



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:42 AM UTC

PDB ID : 2Z8J / pdb_00002z8j
Title : Crystal Structure of Escherichia coli gamma-Glutamyltranspeptidase in Complex with Azaserine prepared in the dark
Authors : Wada, K.; Irie, M.; Fukuyama, K.
Deposited on : 2007-09-05
Resolution : 2.05 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

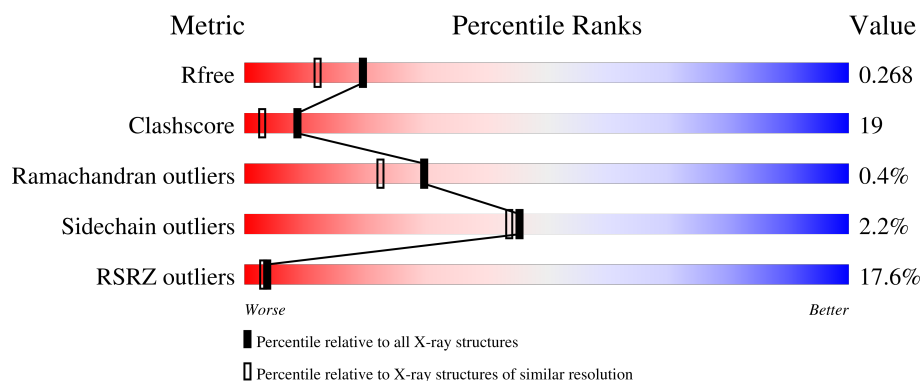
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	17% 68% 26% • •
1	C	366	16% 69% 25% • •
2	B	190	16% 71% 24% 5% •
2	D	190	20% 65% 31% • •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8555 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.

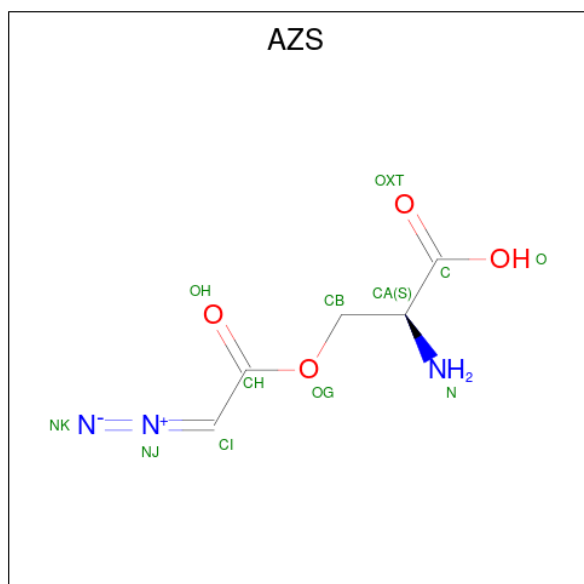
- Molecule 1 is a protein called Gamma-glutamyltranspeptidase.

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	350	Total	C	N	O	S	0	0	0
			2652	1675	447	519	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
			12	5	3	4		
3	D	1	Total	C	N	O	0	0
			12	5	3	4		

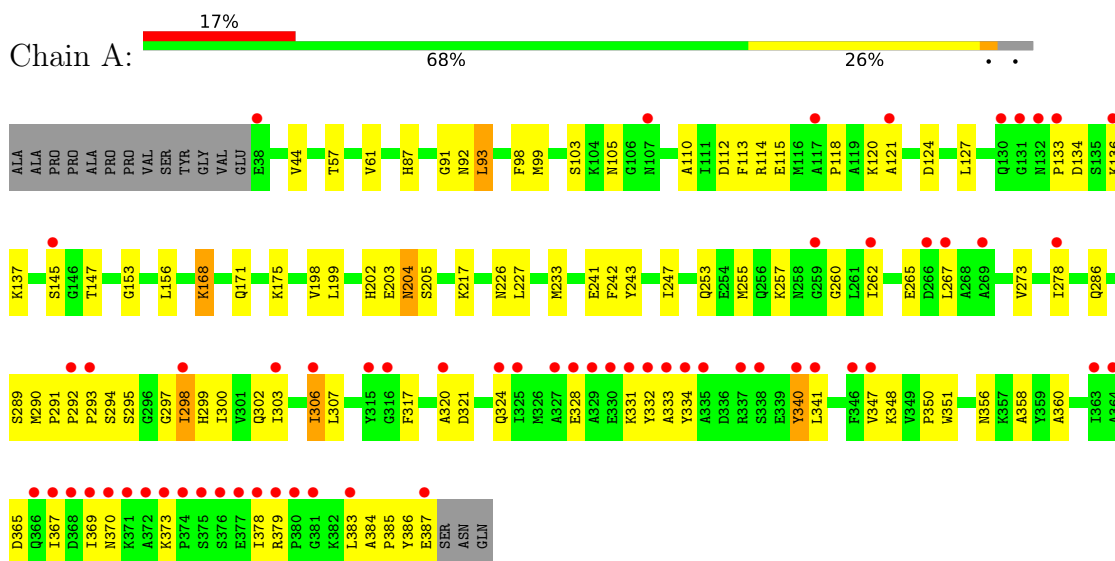
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	0
			124	124		
4	B	70	Total	O	0	0
			70	70		
4	C	149	Total	O	0	0
			149	149		
4	D	70	Total	O	0	0
			70	70		

