



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2025 – 01:16 PM JST

PDB ID : 8Z2A
Title : Crystal structure of *Aspergillus terreus* glutamate dehydrogenase (AtGDH) with sequential mutations
Authors : Godsora, B.K.J.; Bhaumik, P.
Deposited on : 2024-04-12
Resolution : 3.10 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	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

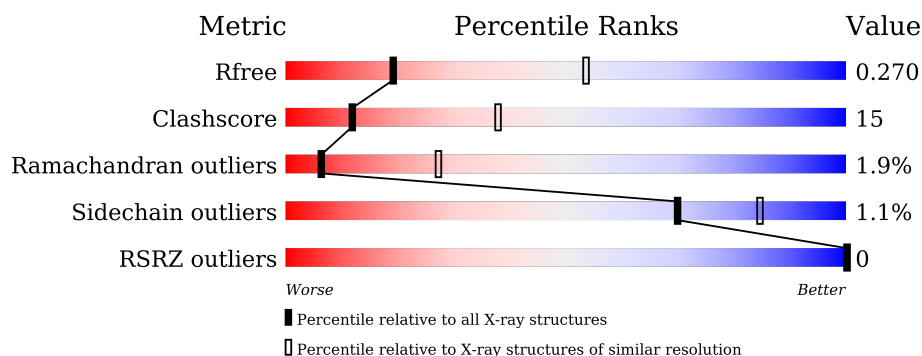
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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	458	<div> <div style="width: 81%; background-color: green;"></div> <div style="width: 17%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>81% 17% .</div>
1	B	458	<div> <div style="width: 64%; background-color: green;"></div> <div style="width: 33%; background-color: yellow;"></div> <div style="width: 3%; background-color: orange;"></div> </div> <div>64% 33% .</div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6936 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 dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	3	0
			3461	2182	600	665	14			
1	B	458	Total	C	N	O	S	0	2	0
			3461	2182	602	664	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	SER	ARG	engineered mutation	UNP T2D1F5
A	260	ASN	LYS	engineered mutation	UNP T2D1F5
A	261	GLY	ASP	engineered mutation	UNP T2D1F5
A	?	-	THR	deletion	UNP T2D1F5
A	?	-	ALA	deletion	UNP T2D1F5
A	262	GLU	LYS	engineered mutation	UNP T2D1F5
A	263	GLY	ASP	engineered mutation	UNP T2D1F5
B	246	SER	ARG	engineered mutation	UNP T2D1F5
B	260	ASN	LYS	engineered mutation	UNP T2D1F5
B	261	GLY	ASP	engineered mutation	UNP T2D1F5
B	?	-	THR	deletion	UNP T2D1F5
B	?	-	ALA	deletion	UNP T2D1F5
B	262	GLU	LYS	engineered mutation	UNP T2D1F5
B	263	GLY	ASP	engineered mutation	UNP T2D1F5

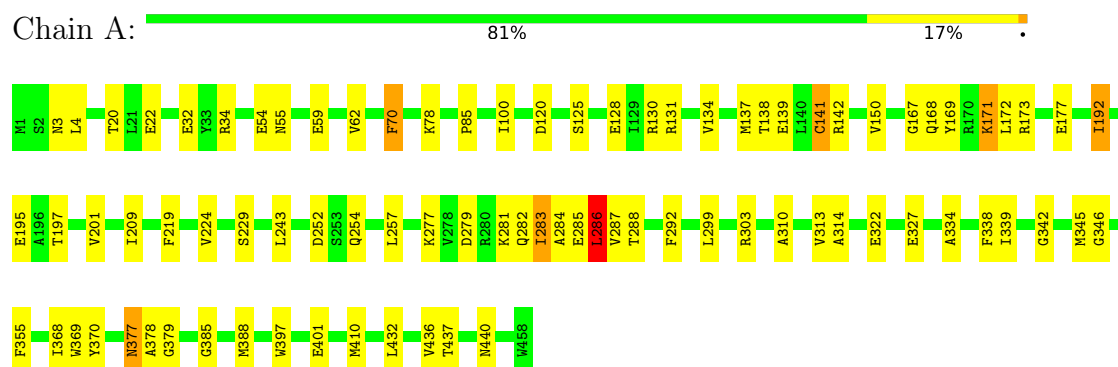
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	4	Total	O	0	0
			4	4		

