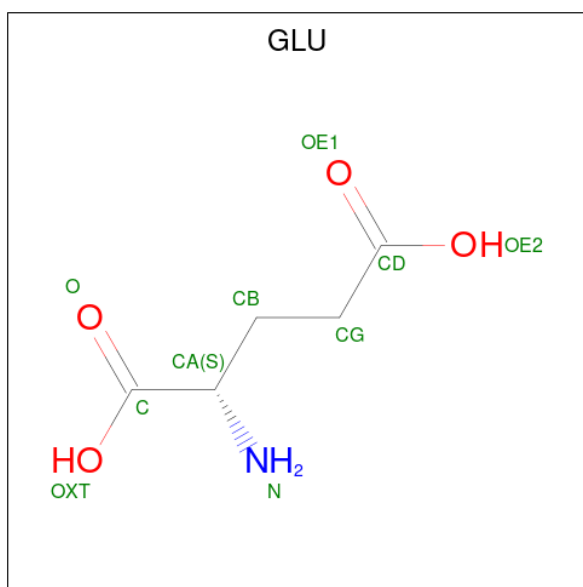
Chain	Residue	Modelled	Actual	Comment	Reference
C	233	HIS	-	expression tag	UNP C3SWD2
C	234	HIS	-	expression tag	UNP C3SWD2
C	235	HIS	-	expression tag	UNP C3SWD2
C	236	HIS	-	expression tag	UNP C3SWD2
C	237	HIS	-	expression tag	UNP C3SWD2
C	238	HIS	-	expression tag	UNP C3SWD2
D	197	SER	CYS	conflict	UNP C3SWD2
D	231	LEU	-	expression tag	UNP C3SWD2
D	232	GLU	-	expression tag	UNP C3SWD2
D	233	HIS	-	expression tag	UNP C3SWD2
D	234	HIS	-	expression tag	UNP C3SWD2
D	235	HIS	-	expression tag	UNP C3SWD2
D	236	HIS	-	expression tag	UNP C3SWD2
D	237	HIS	-	expression tag	UNP C3SWD2
D	238	HIS	-	expression tag	UNP C3SWD2

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



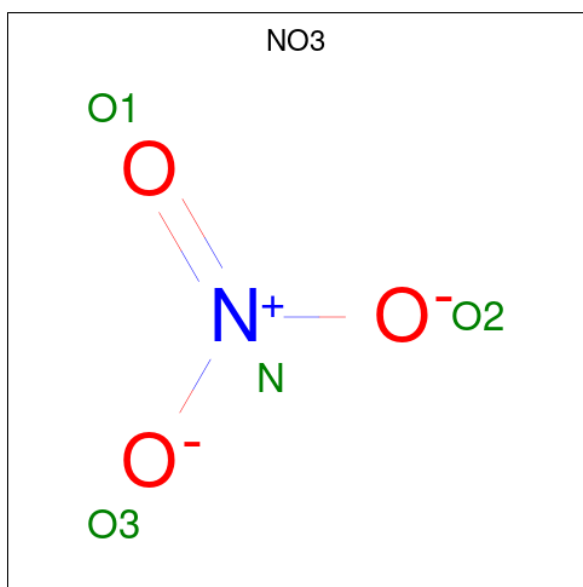
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



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

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	N	O	0	0
			4	1	3		

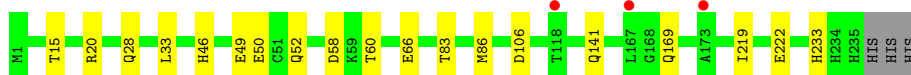
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total 156	O 156	0	0
5	B	124	Total 124	O 124	0	0
5	C	136	Total 136	O 136	0	0
5	D	173	Total 173	O 173	0	0