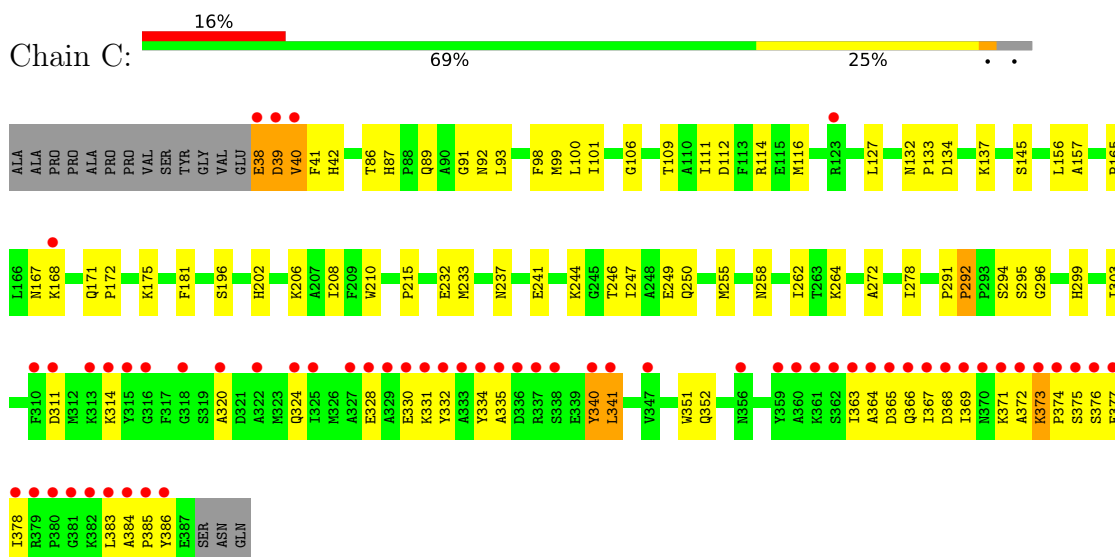
3 Residue-property plots [i](#)

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

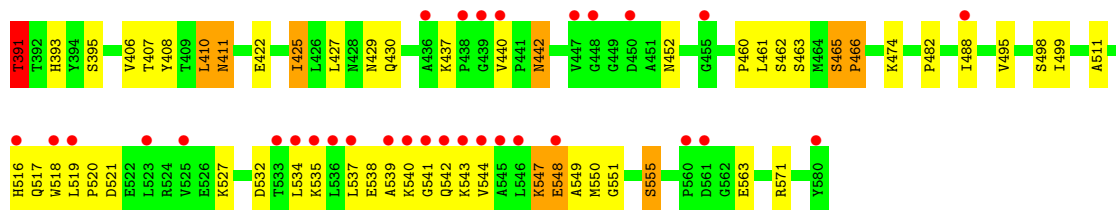


• Molecule 1: Gamma-glutamyltranspeptidase



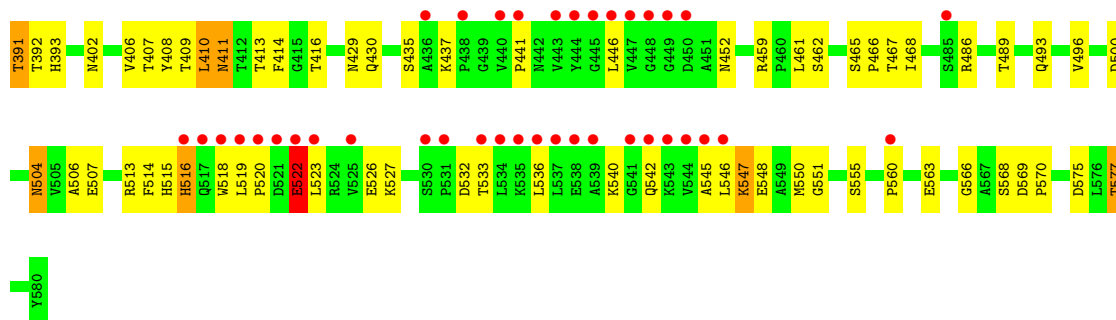
• Molecule 2: Gamma-glutamyltranspeptidase

Chain B: 



• Molecule 2: Gamma-glutamyltranspeptidase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.26Å 126.80Å 128.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.14 – 2.05 40.14 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.14-2.05) 98.5 (40.14-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.66 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.267 0.227 , 0.268	Depositor DCC
R_{free} test set	3972 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8555	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: 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	0.43	0/2705	0.94	11/3660 (0.3%)
1	C	0.51	2/2705 (0.1%)	0.99	16/3660 (0.4%)
2	B	0.56	1/1434 (0.1%)	1.10	14/1952 (0.7%)
2	D	0.51	1/1434 (0.1%)	1.06	8/1952 (0.4%)
All	All	0.50	4/8278 (0.0%)	1.01	49/11224 (0.4%)

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
2	B	1	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	391	THR	C-O	9.74	1.43	1.23
1	C	40	VAL	CA-CB	6.09	1.62	1.54
1	C	40	VAL	C-N	5.47	1.40	1.33
2	D	391	THR	CA-CB	5.33	1.68	1.54