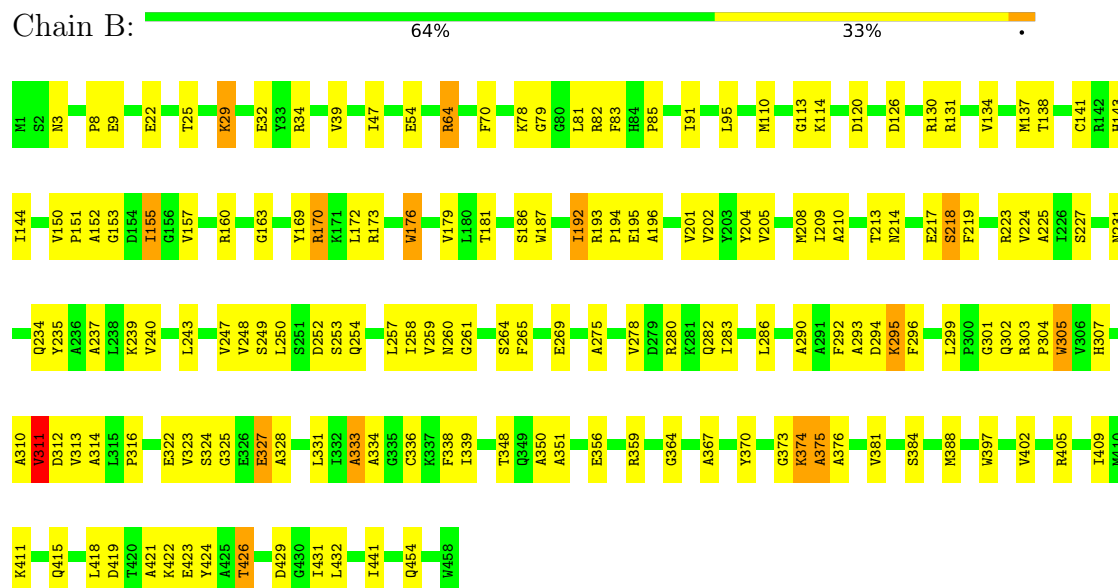
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	143.59Å 143.59Å 143.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 3.10 19.91 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.91-3.10) 92.0 (19.91-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.09Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PDB-REDO	Depositor
R, R_{free}	0.200 , 0.271 0.200 , 0.270	Depositor DCC
R_{free} test set	906 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 17.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
Reported twinning fraction	0.571 for H, K, L 0.429 for -K, -H, -L	Depositor
Outliers	0 of 18106 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6936	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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

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	0.59	2/3531 (0.1%)	0.73	1/4776 (0.0%)
1	B	0.73	1/3531 (0.0%)	0.84	2/4776 (0.0%)
All	All	0.67	3/7062 (0.0%)	0.78	3/9552 (0.0%)

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	A	0	1
1	B	0	5
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	GLU	CG-CD	-6.39	1.42	1.51
1	A	141	CYS	CB-SG	-5.71	1.72	1.81
1	B	327	GLU	CB-CG	5.10	1.61	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	454	GLN	C-N-CA	-6.90	107.81	122.30
1	B	29	LYS	CD-CE-NZ	5.89	125.25	111.70
1	A	286	LEU	CB-CG-CD2	5.12	119.71	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	ASN	Peptide
1	B	170	ARG	Sidechain
1	B	253	SER	Peptide
1	B	311	VAL	Peptide
1	B	333	ALA	Peptide
1	B	64[A]	ARG	Sidechain

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	3461	0	3392	64	0
1	B	3461	0	3393	152	0
2	A	10	0	0	0	0
2	B	4	0	0	0	0
All	All	6936	0	6785	212	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 15.