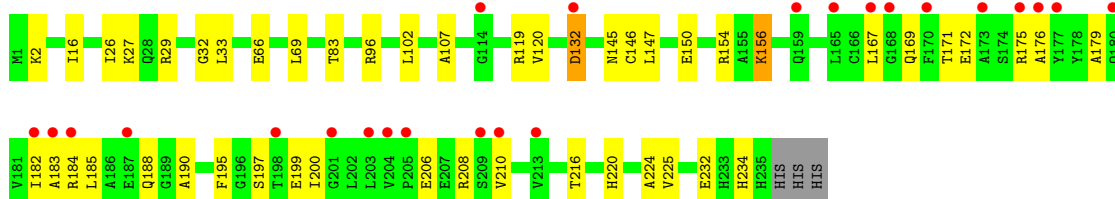
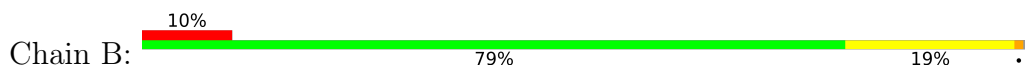
3 Residue-property plots [i](#)

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.

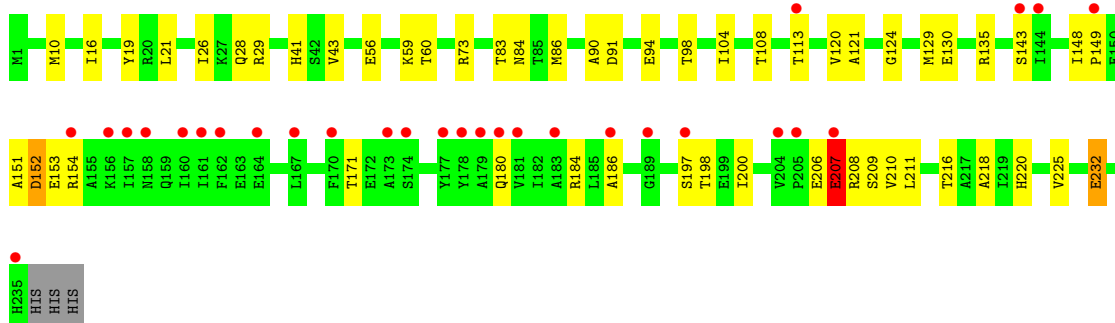
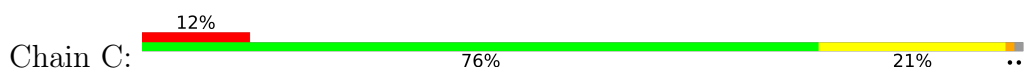
- Molecule 1: Asp/Glu_racemase family protein



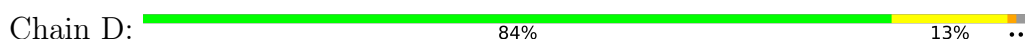
- Molecule 1: Asp/Glu_racemase family protein

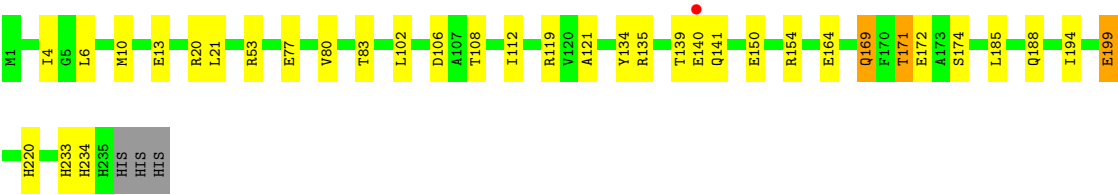


- Molecule 1: Asp/Glu_racemase family protein



- Molecule 1: Asp/Glu_racemase family protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.53Å 81.25Å 83.96Å 90.00° 111.39° 90.00°	Depositor
Resolution (Å)	29.32 – 2.00 29.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.32-2.00) 98.1 (29.32-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.50 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.173 , 0.236 0.182 , 0.241	Depositor DCC
R_{free} test set	2833 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7990	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: GOL, NO3

