



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:03 AM UTC

PDB ID : 2Z8I / pdb_00002z8i
Title : Crystal Structure of Escherichia coli Gamma-Glutamyltranspeptidase in Complex with Azaserine
Authors : Wada, K.; Irie, M.; Fukuyama, K.
Deposited on : 2007-09-05
Resolution : 1.65 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

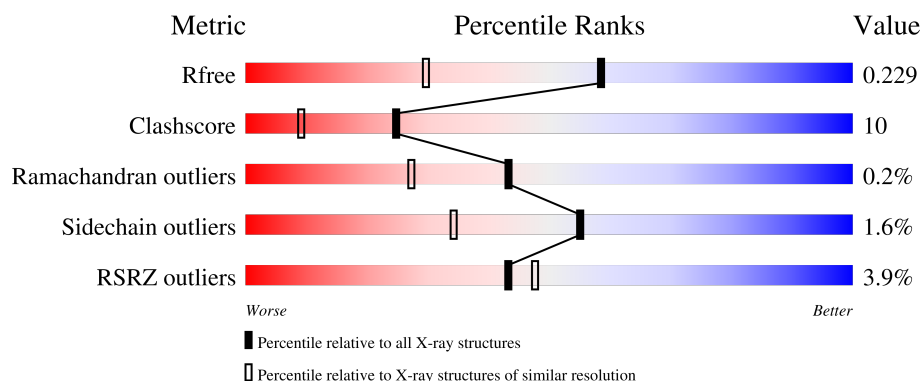
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	366	 4% 77% 17% ..
1	C	366	 4% 79% 16% . 5%
2	B	190	 3% 77% 21% ..
2	D	190	 3% 79% 19% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8602 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.

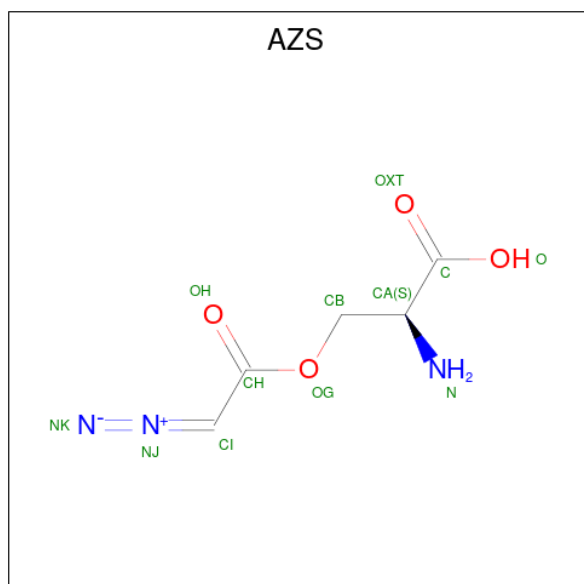
- Molecule 1 is a protein called Gamma-glutamyltranspeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2652	1675	447	519	11			
1	C	349	Total	C	N	O	S	0	0	0
			2643	1670	446	516	11			

- Molecule 2 is a protein called Gamma-glutamyltranspeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	0	0	0
			1407	882	238	282	5			
2	D	190	Total	C	N	O	S	0	0	0
			1407	882	238	282	5			

- Molecule 3 is O-DIAZOACETYL-L-SERINE (CCD ID: AZS) (formula: C₅H₇N₃O₄).



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

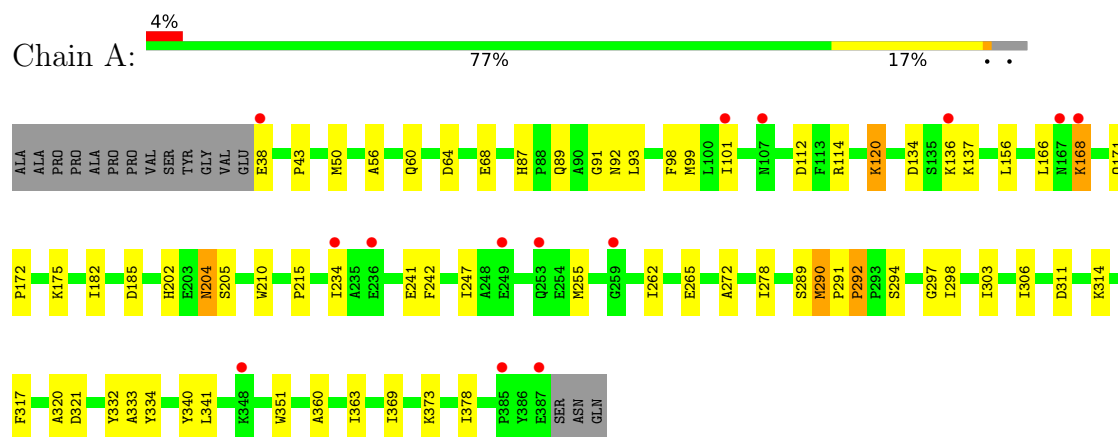
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total	O	0	0
			136	136		
4	B	90	Total	O	0	0
			90	90		
4	C	148	Total	O	0	0
			148	148		
4	D	99	Total	O	0	0
			99	99		