All (212) 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:A:254:GLN:HE21	1:A:282:GLN:CD	1.04	1.52
1:A:254:GLN:NE2	1:A:282:GLN:CD	1.73	1.38
1:A:254:GLN:NE2	1:A:282:GLN:NE2	1.86	1.22
1:B:299:LEU:HD22	1:B:302:GLN:HB3	1.29	1.14
1:A:254:GLN:NE2	1:A:282:GLN:OE1	1.84	1.03
1:B:299:LEU:HD21	1:B:302:GLN:OE1	1.56	1.03
1:A:254:GLN:HE22	1:A:282:GLN:NE2	1.47	1.01
1:A:279:ASP:HB3	1:A:281:LYS:HE3	1.46	0.94
1:B:257:LEU:HD11	1:B:296:PHE:HB3	1.50	0.93
1:B:201:VAL:HG12	1:B:376:ALA:HB1	1.58	0.85
1:B:275:ALA:O	1:B:278:VAL:HG22	1.79	0.83
1:B:302:GLN:HE22	1:B:307:HIS:HE1	1.27	0.82
1:B:311:VAL:H	1:B:334:ALA:HB1	1.45	0.82
1:B:302:GLN:HE22	1:B:307:HIS:CE1	2.00	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LEU:O	1:B:157:VAL:HG22	1.83	0.78
1:B:424:TYR:HB2	1:B:441:ILE:HD11	1.68	0.76
1:B:299:LEU:CD2	1:B:302:GLN:HB3	2.14	0.76
1:B:29:LYS:NZ	1:B:423:GLU:OE2	2.18	0.74
1:B:137:MET:HE2	1:B:141:CYS:HB3	1.68	0.74
1:B:299:LEU:CD2	1:B:302:GLN:OE1	2.35	0.74
1:A:377:ASN:O	1:A:379:GLY:N	2.21	0.73
1:A:254:GLN:HE22	1:A:282:GLN:HE22	1.34	0.73
1:A:130:ARG:O	1:A:134:VAL:HG23	1.89	0.72
1:A:286:LEU:HD23	1:A:287:VAL:N	2.05	0.72
1:B:303:ARG:HH22	1:B:322:GLU:HA	1.55	0.72
1:A:137:MET:HE2	1:A:141:CYS:HB3	1.71	0.71
1:B:299:LEU:HD22	1:B:302:GLN:CB	2.14	0.70
1:B:305:TRP:CD1	1:B:331:LEU:HD11	2.25	0.70
1:B:22:GLU:OE1	1:B:34:ARG:NH1	2.22	0.70
1:B:137:MET:HE1	1:B:169:TYR:HD2	1.55	0.70
1:B:419:ASP:O	1:B:422:LYS:HG2	1.92	0.69
1:A:22:GLU:OE2	1:A:34:ARG:NH1	2.19	0.68
1:A:279:ASP:HB3	1:A:281:LYS:CE	2.23	0.68
1:A:342:GLY:O	1:A:377:ASN:ND2	2.26	0.68
1:B:195:GLU:HG3	1:B:235:TYR:CE1	2.29	0.67
1:B:223:ARG:HB3	1:B:248:VAL:HG11	1.78	0.66
1:B:324:SER:HA	1:B:327:GLU:CD	2.15	0.66
1:B:286:LEU:HA	1:B:292:PHE:HB3	1.78	0.66
1:A:197:THR:O	1:A:201:VAL:HG23	1.96	0.65
1:B:310:ALA:O	1:B:311:VAL:HG13	1.98	0.64
1:B:324:SER:HA	1:B:327:GLU:OE2	1.98	0.64
1:B:195:GLU:HG3	1:B:235:TYR:CD1	2.33	0.64
1:A:286:LEU:HD23	1:A:287:VAL:H	1.63	0.63
1:B:170:ARG:HD3	1:B:176:TRP:HD1	1.63	0.63
1:B:224:VAL:HG21	1:B:240:VAL:HG21	1.81	0.63
1:A:283:ILE:O	1:A:286:LEU:HD22	1.99	0.62