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	LEU	N-CA-C	-10.06	101.34	114.31
2	D	391	THR	CA-CB-CG2	-9.87	93.72	110.50
1	C	91	GLY	N-CA-C	-8.83	101.77	111.93
1	A	93	LEU	N-CA-C	-8.79	103.40	114.56
2	B	391	THR	CA-C-O	-8.04	107.14	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	GLY	N-CA-C	-7.45	103.36	111.93
2	B	410	LEU	N-CA-C	-7.23	103.62	113.30
2	B	391	THR	N-CA-CB	6.99	123.39	111.50
1	A	295	SER	N-CA-C	-6.98	104.37	113.17
1	C	340	TYR	N-CA-C	6.76	120.51	112.93
2	D	410	LEU	N-CA-C	-6.64	104.40	113.30
1	C	92	ASN	N-CA-C	6.45	117.95	108.14
1	C	145	SER	N-CA-C	6.39	120.69	109.96
1	A	92	ASN	N-CA-C	6.35	117.79	108.14
1	C	272	ALA	N-CA-C	-6.15	101.38	110.48
1	C	38	GLU	CA-C-N	6.09	133.17	121.54
1	C	38	GLU	C-N-CA	6.09	133.17	121.54
1	A	44	VAL	N-CA-C	-6.00	101.82	109.80
1	C	39	ASP	N-CA-C	5.96	123.49	110.80
2	B	465	SER	CA-C-N	-5.80	113.79	119.76
2	B	465	SER	C-N-CA	-5.80	113.79	119.76
2	D	527	LYS	N-CA-C	-5.80	102.33	110.50
2	B	391	THR	O-C-N	-5.75	113.79	123.00
1	A	340	TYR	N-CA-C	5.63	120.14	113.28
2	B	391	THR	N-CA-C	5.61	126.70	111.00
1	A	298	ILE	N-CA-C	5.58	116.22	110.36
2	B	555	SER	N-CA-C	5.53	118.09	109.52
2	D	526	GLU	N-CA-C	-5.50	102.05	110.14
1	C	40	VAL	CA-C-N	-5.49	115.42	123.00
1	C	40	VAL	C-N-CA	-5.49	115.42	123.00
2	B	466	PRO	N-CA-C	-5.49	102.58	111.14
2	D	551	GLY	N-CA-C	5.48	122.44	112.58
1	A	341	LEU	N-CA-C	5.43	118.08	109.24
2	B	551	GLY	N-CA-C	5.39	122.29	112.58
1	C	106	GLY	N-CA-C	5.38	121.09	114.69
2	B	425	ILE	N-CA-C	5.32	115.76	107.99
1	C	41	PHE	N-CA-CB	5.31	118.91	110.57
1	C	208	ILE	N-CA-C	5.30	116.71	111.67
2	D	435	SER	N-CA-C	-5.24	100.55	108.67
1	A	145	SER	N-CA-C	5.23	118.46	110.20
1	A	273	VAL	N-CA-C	5.17	115.43	107.77
2	D	577	THR	N-CA-C	-5.16	100.49	108.90
2	B	547	LYS	N-CA-C	5.12	115.29	108.38
2	D	466	PRO	N-CA-C	-5.10	103.18	111.03
2	B	550	MET	N-CA-C	5.09	116.82	108.52
1	C	258	ASN	N-CA-C	5.09	118.98	112.26
1	A	203	GLU	N-CA-C	5.08	117.20	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	527	LYS	N-CA-C	-5.04	103.40	110.50
1	C	341	LEU	N-CA-C	5.03	117.59	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	391	THR	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2652	0	2620	107	0
1	C	2652	0	2620	96	0
2	B	1407	0	1391	65	0
2	D	1407	0	1391	83	0
3	B	12	0	6	2	0
3	D	12	0	6	3	0
4	A	124	0	0	11	0
4	B	70	0	0	0	0
4	C	149	0	0	6	0
4	D	70	0	0	6	0
All	All	8555	0	8034	302	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 (302) 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:302:GLN:O	1:A:306:ILE:HD13	1.57	1.04
2:B:391:THR:N	3:B:390:AZS:HI	1.80	0.96
2:B:532:ASP:O	2:B:535:LYS:HG2	1.63	0.96
2:D:411:ASN:O	3:D:390:AZS:HI	1.64	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LYS:HD2	1:A:378:ILE:HD11	1.49	0.94
1:C:39:ASP:O	1:C:42:HIS:CE1	2.22	0.92
1:A:306:ILE:HD12	1:A:360:ALA:HB1	1.51	0.92
1:C:165:PRO:HG2	1:C:168:LYS:HG2	1.49	0.91
1:C:255:MET:HE3	1:C:262:ILE:HD12	1.54	0.90
1:A:289:SER:HB3	1:A:297:GLY:HA2	1.59	0.85
2:D:391:THR:HG22	2:D:392:THR:N	1.93	0.84
2:B:547:LYS:HG2	2:B:548:GLU:H	1.47	0.79
1:A:118:PRO:HG3	1:A:262:ILE:HD13	1.65	0.78
1:A:328:GLU:HB3	1:A:367:ILE:HD12	1.67	0.77
2:B:548:GLU:HG3	1:C:38:GLU:N	2.01	0.76
1:C:373:LYS:HB2	1:C:373:LYS:NZ	2.01	0.76
4:A:484:HOH:O	2:B:537:LEU:HD22	1.86	0.76