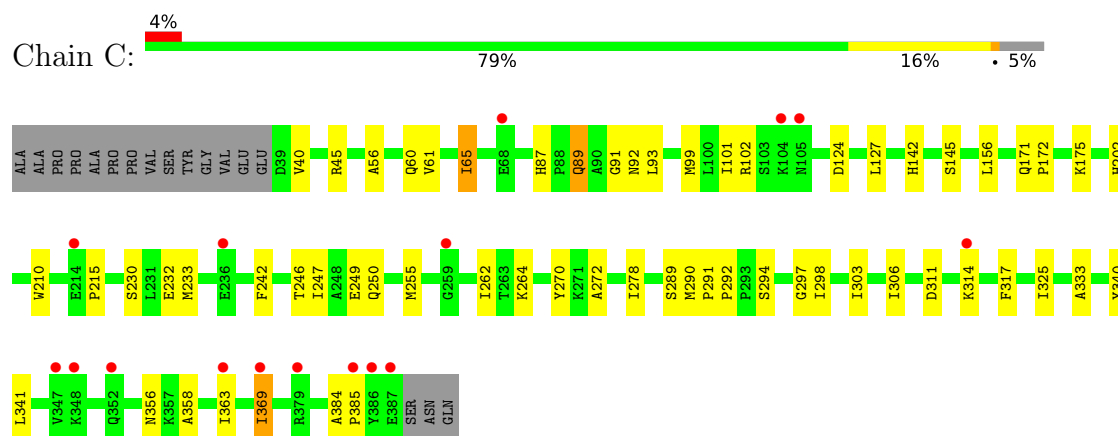
3 Residue-property plots [i](#)

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.

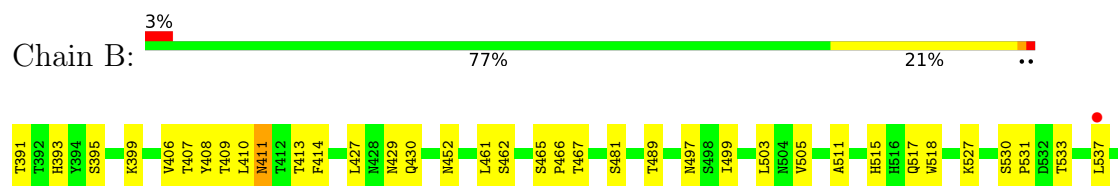
• Molecule 1: Gamma-glutamyltranspeptidase

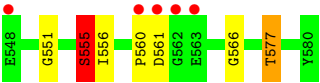


• Molecule 1: Gamma-glutamyltranspeptidase

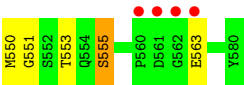
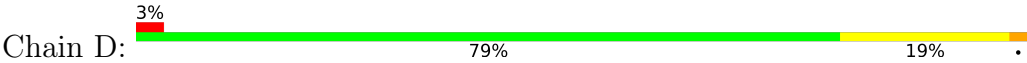


• Molecule 2: Gamma-glutamyltranspeptidase





● Molecule 2: Gamma-glutamyltranspeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.51Å 126.20Å 129.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.41 – 1.65 29.41 – 1.65	Depositor EDS
% Data completeness (in resolution range)	91.0 (29.41-1.65) 91.1 (29.41-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.236 0.213 , 0.229	Depositor DCC
R_{free} test set	7453 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.787	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8602	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: AZS