1:B:339:ILE:HG23	1:B:370:TYR:HA	1.79	0.62
1:B:419:ASP:HA	1:B:422:LYS:HG2	1.81	0.62
1:B:324:SER:HB2	1:B:348:THR:HG22	1.80	0.62
1:B:153:GLY:HA2	1:B:157:VAL:HG23	1.81	0.62
1:B:302:GLN:NE2	1:B:307:HIS:HE1	1.96	0.61
1:B:223:ARG:HB2	1:B:311:VAL:CG2	2.30	0.61
1:B:231:ASN:HA	1:B:234:GLN:HG2	1.81	0.60
1:B:311:VAL:HB	1:B:312:ASP:CG	2.22	0.60
1:A:385:GLY:HA2	1:A:388[B]:MET:HE3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ILE:HA	1:A:195:GLU:OE1	2.02	0.59
1:B:81:LEU:HB2	1:B:157:VAL:HG21	1.85	0.59
1:B:186:SER:HG	1:B:187:TRP:HD1	1.51	0.59
1:A:139:GLU:OE1	1:A:142:ARG:NH1	2.37	0.58
1:B:348:THR:HG23	1:B:350:ALA:H	1.68	0.58
1:B:202:VAL:HG11	1:B:239:LYS:HG3	1.86	0.58
1:B:223:ARG:O	1:B:311:VAL:HG23	2.04	0.57
1:B:209:ILE:HG21	1:B:218:SER:HA	1.87	0.57
1:B:419:ASP:O	1:B:422:LYS:CG	2.53	0.57
1:B:324:SER:HB3	1:B:351:ALA:HB2	1.87	0.57
1:B:421:ALA:O	1:B:426:THR:N	2.39	0.56
1:B:252:ASP:HB3	1:B:282:GLN:HE21	1.71	0.55
1:B:193:ARG:HB3	1:B:194:PRO:HD3	1.87	0.55
1:B:223:ARG:HB2	1:B:311:VAL:HG21	1.89	0.55
1:B:324:SER:HA	1:B:327:GLU:OE1	2.07	0.55
1:A:282:GLN:O	1:A:284:ALA:N	2.40	0.55
1:B:130:ARG:O	1:B:134:VAL:HG23	2.07	0.55
1:B:223:ARG:HB3	1:B:248:VAL:CG1	2.37	0.55
1:B:237:ALA:HB1	1:B:247:VAL:HG21	1.89	0.55
1:B:259:VAL:HA	1:B:295:LYS:O	2.07	0.55
1:B:312:ASP:HA	1:B:336:CYS:HA	1.89	0.55
1:B:25:THR:HG22	1:B:424:TYR:HA	1.90	0.54
1:B:78:LYS:HD2	1:B:150:VAL:O	2.06	0.54
1:B:250:LEU:HD23	1:B:265:PHE:CE2	2.43	0.54
1:A:339:ILE:HG23	1:A:370:TYR:HA	1.90	0.54
1:B:110:MET:HE1	1:B:381:VAL:HG12	1.89	0.54
1:B:314:ALA:HB3	1:B:339:ILE:HD13	1.89	0.54
1:B:209:ILE:HD13	1:B:338:PHE:CE1	2.43	0.54
1:B:356:GLU:OE1	1:B:359:ARG:NE	2.36	0.53
1:B:79:GLY:HA3	1:B:113:GLY:O	2.09	0.53
1:A:32:GLU:H	1:A:32:GLU:CD	2.12	0.53
1:B:254:GLN:HA	1:B:301:GLY:HA2	1.90	0.53
1:A:229:SER:HB2	1:A:277:LYS:HD2	1.91	0.53
1:B:205:VAL:HA	1:B:208:MET:HE2	1.91	0.53
1:B:311:VAL:N	1:B:334:ALA:HB1	2.19	0.52
1:B:126:ASP:OD1	1:B:160:ARG:HD2	2.10	0.52
1:B:405:ARG:O	1:B:409:ILE:HG13	2.10	0.52
1:B:32:GLU:CD	1:B:32:GLU:H	2.11	0.52
1:B:85:PRO:HG3	1:B:120:ASP:HB2	1.92	0.52
1:B:82:ARG:HG3	1:B:155:ILE:HB	1.92	0.51