1:A:93:LEU:HD12	2:B:425:ILE:HD11	1.68	0.75
1:A:306:ILE:HD12	1:A:360:ALA:CB	2.17	0.75
1:A:324:GLN:OE1	2:B:540:LYS:HD3	1.86	0.75
1:A:93:LEU:HB2	2:B:425:ILE:HD12	1.70	0.74
1:A:332:TYR:CE1	1:A:378:ILE:HD12	2.23	0.74
1:A:303:ILE:HD11	1:A:333:ALA:HB2	1.68	0.73
1:A:124:ASP:HB3	1:A:127:LEU:HD12	1.68	0.73
1:A:369:ILE:HG23	1:A:370:ASN:OD1	1.89	0.72
1:C:331:LYS:HE2	2:D:516:HIS:NE2	2.03	0.72
1:C:100:LEU:HD23	2:D:468:ILE:HD13	1.70	0.72
1:A:99:MET:HG3	2:B:406:VAL:HG22	1.72	0.72
2:D:547:LYS:HE2	2:D:548:GLU:H	1.55	0.72
2:D:547:LYS:CE	2:D:548:GLU:H	2.04	0.70
1:C:42:HIS:HD2	4:C:429:HOH:O	1.74	0.70
1:C:39:ASP:O	1:C:42:HIS:NE2	2.23	0.70
1:C:171:GLN:HG3	1:C:175:LYS:HE2	1.73	0.70
1:A:378:ILE:O	1:A:379:ARG:HD2	1.93	0.69
2:D:504:ASN:ND2	2:D:507:GLU:H	1.89	0.69
1:A:373:LYS:CD	1:A:378:ILE:HD11	2.23	0.69
2:D:393:HIS:HD2	2:D:407:THR:OG1	1.76	0.68
1:A:98:PHE:CE2	1:A:294:SER:HB2	2.28	0.68
1:C:241:GLU:HG3	1:C:247:ILE:HD12	1.75	0.68
1:C:373:LYS:HD3	1:C:377:GLU:O	1.94	0.68
1:A:147:THR:HG23	1:A:267:LEU:HD23	1.76	0.67
2:D:452:ASN:HD21	2:D:461:LEU:H	1.42	0.67
1:A:134:ASP:HB3	1:A:137:LYS:HD3	1.75	0.67
2:B:463:SER:HB3	2:B:488:ILE:CD1	2.24	0.67
2:B:549:ALA:CB	1:C:40:VAL:HG22	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:SER:HB3	2:B:488:ILE:HD11	1.76	0.66
1:A:93:LEU:HD12	2:B:425:ILE:CD1	2.25	0.66
2:D:459:ARG:NE	4:D:632:HOH:O	2.28	0.66
2:D:547:LYS:HG3	2:D:548:GLU:H	1.61	0.65
1:A:303:ILE:HD11	1:A:333:ALA:CB	2.25	0.65
1:C:89:GLN:HB2	2:D:413:THR:HG23	1.78	0.65
1:C:364:ALA:HA	1:C:367:ILE:HD12	1.78	0.65
2:D:563:GLU:HB3	4:D:636:HOH:O	1.97	0.64
1:A:290:MET:HE3	1:A:291:PRO:HD2	1.80	0.64
2:D:467:THR:C	2:D:468:ILE:HD12	2.23	0.64
2:D:459:ARG:HG3	2:D:459:ARG:HH11	1.62	0.64
2:B:495:VAL:O	2:B:499:ILE:HD13	1.99	0.63
1:C:296:GLY:HA3	2:D:465:SER:OG	1.99	0.63
1:A:204:ASN:N	1:A:204:ASN:HD22	1.97	0.62
2:B:391:THR:N	3:B:390:AZS:CI	2.58	0.62
2:D:547:LYS:HG3	2:D:548:GLU:N	2.13	0.62
1:A:278:ILE:HG12	1:A:291:PRO:HB3	1.81	0.62
1:A:227:LEU:HD13	2:B:425:ILE:HD13	1.82	0.61
2:B:549:ALA:HB1	1:C:40:VAL:HG22	1.83	0.61
2:B:393:HIS:HD2	2:B:407:THR:OG1	1.82	0.61
1:C:249:GLU:OE1	1:C:264:LYS:HD2	2.00	0.61
1:C:255:MET:HG3	1:C:262:ILE:HB	1.82	0.61
2:D:504:ASN:HD22	2:D:506:ALA:H	1.47	0.61
1:A:255:MET:HG3	1:A:262:ILE:HB	1.83	0.61
1:A:118:PRO:HG3	1:A:262:ILE:CD1	2.29	0.60
1:C:114:ARG:CZ	2:D:462:SER:HB2	2.32	0.60
2:D:411:ASN:O	3:D:390:AZS:CI	2.47	0.60
1:A:204:ASN:HD22	1:A:205:SER:H	1.50	0.60
4:A:477:HOH:O	2:B:563:GLU:HG3	2.00	0.60
1:A:299:HIS:O	1:A:303:ILE:HG12	2.02	0.59
1:A:98:PHE:CD1	1:A:290:MET:HE2	2.38	0.59
1:C:373:LYS:HB2	1:C:373:LYS:HZ2	1.66	0.59
2:B:452:ASN:HD21	2:B:461:LEU:H	1.51	0.58
1:A:134:ASP:CB	1:A:137:LYS:HD3	2.33	0.58
1:A:321:ASP:HB3	1:A:369:ILE:HD11	1.86	0.58
1:A:156:LEU:C	1:A:156:LEU:HD23	2.28	0.57
1:C:368:ASP:HB3	1:C:371:LYS:O	2.04	0.57
1:C:378:ILE:O	2:D:518:TRP:HZ2	1.87	0.57
1:A:320:ALA:HB1	4:A:484:HOH:O	2.03	0.57
1:C:324:GLN:HG2	1:C:369:ILE:O	2.04	0.57
2:D:391:THR:CG2	2:D:392:THR:N	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:CB	1:A:367:ILE:HD12	2.34	0.56
2:B:538:GLU:HA	2:B:542:GLN:O	2.04	0.56
1:C:368:ASP:CG	1:C:371:LYS:HB3	2.30	0.56
2:B:547:LYS:HG2	2:B:548:GLU:N	2.19	0.56
1:C:116:MET:HG2	2:D:459:ARG:NH1	2.20	0.56