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	0.37	0/2705	0.91	8/3660 (0.2%)
1	C	0.37	0/2696	0.90	8/3648 (0.2%)
2	B	0.40	0/1434	1.04	11/1952 (0.6%)
2	D	0.40	0/1434	1.02	8/1952 (0.4%)
All	All	0.38	0/8269	0.95	35/11212 (0.3%)

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	C	0	1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	GLY	N-CA-C	-9.71	100.76	111.93
1	C	93	LEU	N-CA-C	-9.13	102.53	114.31
1	A	93	LEU	N-CA-C	-8.77	103.00	114.31
2	B	410	LEU	N-CA-C	-7.12	103.76	113.30
2	D	465	SER	N-CA-C	7.06	121.09	109.79
1	A	92	ASN	N-CA-C	7.05	118.89	108.60
1	A	91	GLY	N-CA-C	-7.02	103.14	111.36
2	B	481	SER	N-CA-C	6.77	114.22	108.13
1	A	340	TYR	N-CA-C	6.11	120.89	113.38
2	D	551	GLY	N-CA-C	5.95	123.11	112.22
2	B	465	SER	N-CA-C	5.93	119.28	109.79
2	D	410	LEU	N-CA-C	-5.88	105.42	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ASN	N-CA-C	5.83	117.00	108.14
2	D	481	SER	N-CA-C	5.77	113.32	108.13
2	B	555	SER	N-CA-C	5.75	118.43	109.52
1	C	145	SER	N-CA-C	5.72	119.14	109.76
2	D	555	SER	N-CA-C	5.53	118.08	109.52
1	A	292	PRO	N-CA-C	-5.49	105.20	110.47
2	B	466	PRO	N-CA-C	-5.49	102.58	111.03
1	C	278	ILE	N-CA-C	-5.41	101.86	109.21
1	C	40	VAL	N-CA-C	-5.40	104.73	112.35
2	B	527	LYS	N-CA-C	-5.36	102.95	110.50
2	D	499	ILE	N-CA-C	5.34	116.00	110.82
2	B	577	THR	N-CA-C	-5.33	100.21	108.90
1	A	290	MET	N-CA-C	5.24	116.42	109.93
1	C	272	ALA	N-CA-C	-5.21	101.96	110.20
2	B	467	THR	N-CA-C	5.21	117.31	109.23
2	D	466	PRO	N-CA-C	-5.21	103.01	111.03
1	C	340	TYR	N-CA-C	5.18	119.75	113.38
1	A	341	LEU	N-CA-C	5.17	117.67	109.24
1	A	272	ALA	N-CA-C	-5.10	102.94	110.48
2	B	551	GLY	N-CA-C	5.09	121.74	112.58
2	B	409	THR	N-CA-C	5.05	115.81	108.14
2	B	499	ILE	N-CA-C	5.04	115.71	110.82
2	D	409	THR	N-CA-C	5.02	115.77	108.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	270	TYR	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	2652	0	2620	65	0
1	C	2643	0	2614	51	0
2	B	1407	0	1391	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1407	0	1391	31	0
3	B	10	0	5	2	0
3	D	10	0	5	2	0
4	A	136	0	0	4	0
4	B	90	0	0	2	0
4	C	148	0	0	9	0
4	D	99	0	0	6	0
All	All	8602	0	8026	158	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 10.