1:B:299:LEU:CD2	1:B:302:GLN:CB	2.83	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:HA	1:A:172:LEU:HD11	1.91	0.51
1:B:303:ARG:HH12	1:B:322:GLU:HB3	1.75	0.51
1:B:192:ILE:HA	1:B:195:GLU:OE1	2.11	0.51
1:A:167:GLY:O	1:A:171:LYS:HD3	2.11	0.51
1:B:81:LEU:O	1:B:157:VAL:CG2	2.57	0.51
1:B:290:ALA:HA	1:B:293:ALA:HB3	1.93	0.51
1:B:411:LYS:O	1:B:415:GLN:HG2	2.12	0.50
1:A:282:GLN:C	1:A:284:ALA:H	2.14	0.50
1:B:381:VAL:O	1:B:384:SER:OG	2.26	0.50
1:A:397:TRP:HB3	1:A:401:GLU:HB2	1.93	0.50
1:B:292:PHE:O	1:B:296:PHE:HB2	2.11	0.50
1:B:9[B]:GLU:HG3	1:B:91:ILE:HG12	1.94	0.49
1:B:209:ILE:CG2	1:B:218:SER:HA	2.42	0.49
1:B:258:ILE:CD1	1:B:307:HIS:HB2	2.41	0.49
1:B:213:THR:OG1	1:B:217:GLU:HB3	2.12	0.49
1:A:254:GLN:NE2	1:A:282:GLN:HE22	1.91	0.49
1:A:314:ALA:HB3	1:A:339:ILE:HD12	1.94	0.49
1:B:137:MET:CE	1:B:169:TYR:HD2	2.23	0.49
1:B:303:ARG:NH1	1:B:305:TRP:CZ3	2.81	0.49
1:B:219:PHE:CD1	1:B:240:VAL:HG23	2.48	0.49
1:B:64[B]:ARG:N	1:B:64[B]:ARG:HD3	2.28	0.49
1:B:325:GLY:O	1:B:328:ALA:HB3	2.12	0.48
1:B:25:THR:O	1:B:29:LYS:HG3	2.14	0.48
1:B:47:ILE:HD13	1:B:143:HIS:CG	2.48	0.48
1:A:303:ARG:HD2	1:A:327:GLU:OE2	2.13	0.48
1:B:169:TYR:CE2	1:B:179:VAL:HG21	2.49	0.48
1:B:303:ARG:CD	1:B:323:VAL:HG22	2.43	0.48
1:B:22:GLU:CD	1:B:34:ARG:HH12	2.12	0.48
1:B:239:LYS:O	1:B:243:LEU:HD13	2.13	0.48
1:B:257:LEU:HD12	1:B:258:ILE:H	1.79	0.48
1:A:310:ALA:HA	1:A:334:ALA:HB1	1.95	0.47
1:B:225:ALA:HA	1:B:249:SER:OG	2.14	0.47
1:B:79:GLY:O	1:B:151:PRO:HA	2.14	0.47
1:A:257:LEU:HD22	1:A:286:LEU:HD21	1.95	0.47
1:B:227:SER:OG	1:B:316:PRO:HA	2.14	0.47
1:B:305:TRP:HH2	1:B:322:GLU:HG2	1.80	0.47
1:B:223:ARG:CB	1:B:311:VAL:HG21	2.44	0.47
1:B:418:LEU:HD13	1:B:422:LYS:HE3	1.97	0.47
1:A:286:LEU:HD12	1:A:292:PHE:CZ	2.50	0.47
1:B:137:MET:HE1	1:B:144:ILE:HD11	1.97	0.46
1:B:303:ARG:HH22	1:B:322:GLU:CA	2.26	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:SER:OG	1:A:128:GLU:HG3	2.15	0.46
1:A:282:GLN:C	1:A:284:ALA:N	2.68	0.46
1:A:62:VAL:HG21	1:B:39:VAL:HG22	1.97	0.46
1:B:85:PRO:HG3	1:B:120:ASP:CB	2.45	0.46
1:A:209:ILE:HA	1:A:338:PHE:CZ	2.50	0.46