1:A:136:LYS:HD3	1:A:136:LYS:C	2.31	0.56
1:A:332:TYR:HE2	1:A:367:ILE:HD11	1.69	0.56
2:D:522:GLU:HG3	2:D:545:ALA:HB3	1.87	0.56
1:C:202:HIS:HD2	4:C:498:HOH:O	1.87	0.56
1:A:114:ARG:CZ	2:B:462:SER:HB2	2.35	0.56
1:A:253:GLN:HB3	1:A:257:LYS:HE3	1.88	0.56
1:A:303:ILE:O	1:A:307:LEU:HG	2.06	0.55
1:C:311:ASP:HB3	1:C:314:LYS:NZ	2.22	0.55
2:D:504:ASN:HD22	2:D:506:ALA:N	2.04	0.55
1:A:255:MET:HE2	2:B:427:LEU:HD13	1.88	0.55
2:D:411:ASN:HB3	2:D:429:ASN:OD1	2.07	0.55
2:B:543:LYS:HE2	2:B:543:LYS:HA	1.88	0.54
2:B:549:ALA:HB2	1:C:40:VAL:CG2	2.38	0.54
2:D:391:THR:HG23	2:D:409:THR:HB	1.89	0.54
2:D:486:ARG:HG2	2:D:550:MET:SD	2.48	0.54
2:B:499:ILE:HD12	2:B:499:ILE:N	2.23	0.53
2:D:519:LEU:HA	2:D:520:PRO:C	2.33	0.53
1:A:113:PHE:HB3	1:A:153:GLY:HA3	1.91	0.53
1:C:232:GLU:HG2	1:C:233:MET:HE2	1.91	0.53
2:D:515:HIS:CG	2:D:516:HIS:N	2.77	0.53
1:C:328:GLU:OE2	1:C:372:ALA:HA	2.09	0.53
2:D:413:THR:O	2:D:414:PHE:HB2	2.08	0.53
1:C:340:TYR:O	1:C:341:LEU:HD22	2.09	0.53
2:D:560:PRO:HA	4:D:630:HOH:O	2.09	0.53
1:C:87:HIS:HD2	4:C:475:HOH:O	1.91	0.53
2:D:493:GLN:HE22	2:D:514:PHE:H	1.57	0.53
1:C:246:THR:O	1:C:250:GLN:HG3	2.08	0.53
2:D:546:LEU:C	2:D:546:LEU:HD13	2.35	0.52
2:B:411:ASN:HB3	2:B:429:ASN:OD1	2.09	0.52
1:C:292:PRO:HA	1:C:294:SER:N	2.24	0.52
1:A:340:TYR:HB3	1:A:350:PRO:HD2	1.91	0.52
1:A:320:ALA:HB2	2:D:532:ASP:OD1	2.09	0.52
1:A:356:ASN:OD1	1:A:358:ALA:HB3	2.10	0.52
1:C:101:ILE:N	1:C:101:ILE:HD12	2.24	0.52
1:C:375:SER:HB3	2:D:519:LEU:CD1	2.40	0.52
1:A:293:PRO:O	2:B:461:LEU:HD12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TYR:CD2	2:B:517:GLN:HA	2.46	0.51
1:C:112:ASP:OD1	1:C:112:ASP:C	2.52	0.51
1:A:204:ASN:N	1:A:204:ASN:ND2	2.59	0.51
1:C:311:ASP:CG	1:C:314:LYS:HG3	2.35	0.51
1:A:57:THR:O	1:A:61:VAL:HG23	2.11	0.51
2:B:542:GLN:O	2:B:543:LYS:HE2	2.11	0.51
1:C:100:LEU:CD2	2:D:468:ILE:HD13	2.38	0.51
1:C:100:LEU:HD23	2:D:468:ILE:CD1	2.38	0.51
2:D:391:THR:N	3:D:390:AZS:CI	2.74	0.51
1:A:324:GLN:HG2	1:A:369:ILE:O	2.10	0.51
1:A:331:LYS:HE2	2:B:516:HIS:NE2	2.26	0.50
2:B:547:LYS:CG	2:B:548:GLU:H	2.20	0.50
1:C:167:ASN:HD21	1:C:168:LYS:HE2	1.75	0.50
1:A:300:ILE:HD11	2:B:488:ILE:O	2.12	0.50
1:C:365:ASP:C	1:C:367:ILE:H	2.18	0.50
1:A:103:SER:HB2	1:A:105:ASN:OD1	2.11	0.50
1:C:232:GLU:HG2	1:C:233:MET:CE	2.42	0.50
1:C:383:LEU:C	1:C:385:PRO:HD2	2.36	0.50
1:C:134:ASP:OD2	1:C:137:LYS:HG3	2.11	0.50
2:D:452:ASN:ND2	2:D:461:LEU:H	2.08	0.50
1:A:306:ILE:N	1:A:306:ILE:CD1	2.74	0.50
1:C:171:GLN:HB3	1:C:172:PRO:HD3	1.94	0.50
1:A:321:ASP:O	1:A:324:GLN:HB3	2.11	0.50
2:D:391:THR:HA	2:D:409:THR:HB	1.94	0.50
2:B:437:LYS:HD3	2:B:440:VAL:HG21	1.93	0.50
1:A:278:ILE:HG12	1:A:291:PRO:CB	2.41	0.49
1:A:324:GLN:CD	4:A:485:HOH:O	2.56	0.49
2:B:549:ALA:CB	1:C:40:VAL:CG2	2.90	0.49
2:D:504:ASN:HD22	2:D:504:ASN:C	2.20	0.49
2:D:522:GLU:O	2:D:522:GLU:HG2	2.12	0.49
1:A:168:LYS:HB2	1:A:168:LYS:NZ	2.28	0.49
2:D:547:LYS:CG	2:D:548:GLU:H	2.24	0.49
1:A:385:PRO:HG2	1:A:386:TYR:CE2	2.47	0.49
1:C:332:TYR:OH	1:C:366:GLN:HB2	2.12	0.48
1:A:289:SER:HB3	1:A:297:GLY:CA	2.37	0.48
2:D:402:ASN:HB3	4:D:622:HOH:O	2.12	0.48
2:D:566:GLY:HA3	2:D:577:THR:HG21	1.95	0.48
1:A:204:ASN:ND2	1:A:204:ASN:H	2.11	0.48
1:A:298:ILE:HG12	4:A:422:HOH:O	2.13	0.48
2:D:504:ASN:ND2	2:D:506:ALA:H	2.10	0.48