All (158) 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)
2:D:550:MET:HE2	4:D:775:HOH:O	1.59	1.02
1:A:373:LYS:HD2	1:A:378:ILE:HD11	1.43	1.00
1:C:89:GLN:HE21	1:C:89:GLN:H	1.02	1.00
1:C:369:ILE:HD12	1:C:369:ILE:H	1.34	0.93
1:A:234:ILE:HD13	1:A:241:GLU:HB3	1.54	0.88
1:A:50:MET:SD	2:B:556:ILE:HD12	2.18	0.83
1:C:171:GLN:HG3	1:C:175:LYS:HE2	1.61	0.82
2:D:524:ARG:HG2	4:D:775:HOH:O	1.80	0.82
2:D:493:GLN:HE22	2:D:514:PHE:H	1.27	0.81
1:A:98:PHE:CD1	1:A:290:MET:HE2	2.15	0.80
1:C:249:GLU:OE1	1:C:264:LYS:HD2	1.82	0.79
1:C:61:VAL:O	1:C:65:ILE:HD13	1.87	0.74
2:D:411:ASN:O	3:D:390:AZS:CI	2.37	0.72
2:D:411:ASN:HB3	2:D:429:ASN:OD1	1.91	0.71
1:A:373:LYS:CD	1:A:378:ILE:HD11	2.21	0.69
2:D:504:ASN:ND2	2:D:507:GLU:H	1.90	0.69
1:A:136:LYS:HD3	1:A:137:LYS:N	2.08	0.69
2:D:504:ASN:HD22	2:D:504:ASN:C	2.00	0.69
1:C:325:ILE:HD11	1:C:369:ILE:HG13	1.74	0.68
1:A:311:ASP:OD2	1:A:314:LYS:HE3	1.92	0.68
1:A:290:MET:HE3	1:A:291:PRO:HD2	1.75	0.68
1:C:363:ILE:HD11	4:C:475:HOH:O	1.93	0.67
2:B:533:THR:O	2:B:537:LEU:HD23	1.96	0.66
1:C:89:GLN:H	1:C:89:GLN:NE2	1.86	0.66
1:C:306:ILE:HD12	1:C:363:ILE:HB	1.79	0.65
2:B:411:ASN:O	3:B:390:AZS:CI	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ILE:HD12	1:A:363:ILE:HB	1.76	0.65
1:A:332:TYR:CE1	1:A:378:ILE:HD12	2.31	0.65
2:D:518:TRP:CD2	2:D:519:LEU:HD13	2.33	0.64
2:B:555:SER:O	2:B:556:ILE:HD13	1.97	0.64
1:A:320:ALA:HA	2:B:537:LEU:HD21	1.80	0.64
1:A:64:ASP:O	1:A:68:GLU:HG3	1.97	0.63
1:A:136:LYS:HD3	1:A:136:LYS:C	2.24	0.63
1:C:298:ILE:HD12	4:C:511:HOH:O	1.98	0.62
2:D:452:ASN:HD21	2:D:461:LEU:H	1.49	0.61
1:C:311:ASP:OD2	1:C:314:LYS:HG3	2.01	0.61
2:D:393:HIS:HD2	2:D:407:THR:OG1	1.84	0.61
1:C:303:ILE:HD11	1:C:333:ALA:HB2	1.84	0.60
1:A:182:ILE:HD12	1:A:182:ILE:N	2.17	0.60
1:A:182:ILE:HD12	1:A:182:ILE:H	1.67	0.59
1:A:306:ILE:CD1	1:A:363:ILE:HB	2.31	0.59
1:C:306:ILE:CD1	1:C:363:ILE:HB	2.34	0.57
2:B:393:HIS:HD2	2:B:407:THR:OG1	1.85	0.57
2:B:411:ASN:HB3	2:B:429:ASN:OD1	2.04	0.57
2:B:452:ASN:HD21	2:B:461:LEU:H	1.52	0.57
1:A:204:ASN:HD22	1:A:205:SER:H	1.53	0.57
1:C:156:LEU:C	1:C:156:LEU:HD23	2.30	0.56
2:B:489:THR:OG1	2:B:515:HIS:HD2	1.88	0.56
1:C:369:ILE:HD12	1:C:369:ILE:N	2.14	0.56
1:A:278:ILE:HG12	1:A:291:PRO:HB3	1.86	0.56
2:D:521:ASP:O	2:D:543:LYS:HE2	2.07	0.55
1:A:101:ILE:N	1:A:101:ILE:HD12	2.21	0.55
1:A:168:LYS:HB2	1:A:168:LYS:NZ	2.22	0.55
1:A:38:GLU:HA	2:D:548:GLU:HA	1.89	0.54
2:B:399:LYS:HB3	4:B:770:HOH:O	2.06	0.54