1:A:4:LEU:HD21	1:B:64[B]:ARG:NH2	2.30	0.46
1:A:322:GLU:N	1:A:346:GLY:O	2.41	0.46
1:B:85:PRO:HG3	1:B:120:ASP:CG	2.36	0.46
1:A:169:TYR:CE1	1:A:173:ARG:HG3	2.50	0.46
1:B:138:THR:HA	1:B:172:LEU:HD11	1.98	0.46
1:B:364:GLY:HA2	1:B:432:LEU:HG	1.97	0.45
1:B:78:LYS:NZ	1:B:181:THR:OG1	2.49	0.45
1:B:294:ASP:C	1:B:296:PHE:H	2.20	0.45
1:A:54:GLU:O	1:A:131:ARG:HD2	2.17	0.45
1:A:257:LEU:CD2	1:A:286:LEU:HD21	2.47	0.45
1:A:134:VAL:HG13	1:A:168:GLN:CD	2.37	0.45
1:B:269:GLU:HG2	1:B:292:PHE:CZ	2.52	0.45
1:B:305:TRP:CH2	1:B:322:GLU:HG2	2.52	0.45
1:A:224:VAL:HG22	1:A:313:VAL:HB	1.99	0.45
1:A:55:ASN:HD21	1:A:59:GLU:HB2	1.82	0.45
1:B:95:LEU:HB2	1:B:114:LYS:HG2	1.99	0.45
1:B:210:ALA:O	1:B:214:ASN:HA	2.17	0.45
1:B:224:VAL:O	1:B:248:VAL:HG22	2.17	0.45
1:B:193:ARG:HA	1:B:193:ARG:HD2	1.73	0.44
1:B:265:PHE:HA	1:B:269:GLU:OE1	2.18	0.44
1:A:85:PRO:O	1:B:3:ASN:ND2	2.40	0.44
1:B:252:ASP:HB3	1:B:282:GLN:NE2	2.32	0.44
1:A:345:MET:HE3	1:A:345:MET:HB3	1.85	0.44
1:A:20:THR:HG21	1:A:440:ASN:HB3	2.00	0.43
1:A:355:PHE:CD1	1:A:368:ILE:HD13	2.53	0.43
1:B:305:TRP:HD1	1:B:331:LEU:HD11	1.81	0.43
1:A:78:LYS:HD2	1:A:150:VAL:O	2.18	0.43
1:B:163:GLY:HA2	1:B:187:TRP:CH2	2.53	0.43
1:B:294:ASP:O	1:B:296:PHE:N	2.51	0.43
1:B:373:GLY:O	1:B:375:ALA:N	2.50	0.43
1:B:204:TYR:CE1	1:B:375:ALA:HB1	2.53	0.43
1:B:252:ASP:CB	1:B:282:GLN:HE21	2.30	0.43
1:A:197:THR:HG23	1:A:377:ASN:O	2.18	0.43
1:B:324:SER:HB2	1:B:348:THR:CG2	2.47	0.43
1:A:219:PHE:HB2	1:A:243:LEU:HD23	2.00	0.43
1:A:252:ASP:CG	1:A:283:ILE:HG12	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLU:O	1:B:131:ARG:HD2	2.19	0.43
1:B:310:ALA:O	1:B:311:VAL:HG22	2.18	0.42
1:A:252:ASP:OD2	1:A:283:ILE:HG12	2.19	0.42
1:A:379:GLY:CA	1:A:410:MET:HE3	2.49	0.42
1:B:397:TRP:HE3	1:B:402:VAL:HG12	1.84	0.42
1:B:418:LEU:CD1	1:B:422:LYS:HE3	2.49	0.42
1:A:62:VAL:CG2	1:B:39:VAL:HG22	2.50	0.42
1:B:25:THR:CG2	1:B:424:TYR:HA	2.49	0.42
1:B:280:ARG:NH1	1:B:280:ARG:HG3	2.34	0.42
1:A:369:TRP:CD2	1:A:432:LEU:HD13	2.55	0.42
1:B:247:VAL:O	1:B:264:SER:HA	2.20	0.42
1:B:359:ARG:HA	1:B:367:ALA:HB1	2.00	0.41
1:B:254:GLN:HG2	1:B:301:GLY:HA2	2.01	0.41