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	1.21	0/1853	1.09	2/2505 (0.1%)
1	B	1.12	2/1866 (0.1%)	1.08	1/2522 (0.0%)
1	C	1.13	3/1864 (0.2%)	1.07	2/2519 (0.1%)
1	D	1.24	1/1900 (0.1%)	1.15	3/2565 (0.1%)
All	All	1.18	6/7483 (0.1%)	1.10	8/10111 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	16	ILE	C-O	-5.48	1.20	1.24
1	C	16	ILE	CA-CB	5.38	1.57	1.54
1	C	19	TYR	C-O	5.28	1.30	1.24
1	B	224	ALA	N-CA	5.13	1.52	1.46
1	C	108	THR	CA-C	5.07	1.59	1.52
1	D	134	TYR	CA-C	-5.01	1.49	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	VAL	CB-CA-C	-7.86	102.94	111.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	141	GLN	N-CA-C	5.66	120.46	113.50
1	D	4	ILE	CA-C-N	5.24	126.95	122.29
1	D	4	ILE	C-N-CA	5.24	126.95	122.29
1	C	208	ARG	N-CA-C	5.20	121.87	110.80
1	B	16	ILE	CA-C-O	5.14	122.13	118.69
1	A	15	THR	CA-C-N	5.12	123.47	120.24
1	A	15	THR	C-N-CA	5.12	123.47	120.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	234	HIS	Peptide
1	C	207	GLU	Peptide

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	1821	0	1805	19	0
1	B	1834	0	1823	35	0
1	C	1832	0	1817	38	0
1	D	1868	0	1850	39	0
2	A	6	0	8	0	0
2	D	6	0	8	3	0
3	B	10	0	5	3	0
3	C	10	0	5	4	0
3	D	10	0	5	4	0
4	D	4	0	0	0	0
5	A	156	0	0	9	0
5	B	124	0	0	7	3
5	C	136	0	0	8	1
5	D	173	0	0	5	2
All	All	7990	0	7326	128	3

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 9.