1:C:369:ILE:H	1:C:369:ILE:CD1	2.11	0.54
1:C:232:GLU:HG2	1:C:233:MET:HE2	1.88	0.54
1:C:210:TRP:CH2	1:C:215:PRO:HB3	2.42	0.54
1:A:255:MET:HE3	1:A:262:ILE:HD12	1.89	0.54
2:D:501:TYR:HE2	4:D:776:HOH:O	1.91	0.54
1:A:306:ILE:HD13	1:A:360:ALA:O	2.08	0.53
1:A:298:ILE:HD11	1:A:351:TRP:HB2	1.90	0.53
1:C:89:GLN:HE21	1:C:89:GLN:N	1.86	0.53
1:A:156:LEU:C	1:A:156:LEU:HD23	2.33	0.53
1:C:292:PRO:HA	1:C:294:SER:N	2.23	0.53
1:C:142:HIS:HD2	1:C:255:MET:HE2	1.73	0.53
1:C:255:MET:HG3	1:C:262:ILE:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:MET:HG3	2:D:406:VAL:HG22	1.90	0.52
1:C:171:GLN:HB3	1:C:172:PRO:HD3	1.92	0.52
2:B:391:THR:N	3:B:390:AZS:CI	2.73	0.51
1:A:99:MET:HG3	2:B:406:VAL:HG22	1.93	0.51
1:C:292:PRO:HG3	4:C:511:HOH:O	2.10	0.51
2:D:391:THR:N	3:D:390:AZS:CI	2.74	0.50
1:A:317:PHE:CZ	2:B:511:ALA:HB1	2.47	0.50
1:A:87:HIS:HD2	4:A:474:HOH:O	1.95	0.49
1:A:204:ASN:HD22	1:A:204:ASN:N	2.10	0.49
1:A:303:ILE:HD11	1:A:333:ALA:HB2	1.95	0.49
2:B:517:GLN:O	2:B:518:TRP:HB3	2.11	0.49
2:D:517:GLN:O	2:D:518:TRP:HB3	2.11	0.49
1:A:255:MET:HG3	1:A:262:ILE:HB	1.94	0.49
1:A:289:SER:HB3	1:A:297:GLY:HA2	1.94	0.49
2:D:518:TRP:O	2:D:519:LEU:HD12	2.13	0.49
1:A:242:PHE:HA	1:A:247:ILE:HB	1.95	0.48
1:A:265:GLU:HG3	4:A:522:HOH:O	2.12	0.48
1:C:290:MET:HE3	1:C:291:PRO:HD2	1.95	0.48
1:A:278:ILE:HD12	1:A:298:ILE:HD11	1.94	0.48
1:C:303:ILE:HD11	1:C:333:ALA:CB	2.42	0.48
1:A:98:PHE:HD1	1:A:290:MET:HE2	1.74	0.48
1:A:185:ASP:HB3	1:C:45:ARG:NH1	2.29	0.48
2:B:560:PRO:HG2	2:B:561:ASP:OD1	2.14	0.48
2:D:504:ASN:HD22	2:D:506:ALA:H	1.60	0.48
1:C:124:ASP:HB3	1:C:127:LEU:HD12	1.96	0.48
1:C:311:ASP:CG	1:C:314:LYS:HG3	2.39	0.47
1:C:232:GLU:HG2	1:C:233:MET:CE	2.44	0.47
1:C:289:SER:HB3	1:C:297:GLY:HA2	1.96	0.47
1:A:185:ASP:HB3	1:C:45:ARG:HH11	1.79	0.47
1:A:204:ASN:HD22	1:A:205:SER:N	2.12	0.47
4:C:510:HOH:O	2:D:451:ALA:HB3	2.15	0.46
2:D:504:ASN:HD22	2:D:506:ALA:N	2.13	0.46
1:C:87:HIS:HD2	4:C:542:HOH:O	1.98	0.46
1:C:102:ARG:HD3	2:D:475:THR:OG1	2.16	0.46
2:D:504:ASN:ND2	2:D:506:ALA:H	2.14	0.46
2:D:504:ASN:HD21	2:D:506:ALA:HB3	1.79	0.46
1:C:171:GLN:HG3	1:C:175:LYS:CE	2.39	0.46
1:C:242:PHE:HA	1:C:247:ILE:HB	1.97	0.45
1:C:317:PHE:CZ	2:D:511:ALA:HB1	2.52	0.45
1:A:171:GLN:HB3	1:A:172:PRO:HD3	1.99	0.45
1:C:363:ILE:CD1	4:C:475:HOH:O	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:CZ	2:B:462:SER:HB2	2.47	0.45
2:D:550:MET:CE	4:D:775:HOH:O	2.38	0.45