1:A:436:VAL:HG13	1:A:437:THR:N	2.36	0.41
1:B:305:TRP:HD1	1:B:331:LEU:HD21	1.85	0.41
1:A:55:ASN:ND2	1:A:59:GLU:HB2	2.36	0.41
1:A:285:GLU:O	1:A:288:THR:HG22	2.20	0.41
1:A:299:LEU:HD12	1:A:299:LEU:N	2.36	0.41
1:B:83:PHE:CD2	1:B:157:VAL:HG12	2.56	0.41
1:B:137:MET:HE1	1:B:169:TYR:CD2	2.45	0.41
1:B:169:TYR:CZ	1:B:173:ARG:HG3	2.56	0.41
1:B:205:VAL:HG23	1:B:219:PHE:CE2	2.55	0.41
1:B:286:LEU:HB2	1:B:292:PHE:O	2.21	0.41
1:B:313:VAL:HG13	1:B:338:PHE:HB2	2.03	0.41
1:B:259:VAL:HG12	1:B:261:GLY:O	2.21	0.41
1:A:70:PHE:CD1	1:A:100:ILE:HD11	2.57	0.40
1:B:280:ARG:HG3	1:B:280:ARG:HH11	1.85	0.40
1:B:431:ILE:HG22	1:B:432:LEU:O	2.21	0.40
1:A:85:PRO:HG3	1:A:120:ASP:HB2	2.04	0.40
1:B:78:LYS:HZ2	1:B:152:ALA:HB2	1.85	0.40
1:B:419:ASP:CA	1:B:422:LYS:HG2	2.47	0.40
1:B:257:LEU:HD12	1:B:258:ILE:N	2.35	0.40
1:B:260:ASN:OD1	1:B:295:LYS:HA	2.22	0.40
1:B:384:SER:O	1:B:388:MET:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/458 (100%)	435 (95%)	21 (5%)	3 (1%)	19	51
1	B	458/458 (100%)	396 (86%)	48 (10%)	14 (3%)	3	19
All	All	917/916 (100%)	831 (91%)	69 (8%)	17 (2%)	6	27

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ILE
1	B	196	ALA
1	B	283	ILE
1	B	311	VAL
1	B	374	LYS
1	A	378	ALA
1	B	192	ILE
1	B	295	LYS
1	B	333	ALA
1	B	375	ALA
1	B	304	PRO
1	B	426	THR
1	B	305	TRP
1	A	283	ILE
1	B	218	SER
1	B	155	ILE
1	B	8	PRO

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	351/348 (101%)	347 (99%)	4 (1%)	70	84
1	B	350/348 (101%)	346 (99%)	4 (1%)	70	84
All	All	701/696 (101%)	693 (99%)	8 (1%)	70	84

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	70	PHE
1	A	171	LYS
1	A	286	LEU
1	B	70	PHE
1	B	176	TRP
1	B	374	LYS
1	B	429	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	307	HIS
1	A	358	HIS
1	B	282	GLN
1	B	307	HIS

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

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	458/458 (100%)	-0.81	0 100 100	26, 54, 64, 83	3 (0%)
1	B	458/458 (100%)	-0.62	0 100 100	27, 66, 84, 99	2 (0%)
All	All	916/916 (100%)	-0.72	0 100 100	26, 58, 82, 99	5 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.