All (128) 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:172[B]:GLU:N	1:D:172[B]:GLU:OE2	1.70	1.25
1:D:13:GLU:HG2	5:D:488:HOH:O	1.47	1.10
1:C:60:THR:HG21	1:C:86:MET:HE1	1.35	1.05
1:C:135:ARG:HD3	5:C:464:HOH:O	1.58	1.04
1:A:66:GLU:OE1	5:A:401:HOH:O	1.83	0.95
1:A:60:THR:HG21	1:A:86:MET:HE1	1.55	0.89
1:C:60:THR:CG2	1:C:86:MET:HE1	2.02	0.88
1:D:171:THR:HG21	5:D:461:HOH:O	1.72	0.88
1:A:233:HIS:O	5:A:402:HOH:O	1.92	0.88
1:D:20[B]:ARG:CG	1:D:20[B]:ARG:HH21	1.87	0.87
1:D:20[B]:ARG:HH21	1:D:20[B]:ARG:HG2	1.40	0.87
1:C:60:THR:CG2	1:C:86:MET:CE	2.56	0.84
1:C:60:THR:HG21	1:C:86:MET:CE	2.10	0.80
1:D:77:GLU:OE1	5:D:401:HOH:O	2.01	0.76
1:C:98:THR:OG1	5:C:401:HOH:O	2.04	0.76
1:D:199:GLU:OE2	3:D:301:GLU:HA	1.86	0.75
1:D:171:THR:CG2	1:D:174:SER:H	2.01	0.73
1:C:152:ASP:N	1:C:152:ASP:OD1	2.23	0.71
1:D:171:THR:HG22	1:D:174:SER:HB2	1.73	0.71
1:D:20[B]:ARG:HH21	1:D:20[B]:ARG:CB	2.04	0.70
1:B:2[A]:LYS:HE3	5:B:437:HOH:O	1.91	0.70
1:D:172[B]:GLU:OE2	1:D:172[B]:GLU:CA	2.40	0.70
1:D:20[A]:ARG:NH2	5:D:402:HOH:O	2.16	0.69
1:A:60:THR:HG21	1:A:86:MET:CE	2.21	0.69
1:D:20[B]:ARG:HG2	1:D:20[B]:ARG:NH2	2.04	0.68
1:A:33:LEU:HD21	5:B:470:HOH:O	1.93	0.68
1:A:28:GLN:OE1	5:A:403:HOH:O	2.10	0.67
1:B:27:LYS:HE3	1:B:32:GLY:O	1.94	0.67
1:D:20[B]:ARG:HH21	1:D:20[B]:ARG:HB3	1.61	0.65
1:D:20[B]:ARG:NH2	1:D:21:LEU:HG	2.12	0.65
1:D:199:GLU:OE2	3:D:301:GLU:CA	2.46	0.64
1:B:27:LYS:CE	1:B:32:GLY:O	2.46	0.64
1:A:58:ASP:HB2	5:A:514:HOH:O	2.01	0.61
1:C:198:THR:H	3:C:301:GLU:N	1.98	0.61
1:C:84:ASN:H	3:C:301:GLU:N	1.99	0.60
1:D:13:GLU:CG	5:D:488:HOH:O	2.25	0.60
1:B:107:ALA:HB2	5:B:406:HOH:O	2.03	0.59
1:D:199:GLU:OE2	3:D:301:GLU:N	2.36	0.59
1:B:150:GLU:HA	1:B:150:GLU:OE1	2.03	0.58
1:B:195:PHE:CD2	1:B:200:ILE:HG22	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLN:HE21	1:B:171:THR:HG21	1.67	0.58
1:B:132:ASP:N	1:B:132:ASP:OD1	2.37	0.58
3:B:301:GLU:N	5:B:405:HOH:O	2.40	0.55
1:C:198:THR:HG1	3:C:301:GLU:N	2.04	0.55
1:D:20[B]:ARG:NH2	1:D:20[B]:ARG:HB3	2.21	0.55
1:D:20[B]:ARG:HH22	1:D:21:LEU:HG	1.72	0.54
1:B:199:GLU:OE2	3:B:301:GLU:N	2.41	0.54
1:A:106:ASP:OD1	1:A:141:GLN:HG3	2.08	0.53
1:D:10:MET:O	3:D:301:GLU:HB2	2.09	0.53
1:B:179:ALA:HB2	1:B:208:ARG:HD2	1.91	0.53
1:D:20[B]:ARG:CG	1:D:20[B]:ARG:NH2	2.57	0.53
1:D:171:THR:HG22	1:D:174:SER:H	1.70	0.52
1:D:121:ALA:HB1	1:D:185:LEU:HD13	1.91	0.52
1:A:33:LEU:HD12	1:B:167:LEU:HD21	1.90	0.52
1:B:179:ALA:HB2	1:B:208:ARG:CD	2.40	0.52
1:C:90:ALA:O	1:C:94:GLU:HG3	2.09	0.52
1:B:172:GLU:HB3	1:C:207:GLU:HB3	1.91	0.51
1:D:119:ARG:NH2	1:D:188:GLN:O	2.44	0.51
1:C:104:ILE:HD11	1:C:216:THR:HB	1.93	0.51
1:D:171:THR:HG22	1:D:174:SER:CB	2.41	0.50
1:D:6:LEU:HD23	1:D:80:VAL:HB	1.92	0.50
1:D:164:GLU:O	1:D:169:GLN:HG2	2.12	0.50
1:D:171:THR:C	1:D:172[B]:GLU:OE2	2.49	0.50
1:B:66:GLU:OE2	1:B:96:ARG:NH1	2.45	0.50
1:B:183:ALA:HA	1:B:210:VAL:HG11	1.93	0.49