1:C:341:LEU:HD11	4:C:511:HOH:O	2.16	0.45
1:A:306:ILE:CD1	1:A:360:ALA:HA	2.46	0.45
2:B:413:THR:O	2:B:414:PHE:HB2	2.16	0.45
1:A:89:GLN:HB3	2:B:413:THR:HG23	1.99	0.45
1:A:120:LYS:NZ	1:A:120:LYS:HB2	2.33	0.44
1:C:247:ILE:CD1	4:C:427:HOH:O	2.65	0.44
2:B:489:THR:OG1	2:B:515:HIS:CD2	2.71	0.44
1:C:356:ASN:OD1	1:C:358:ALA:HB3	2.18	0.44
1:A:43:PRO:HB3	2:B:505:VAL:HG12	2.00	0.44
1:A:56:ALA:O	1:A:60:GLN:HG3	2.18	0.44
1:A:255:MET:HE2	2:B:427:LEU:HD13	1.99	0.43
1:A:134:ASP:OD2	1:A:136:LYS:HB3	2.19	0.43
1:A:166:LEU:HD21	4:A:508:HOH:O	2.18	0.43
2:D:452:ASN:ND2	2:D:461:LEU:H	2.17	0.43
1:A:204:ASN:N	1:A:204:ASN:ND2	2.67	0.43
1:A:210:TRP:CH2	1:A:215:PRO:HB3	2.54	0.42
1:C:87:HIS:HA	1:C:89:GLN:HE22	1.84	0.42
1:A:112:ASP:OD1	1:A:112:ASP:C	2.62	0.42
1:A:171:GLN:HG3	1:A:175:LYS:NZ	2.34	0.42
1:A:156:LEU:HD23	1:A:156:LEU:O	2.19	0.42
2:D:504:ASN:ND2	2:D:504:ASN:C	2.69	0.42
1:A:321:ASP:HB3	1:A:369:ILE:HD11	2.00	0.42
1:C:56:ALA:O	1:C:60:GLN:HG3	2.19	0.42
1:C:172:PRO:HA	1:C:175:LYS:HE3	2.02	0.42
2:B:393:HIS:HE1	2:B:395:SER:OG	2.02	0.42
2:B:566:GLY:HA3	2:B:577:THR:HG21	2.02	0.42
1:A:247:ILE:CD1	4:A:463:HOH:O	2.68	0.41
1:A:303:ILE:HD11	1:A:333:ALA:CB	2.49	0.41
1:A:171:GLN:HA	1:A:171:GLN:HE21	1.85	0.41
1:A:306:ILE:HD11	1:A:360:ALA:HA	2.03	0.41
1:C:246:THR:O	1:C:250:GLN:HG3	2.21	0.41
1:A:171:GLN:HA	1:A:171:GLN:NE2	2.35	0.41
1:C:202:HIS:HE1	4:C:548:HOH:O	2.02	0.41
1:C:230:SER:OG	1:C:247:ILE:HD11	2.20	0.41
1:C:156:LEU:HD23	1:C:156:LEU:O	2.21	0.41
2:D:493:GLN:HE22	2:D:514:PHE:N	2.06	0.41
1:A:306:ILE:HD11	1:A:363:ILE:HD12	2.02	0.41
2:B:497:ASN:HB3	2:B:503:LEU:HD12	2.03	0.41
2:B:530:SER:HA	2:B:531:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:ALA:N	1:C:385:PRO:HD2	2.36	0.41
2:D:442:ASN:ND2	4:D:773:HOH:O	2.53	0.41
2:D:525:VAL:C	4:D:775:HOH:O	2.63	0.41
1:A:292:PRO:HA	1:A:294:SER:N	2.35	0.41
1:A:202:HIS:HE1	4:B:786:HOH:O	2.04	0.40
1:A:306:ILE:HD13	1:A:360:ALA:CA	2.50	0.40
1:C:99:MET:SD	1:C:101:ILE:HD11	2.62	0.40
1:A:334:TYR:CD2	2:B:517:GLN:HA	2.56	0.40
2:D:509:THR:HG23	2:D:553:THR:OG1	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	348/366 (95%)	339 (97%)	9 (3%)	0	100	100
1	C	347/366 (95%)	341 (98%)	6 (2%)	0	100	100
2	B	188/190 (99%)	182 (97%)	5 (3%)	1 (0%)	24	10
2	D	188/190 (99%)	182 (97%)	5 (3%)	1 (0%)	24	10
All	All	1071/1112 (96%)	1044 (98%)	25 (2%)	2 (0%)	43	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	411	ASN
2	D	411	ASN