1:A:384:ALA:HB3	1:A:385:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:518:TRP:O	2:D:519:LEU:HD12	2.13	0.48
2:D:486:ARG:HD3	2:D:486:ARG:N	2.29	0.48
2:B:534:LEU:HD22	2:B:544:VAL:HG11	1.95	0.47
1:A:136:LYS:HD3	1:A:137:LYS:N	2.29	0.47
1:A:202:HIS:HD2	4:A:478:HOH:O	1.96	0.47
2:B:465:SER:O	2:B:466:PRO:C	2.55	0.47
2:D:536:LEU:O	2:D:540:LYS:HG3	2.14	0.47
1:C:196:SER:HA	1:C:210:TRP:CH2	2.50	0.47
2:D:459:ARG:NH2	4:D:632:HOH:O	2.47	0.47
2:D:504:ASN:HD21	2:D:506:ALA:HB3	1.79	0.47
1:A:324:GLN:NE2	4:A:485:HOH:O	2.47	0.47
1:A:384:ALA:HB3	1:A:385:PRO:CD	2.44	0.47
2:B:442:ASN:C	2:B:442:ASN:HD22	2.23	0.47
2:D:391:THR:HG22	2:D:392:THR:H	1.72	0.47
1:A:265:GLU:HG3	4:A:482:HOH:O	2.14	0.47
4:A:485:HOH:O	2:B:542:GLN:CG	2.63	0.47
2:B:391:THR:HB	2:B:482:PRO:CB	2.45	0.47
2:D:459:ARG:CZ	4:D:632:HOH:O	2.63	0.47
1:C:127:LEU:HD21	2:D:437:LYS:HB2	1.95	0.47
1:C:320:ALA:HB2	2:D:533:THR:HG23	1.97	0.47
2:D:504:ASN:HD21	2:D:507:GLU:H	1.59	0.47
1:C:167:ASN:HD21	1:C:168:LYS:CE	2.27	0.47
2:B:442:ASN:C	2:B:442:ASN:ND2	2.73	0.47
1:C:295:SER:O	1:C:299:HIS:HD2	1.98	0.47
1:C:332:TYR:CD2	1:C:363:ILE:HG23	2.51	0.46
2:D:515:HIS:CG	2:D:516:HIS:H	2.33	0.46
1:A:300:ILE:CD1	2:B:488:ILE:O	2.63	0.46
1:A:383:LEU:O	1:A:387:GLU:HG2	2.15	0.46
2:D:416:THR:HG22	2:D:429:ASN:HB3	1.96	0.46
1:A:242:PHE:HA	1:A:247:ILE:HB	1.96	0.46
2:D:493:GLN:HE22	2:D:513:ARG:HA	1.80	0.46
1:A:292:PRO:HA	1:A:294:SER:N	2.31	0.46
2:D:569:ASP:OD1	2:D:570:PRO:HD2	2.15	0.46
2:D:547:LYS:CG	2:D:548:GLU:N	2.78	0.46
1:A:243:TYR:HB3	1:A:267:LEU:O	2.16	0.46
2:D:486:ARG:HG3	2:D:515:HIS:CG	2.50	0.45
2:D:496:VAL:HG13	2:D:500:ASP:OD2	2.17	0.45
1:C:99:MET:HG3	2:D:406:VAL:HG22	1.98	0.45
1:C:244:LYS:NZ	4:C:460:HOH:O	2.50	0.45
1:A:347:VAL:HG22	1:A:348:LYS:N	2.31	0.45
2:B:537:LEU:O	2:B:542:GLN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ILE:HD13	1:A:306:ILE:H	1.81	0.45
2:B:549:ALA:HB2	1:C:40:VAL:HG23	1.97	0.45
2:B:571:ARG:CG	1:C:40:VAL:HG13	2.47	0.45
1:C:384:ALA:N	1:C:385:PRO:HD2	2.32	0.45
1:A:217:LYS:HE2	4:A:469:HOH:O	2.17	0.44
1:A:255:MET:SD	1:A:260:GLY:HA3	2.57	0.44
1:C:324:GLN:HE22	2:D:542:GLN:NE2	2.15	0.44
1:C:332:TYR:O	1:C:335:ALA:HB3	2.17	0.44
2:B:498:SER:HB2	2:B:499:ILE:HD12	1.98	0.44
1:A:204:ASN:HD22	1:A:205:SER:N	2.14	0.44
1:C:365:ASP:C	1:C:367:ILE:N	2.75	0.44
1:A:303:ILE:CD1	1:A:333:ALA:HB2	2.41	0.44
1:C:351:TRP:CZ3	1:C:352:GLN:HG3	2.52	0.44
1:C:383:LEU:O	1:C:386:TYR:N	2.46	0.44
2:B:393:HIS:HE1	2:B:395:SER:OG	2.00	0.44
1:C:156:LEU:C	1:C:156:LEU:HD23	2.43	0.44
1:C:100:LEU:HD12	1:C:109:THR:O	2.17	0.44
1:A:278:ILE:HG21	1:A:298:ILE:HD13	2.00	0.44
1:A:328:GLU:HB3	1:A:367:ILE:CD1	2.41	0.44
1:C:98:PHE:CE2	1:C:294:SER:HB2	2.52	0.43
1:C:378:ILE:HB	2:D:518:TRP:HE1	1.83	0.43
2:D:486:ARG:HG3	2:D:515:HIS:CD2	2.53	0.43
1:A:118:PRO:HD2	1:A:121:ALA:HB2	2.01	0.43
1:C:330:GLU:O	1:C:334:TYR:HD2	2.01	0.43
2:B:518:TRP:O	2:B:519:LEU:HD12	2.19	0.43
1:C:340:TYR:C	1:C:341:LEU:HD22	2.43	0.43
1:C:331:LYS:HE2	2:D:516:HIS:CE1	2.54	0.43
2:B:410:LEU:O	2:B:411:ASN:HB3	2.19	0.43
2:B:571:ARG:HG2	1:C:40:VAL:HG13	1.99	0.43
1:C:111:ILE:HD13	1:C:157:ALA:HB2	1.99	0.43
1:A:113:PHE:CB	1:A:153:GLY:HA3	2.49	0.43
1:C:206:LYS:HE2	4:C:452:HOH:O	2.19	0.43
1:A:156:LEU:C	1:A:156:LEU:CD2	2.91	0.43