1:C:21:LEU:HD13	1:C:218:ALA:HA	1.93	0.49
1:B:147:LEU:HD12	1:B:190:ALA:HB2	1.94	0.49
1:C:129:MET:O	1:C:135:ARG:HD2	2.11	0.49
1:A:20:ARG:NE	5:A:416:HOH:O	2.45	0.49
1:C:207:GLU:HA	1:C:209:SER:N	2.27	0.49
1:B:107:ALA:CB	5:B:406:HOH:O	2.59	0.49
1:B:197:SER:HG	3:B:301:GLU:N	2.10	0.49
1:B:69:LEU:HD21	1:B:96:ARG:O	2.13	0.48
1:B:150:GLU:O	1:B:154:ARG:HG3	2.14	0.48
1:D:171:THR:HG23	1:D:174:SER:H	1.77	0.48
1:D:102:LEU:HA	2:D:303:GOL:H12	1.96	0.48
1:C:60:THR:HG23	1:C:86:MET:CE	2.43	0.48
1:D:80:VAL:HG13	1:D:220:HIS:CE1	2.48	0.48
1:C:73:ARG:NH2	5:C:403:HOH:O	2.22	0.48
1:A:46:HIS:O	1:A:50:GLU:HG2	2.13	0.47
1:B:119:ARG:HA	1:B:145:ASN:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:CD	5:A:416:HOH:O	2.62	0.46
1:B:182:ILE:HG22	1:B:210:VAL:HG12	1.98	0.46
1:C:210:VAL:O	1:C:210:VAL:HG12	2.15	0.46
1:B:120:VAL:O	1:B:146:CYS:HA	2.16	0.46
1:B:208:ARG:NH1	5:B:409:HOH:O	2.48	0.46
1:A:60:THR:CG2	1:A:86:MET:CE	2.93	0.45
1:D:106:ASP:HB2	2:D:303:GOL:H2	1.98	0.45
1:C:26:ILE:HD13	1:C:225:VAL:HG13	1.97	0.45
1:D:106:ASP:CB	2:D:303:GOL:H2	2.47	0.45
1:C:206:GLU:HG3	5:C:469:HOH:O	2.16	0.45
1:B:172:GLU:OE2	1:B:175:ARG:HD2	2.17	0.44
1:D:150:GLU:O	1:D:154:ARG:HG3	2.18	0.44
1:A:52:GLN:OE1	1:A:52:GLN:HA	2.18	0.44
1:B:102[A]:LEU:N	1:B:102[A]:LEU:HD12	2.32	0.44
1:B:176:ALA:O	1:B:179:ALA:HB3	2.18	0.44
1:C:29:ARG:NH2	5:C:417:HOH:O	2.51	0.44
1:D:108:THR:HG22	1:D:112:ILE:HD12	2.00	0.44
1:A:20:ARG:HD3	5:A:416:HOH:O	2.17	0.44
1:B:29:ARG:NE	5:B:414:HOH:O	2.51	0.43
1:C:124:GLY:O	1:C:129:MET:HE2	2.17	0.43
1:C:56:GLU:HG3	5:C:503:HOH:O	2.17	0.43
1:C:104:ILE:HD12	1:C:220:HIS:ND1	2.33	0.43
1:B:156:LYS:N	1:B:156:LYS:HD2	2.32	0.43
1:C:148:ILE:HB	1:C:149:PRO:HD2	2.01	0.43
1:C:120:VAL:HG22	1:C:121:ALA:N	2.34	0.42
1:B:216:THR:O	1:B:220:HIS:HB2	2.19	0.42
1:A:28:GLN:HG3	5:A:458:HOH:O	2.18	0.42
1:A:49:GLU:HG2	1:B:33:LEU:HD12	2.02	0.42
1:C:151:ALA:HA	1:C:154:ARG:NH1	2.34	0.42
1:B:208:ARG:HH22	1:C:210:VAL:HG22	1.84	0.42
1:C:197:SER:HB3	1:C:200:ILE:HG13	2.01	0.42
1:A:219:ILE:O	1:A:222:GLU:HG2	2.20	0.42
1:D:233:HIS:CD2	1:D:234:HIS:CD2	3.08	0.42
1:C:210:VAL:O	1:C:210:VAL:CG1	2.68	0.42
1:B:184:ARG:O	1:B:188:GLN:HG2	2.20	0.41
1:C:207:GLU:CA	1:C:209:SER:H	2.33	0.41
1:C:10:MET:O	3:C:301:GLU:HB2	2.20	0.41
1:C:216:THR:O	1:C:220:HIS:HB2	2.20	0.41
1:C:28:GLN:NE2	5:C:419:HOH:O	2.52	0.41
1:B:26:ILE:HD13	1:B:225:VAL:HG13	2.03	0.41
1:C:207:GLU:HA	1:C:209:SER:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:THR:O	1:D:140:GLU:C	2.64	0.41
1:C:41:HIS:CE1	5:C:460:HOH:O	2.73	0.40
1:C:186:ALA:HB2	1:C:211:LEU:HD21	2.03	0.40
1:D:194:ILE:HD13	1:D:194:ILE:HG21	1.92	0.40
1:A:169:GLN:O	5:A:404:HOH:O	2.22	0.40
1:B:185:LEU:HA	1:B:188:GLN:HG2	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:471:HOH:O	5:C:475:HOH:O[2_555]	1.89	0.31
5:B:411:HOH:O	5:D:430:HOH:O[1_556]	1.92	0.28
5:B:523:HOH:O	5:D:543:HOH:O[1_556]	1.97	0.23