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	275/287 (96%)	272 (99%)	3 (1%)	65	48
1	C	274/287 (96%)	271 (99%)	3 (1%)	65	48
2	B	154/154 (100%)	151 (98%)	3 (2%)	50	28
2	D	154/154 (100%)	149 (97%)	5 (3%)	34	12
All	All	857/882 (97%)	843 (98%)	14 (2%)	55	34

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	LYS
1	A	168	LYS
1	A	204	ASN
2	B	408	TYR
2	B	430	GLN
2	B	555	SER
1	C	65	ILE
1	C	89	GLN
1	C	369	ILE
2	D	408	TYR
2	D	430	GLN
2	D	504	ASN
2	D	555	SER
2	D	563	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	60	GLN
1	A	87	HIS
1	A	107	ASN
1	A	202	HIS

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Mol	Chain	Res	Type
1	A	204	ASN
1	A	250	GLN
1	A	253	GLN
1	A	370	ASN
2	B	393	HIS
2	B	452	ASN
2	B	515	HIS
1	C	87	HIS
1	C	89	GLN
1	C	107	ASN
1	C	167	ASN
1	C	171	GLN
1	C	201	ASN
1	C	202	HIS
1	C	237	ASN
1	C	366	GLN
2	D	393	HIS
2	D	452	ASN
2	D	493	GLN
2	D	504	ASN

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](#)

2 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	AZS	D	390	2	8,9,11	2.49	2 (25%)	7,11,13	1.82	2 (28%)
3	AZS	B	390	2	8,9,11	2.48	2 (25%)	7,11,13	2.15	3 (42%)

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	AZS	D	390	2	-	1/9/9/12	-
3	AZS	B	390	2	-	1/9/9/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	390	AZS	OH-CH	6.28	1.43	1.21
3	B	390	AZS	OH-CH	6.26	1.43	1.21
3	D	390	AZS	OG-CH	2.14	1.43	1.33
3	B	390	AZS	OG-CH	2.12	1.43	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	390	AZS	OH-CH-CI	-4.31	109.49	124.77
3	D	390	AZS	OH-CH-CI	-3.58	112.08	124.77
3	D	390	AZS	OG-CH-OH	-2.77	107.67	121.59
3	B	390	AZS	OG-CH-OH	-2.45	109.30	121.59
3	B	390	AZS	CB-OG-CH	-2.33	111.34	117.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	390	AZS	OH-CH-OG-CB
3	D	390	AZS	OH-CH-OG-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	390	AZS	2	0
3	B	390	AZS	2	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	350/366 (95%)	0.22	14 (4%) 42 46	9, 14, 24, 38	0
1	C	349/366 (95%)	0.32	16 (4%) 37 41	9, 15, 27, 44	0
2	B	190/190 (100%)	0.04	6 (3%) 50 54	8, 12, 21, 38	0
2	D	190/190 (100%)	0.05	6 (3%) 50 54	8, 13, 25, 39	0
All	All	1079/1112 (97%)	0.19	42 (3%) 43 48	8, 14, 25, 44	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	560	PRO	5.2
1	C	105	ASN	4.2
2	B	561	ASP	4.0
1	C	369	ILE	3.8
1	A	387	GLU	3.5
2	B	563	GLU	3.3
1	C	386	TYR	3.3
2	D	561	ASP	3.2
2	B	548	GLU	3.2
1	C	314	LYS	3.2
2	B	562	GLY	3.2
1	C	387	GLU	3.0
1	A	385	PRO	3.0
2	D	562	GLY	3.0
1	A	136	LYS	2.9
2	D	563	GLU	2.9
2	D	560	PRO	2.9
1	C	385	PRO	2.8
1	A	234	ILE	2.8
1	C	104	LYS	2.8
1	A	38	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	214	GLU	2.7
1	C	363	ILE	2.6
1	C	348	LYS	2.5
1	A	249	GLU	2.5
1	C	379	ARG	2.4
1	A	236	GLU	2.4
1	C	347	VAL	2.4
2	D	543	LYS	2.3
2	B	537	LEU	2.2
1	A	168	LYS	2.2
1	A	167	ASN	2.2
1	C	236	GLU	2.2
1	A	348	LYS	2.2
1	A	107	ASN	2.2
2	D	472	ASP	2.1
1	A	259	GLY	2.1
1	C	68	GLU	2.1
1	C	352	GLN	2.1
1	A	253	GLN	2.0
1	C	259	GLY	2.0
1	A	101	ILE	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	AZS	B	390	10/12	0.87	0.11	10,12,14,15	0
3	AZS	D	390	10/12	0.90	0.10	10,11,14,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.