1:C:99:MET:HG2	1:C:101:ILE:HD11	1.99	0.43
1:C:330:GLU:OE1	2:D:489:THR:HG21	2.18	0.43
2:D:547:LYS:CE	2:D:548:GLU:N	2.78	0.43
1:A:204:ASN:ND2	1:A:205:SER:H	2.15	0.42
1:A:365:ASP:C	1:A:367:ILE:H	2.27	0.42
2:B:539:ALA:C	2:B:541:GLY:N	2.76	0.42
1:C:373:LYS:HB2	1:C:373:LYS:HZ3	1.79	0.42
2:D:518:TRP:C	2:D:519:LEU:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:HG12	1:A:291:PRO:CA	2.49	0.42
1:A:378:ILE:HB	2:B:518:TRP:HE1	1.85	0.42
1:C:311:ASP:HB3	1:C:314:LYS:HZ3	1.83	0.42
2:D:523:LEU:HD23	2:D:523:LEU:C	2.44	0.42
1:C:299:HIS:O	1:C:303:ILE:HG12	2.19	0.42
2:B:474:LYS:HE3	2:B:474:LYS:HB2	1.75	0.42
1:C:373:LYS:NZ	1:C:373:LYS:CB	2.78	0.42
2:B:519:LEU:HA	2:B:520:PRO:C	2.44	0.42
1:C:383:LEU:O	1:C:384:ALA:C	2.62	0.42
1:A:198:VAL:HG23	1:A:199:LEU:N	2.35	0.42
1:C:100:LEU:CG	2:D:468:ILE:HD13	2.50	0.42
1:C:237:ASN:HB2	1:C:241:GLU:HB2	2.02	0.42
1:C:324:GLN:NE2	2:D:542:GLN:NE2	2.67	0.42
1:A:133:PRO:HG2	2:B:440:VAL:HG11	2.02	0.41
1:A:321:ASP:CB	1:A:369:ILE:HD11	2.48	0.41
1:A:110:ALA:HB1	1:A:290:MET:SD	2.60	0.41
1:A:226:ASN:HB3	2:B:422:GLU:O	2.21	0.41
1:A:300:ILE:HD13	2:B:488:ILE:HG23	2.01	0.41
2:B:488:ILE:HD12	2:B:488:ILE:N	2.36	0.41
1:C:331:LYS:HE2	2:D:516:HIS:HE2	1.81	0.41
2:D:391:THR:CG2	2:D:392:THR:H	2.32	0.41
2:D:504:ASN:ND2	2:D:506:ALA:N	2.68	0.41
1:A:278:ILE:HG12	1:A:291:PRO:HA	2.02	0.41
1:A:115:GLU:O	2:B:460:PRO:HD2	2.19	0.41
1:A:286:GLN:CD	1:A:286:GLN:N	2.79	0.41
2:B:521:ASP:OD2	2:B:521:ASP:C	2.63	0.41
1:C:99:MET:SD	1:C:101:ILE:HD11	2.60	0.41
2:D:441:PRO:HA	2:D:446:LEU:O	2.21	0.41
2:D:568:SER:HB3	2:D:575:ASP:OD2	2.21	0.41
1:A:306:ILE:HD13	1:A:306:ILE:N	2.36	0.41
1:C:233:MET:HE2	1:C:233:MET:HA	2.03	0.41
2:D:410:LEU:O	2:D:411:ASN:HB3	2.21	0.41
2:D:518:TRP:CD2	2:D:519:LEU:HD13	2.55	0.41
2:D:547:LYS:HE3	2:D:547:LYS:HA	2.01	0.41
1:A:255:MET:CE	2:B:427:LEU:HD13	2.50	0.41
1:C:210:TRP:CH2	1:C:215:PRO:HB3	2.56	0.41
1:C:278:ILE:HG12	1:C:291:PRO:HB3	2.02	0.41
1:C:372:ALA:O	1:C:374:PRO:HD3	2.20	0.41
1:C:86:THR:HA	1:C:181:PHE:CZ	2.57	0.41
1:A:87:HIS:HD2	4:A:411:HOH:O	2.02	0.40
1:A:171:GLN:HG3	1:A:175:LYS:NZ	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:MET:CE	1:A:291:PRO:HD2	2.47	0.40
1:A:306:ILE:CD1	1:A:360:ALA:CB	2.95	0.40
2:B:410:LEU:O	2:B:411:ASN:CB	2.70	0.40
1:C:374:PRO:C	1:C:376:SER:N	2.77	0.40
1:A:317:PHE:CZ	2:B:511:ALA:HB1	2.56	0.40
1:A:233:MET:HB3	1:A:241:GLU:HG2	2.03	0.40
1:C:132:ASN:HA	1:C:133:PRO:HD3	1.98	0.40
1:C:233:MET:HG3	4:C:474:HOH:O	2.21	0.40
1:A:298:ILE:CD1	1:A:351:TRP:HB2	2.52	0.40
2:B:517:GLN:O	2:B:518:TRP:HB3	2.21	0.40
1:C:374:PRO:C	1:C:376:SER:H	2.30	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	348/366 (95%)	331 (95%)	17 (5%)	0	100	100
1	C	348/366 (95%)	327 (94%)	21 (6%)	0	100	100
2	B	188/190 (99%)	177 (94%)	10 (5%)	1 (0%)	24	16
2	D	188/190 (99%)	174 (93%)	11 (6%)	3 (2%)	7	2
All	All	1072/1112 (96%)	1009 (94%)	59 (6%)	4 (0%)	30	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	411	ASN
2	D	411	ASN
2	D	516	HIS
2	D	522	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	275/287 (96%)	270 (98%)	5 (2%)	51	51
1	C	275/287 (96%)	273 (99%)	2 (1%)	76	80
2	B	154/154 (100%)	148 (96%)	6 (4%)	28	23
2	D	154/154 (100%)	148 (96%)	6 (4%)	28	23
All	All	858/882 (97%)	839 (98%)	19 (2%)	45	44