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/238 (98%)	225 (97%)	8 (3%)	0	100	100
1	B	235/238 (99%)	228 (97%)	6 (3%)	1 (0%)	30	27
1	C	234/238 (98%)	223 (95%)	9 (4%)	2 (1%)	14	9
1	D	238/238 (100%)	232 (98%)	6 (2%)	0	100	100
All	All	940/952 (99%)	908 (97%)	29 (3%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	206	GLU
1	C	232	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	207	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	188/191 (98%)	187 (100%)	1 (0%)	81	87
1	B	189/191 (99%)	185 (98%)	4 (2%)	47	52
1	C	189/191 (99%)	177 (94%)	12 (6%)	16	13
1	D	191/191 (100%)	185 (97%)	6 (3%)	35	37
All	All	757/764 (99%)	734 (97%)	23 (3%)	34	38

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	B	83	THR
1	B	132	ASP
1	B	156	LYS
1	B	232	GLU
1	C	59	LYS
1	C	83	THR
1	C	91	ASP
1	C	113	THR
1	C	130	GLU
1	C	143	SER
1	C	152	ASP
1	C	153	GLU
1	C	171	THR
1	C	180	GLN
1	C	184	ARG
1	C	232	GLU
1	D	53	ARG
1	D	83	THR
1	D	135	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	169	GLN
1	D	171	THR
1	D	199	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	233	HIS
1	B	46	HIS
1	B	72	GLN
1	B	169	GLN
1	C	37	GLN
1	C	84	ASN
1	D	28	GLN
1	D	180	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLU	C	301	-	8,9,9	1.16	0	8,11,11	1.08	0
3	GLU	B	301	-	8,9,9	1.48	1 (12%)	8,11,11	1.01	0
2	GOL	A	301	-	5,5,5	0.29	0	5,5,5	0.32	0
4	NO3	D	302	-	1,3,3	0.25	0	0,3,3	-	-
2	GOL	D	303	-	5,5,5	0.85	0	5,5,5	0.96	0
3	GLU	D	301	-	8,9,9	1.19	1 (12%)	8,11,11	1.41	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
3	GLU	C	301	-	-	2/9/9/9	-
3	GLU	B	301	-	-	2/9/9/9	-
2	GOL	A	301	-	-	0/4/4/4	-
2	GOL	D	303	-	-	3/4/4/4	-
3	GLU	D	301	-	-	3/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	GLU	OXT-C	-3.11	1.20	1.30
3	D	301	GLU	OE2-CD	-2.14	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	GLU	OXT-C-O	-2.74	117.86	124.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	303	GOL	C1-C2-C3-O3
2	D	303	GOL	O2-C2-C3-O3
3	C	301	GLU	CA-CB-CG-CD
2	D	303	GOL	O1-C1-C2-C3
3	B	301	GLU	C-CA-CB-CG
3	B	301	GLU	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	301	GLU	N-CA-CB-CG
3	D	301	GLU	O-C-CA-CB
3	D	301	GLU	OXT-C-CA-CB
3	C	301	GLU	OXT-C-CA-N

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	GLU	4	0
3	B	301	GLU	3	0
2	D	303	GOL	3	0
3	D	301	GLU	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	235/238 (98%)	-0.06	3 (1%) 75 74	7, 17, 31, 47	0
1	B	235/238 (98%)	0.48	24 (10%) 12 11	5, 23, 47, 67	2 (0%)
1	C	235/238 (98%)	0.51	29 (12%) 8 7	4, 23, 54, 62	1 (0%)
1	D	235/238 (98%)	-0.22	1 (0%) 88 88	2, 13, 26, 42	4 (1%)
All	All	940/952 (98%)	0.18	57 (6%) 27 26	2, 17, 47, 67	7 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173	ALA	4.5
1	C	170	PHE	4.2
1	B	204	VAL	3.9
1	B	173	ALA	3.5
1	D	140	GLU	3.4
1	C	167	LEU	3.4
1	B	167	LEU	3.2
1	C	181	VAL	3.1
1	B	182	ILE	3.0
1	C	161	ILE	3.0
1	C	180	GLN	3.0
1	C	235	HIS	3.0
1	C	160	ILE	2.9
1	C	143	SER	2.8
1	B	176	ALA	2.8
1	B	180	GLN	2.8
1	C	178	TYR	2.8
1	B	210	VAL	2.8
1	C	179	ALA	2.7
1	B	205	PRO	2.7
1	C	144	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	156	LYS	2.7
1	B	170	PHE	2.6
1	C	197	SER	2.6
1	C	183	ALA	2.6
1	A	167	LEU	2.6
1	C	157	ILE	2.5
1	B	203	LEU	2.5
1	B	213	VAL	2.5
1	B	201	GLY	2.5
1	B	168	GLY	2.4
1	C	186	ALA	2.4
1	C	162	PHE	2.4
1	C	177	TYR	2.3
1	B	187	GLU	2.3
1	B	159	GLN	2.3
1	B	175	ARG	2.3
1	B	114	GLY	2.3
1	C	174	SER	2.2
1	B	198	THR	2.2
1	C	204	VAL	2.2
1	C	164	GLU	2.2
1	C	189	GLY	2.2
1	B	183	ALA	2.2
1	C	154	ARG	2.2
1	B	132	ASP	2.2
1	C	205	PRO	2.1
1	B	165	LEU	2.1
1	C	158	ASN	2.1
1	C	113	THR	2.1
1	B	209	SER	2.1
1	C	207	GLU	2.0
1	B	184	ARG	2.0
1	A	118	THR	2.0
1	A	173	ALA	2.0
1	C	149	PRO	2.0
1	B	177	TYR	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLU	C	301	10/10	0.81	0.16	28,39,48,52	0
2	GOL	D	303	6/6	0.86	0.13	28,31,32,36	0
3	GLU	B	301	10/10	0.87	0.14	26,35,40,40	0
2	GOL	A	301	6/6	0.87	0.09	34,35,36,36	0
3	GLU	D	301	10/10	0.87	0.12	18,31,41,50	0
4	NO3	D	302	4/4	0.89	0.11	28,29,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.