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ASP
1	A	120	LYS
1	A	168	LYS
1	A	204	ASN
1	A	306	ILE
2	B	391	THR
2	B	408	TYR
2	B	430	GLN
2	B	442	ASN
2	B	548	GLU
2	B	555	SER
1	C	292	PRO
1	C	373	LYS
2	D	408	TYR
2	D	430	GLN
2	D	504	ASN
2	D	522	GLU
2	D	547	LYS
2	D	555	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	48	GLN
1	A	87	HIS
1	A	107	ASN
1	A	132	ASN
1	A	171	GLN
1	A	202	HIS
1	A	204	ASN
1	A	250	GLN
1	A	253	GLN
1	A	366	GLN
2	B	393	HIS
2	B	442	ASN
2	B	452	ASN
2	B	510	ASN
2	B	515	HIS
2	B	542	GLN
1	C	42	HIS
1	C	48	GLN
1	C	60	GLN
1	C	87	HIS
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	250	GLN
1	C	299	HIS
1	C	309	ASN
1	C	366	GLN
2	D	393	HIS
2	D	452	ASN
2	D	493	GLN
2	D	504	ASN
2	D	542	GLN

5.3.3 RNA ⓘ

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	9,11,11	4.90	4 (44%)	7,13,13	3.61	3 (42%)
3	AZS	B	390	2	9,11,11	5.16	3 (33%)	7,13,13	3.60	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	-	3/11/12/12	-
3	AZS	B	390	2	-	4/11/12/12	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	390	AZS	OH-CH	11.07	1.43	1.21
3	D	390	AZS	OH-CH	10.53	1.42	1.21
3	B	390	AZS	CI-NJ	9.70	1.48	1.32
3	D	390	AZS	CI-NJ	8.99	1.47	1.32
3	B	390	AZS	OG-CH	3.91	1.43	1.34
3	D	390	AZS	OG-CH	3.85	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	390	AZS	CI-CH	2.14	1.53	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	390	AZS	OG-CH-OH	-6.56	109.18	122.96
3	D	390	AZS	OG-CH-OH	-6.28	109.76	122.96
3	D	390	AZS	OH-CH-CI	-5.40	109.38	125.00
3	B	390	AZS	OH-CH-CI	-5.35	109.55	125.00
3	D	390	AZS	CB-OG-CH	-4.38	109.42	116.47
3	B	390	AZS	CB-OG-CH	-4.06	109.93	116.47

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	390	AZS	OG-CH-CI-NJ
3	B	390	AZS	OH-CH-CI-NJ
3	D	390	AZS	OG-CH-CI-NJ
3	B	390	AZS	OH-CH-OG-CB
3	D	390	AZS	OH-CH-OG-CB
3	D	390	AZS	O-C-CA-N
3	B	390	AZS	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	390	AZS	3	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%)	0.86	61 (17%) 4 3	20, 37, 60, 75	0
1	C	350/366 (95%)	0.68	60 (17%) 4 3	17, 31, 68, 85	0
2	B	190/190 (100%)	0.67	31 (16%) 4 4	19, 32, 59, 68	0
2	D	190/190 (100%)	0.67	38 (20%) 3 2	17, 29, 66, 78	0
All	All	1080/1112 (97%)	0.74	190 (17%) 4 3	17, 34, 63, 85	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	VAL	8.5
1	C	39	ASP	7.2
1	C	367	ILE	6.9
1	C	369	ILE	6.9
1	C	372	ALA	6.6
2	D	539	ALA	5.8
1	A	369	ILE	5.6
1	C	378	ILE	5.6
1	A	367	ILE	5.4
1	C	333	ALA	5.4
1	C	375	SER	5.3
1	C	376	SER	5.2
1	A	327	ALA	5.0
1	C	334	TYR	5.0
1	A	375	SER	4.9
2	D	544	VAL	4.9
1	C	368	ASP	4.8
2	D	440	VAL	4.8
2	D	519	LEU	4.7
1	C	325	ILE	4.6
2	D	443	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	370	ASN	4.5
1	C	366	GLN	4.5
1	C	379	ARG	4.5
1	C	338	SER	4.5
1	C	363	ILE	4.5
2	D	537	LEU	4.4
1	C	38	GLU	4.4
1	C	332	TYR	4.3
1	C	384	ALA	4.3
1	C	361	LYS	4.3
2	B	447	VAL	4.3
1	C	331	LYS	4.3
1	C	335	ALA	4.2
1	C	374	PRO	4.2
1	A	372	ALA	4.2
1	C	310	PHE	4.2
2	B	519	LEU	4.2
1	C	365	ASP	4.2
2	D	545	ALA	4.1
1	C	364	ALA	4.0
2	D	536	LEU	4.0
1	C	373	LYS	3.9
1	A	378	ILE	3.9
1	C	322	ALA	3.9
1	A	315	TYR	3.8
2	D	523	LEU	3.8
2	D	541	GLY	3.8
2	B	537	LEU	3.7
2	D	446	LEU	3.7
2	D	543	LYS	3.7
2	D	542	GLN	3.7
2	B	539	ALA	3.7
2	D	444	TYR	3.7
1	C	329	ALA	3.7
2	B	536	LEU	3.6
2	D	447	VAL	3.6
1	A	325	ILE	3.6
2	D	520	PRO	3.6
2	D	546	LEU	3.5
2	D	441	PRO	3.4
1	A	363	ILE	3.4
1	C	320	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	580	TYR	3.4
1	C	328	GLU	3.4
2	B	548	GLU	3.4
1	A	379	ARG	3.4
2	B	546	LEU	3.4
2	D	518	TRP	3.3
2	B	516	HIS	3.3
1	A	370	ASN	3.3
2	B	440	VAL	3.3
2	B	544	VAL	3.2
2	D	534	LEU	3.2
1	A	368	ASP	3.2
2	B	436	ALA	3.1
2	D	445	GLY	3.1
2	D	517	GLN	3.1
1	C	315	TYR	3.0
1	C	380	PRO	3.0
1	A	347	VAL	3.0
2	D	521	ASP	3.0
2	D	516	HIS	3.0
1	C	362	SER	2.9
2	B	439	GLY	2.9
1	C	386	TYR	2.9
1	A	371	LYS	2.9
1	A	133	PRO	2.9
1	C	360	ALA	2.9
2	D	522	GLU	2.8
2	B	540	LYS	2.8
2	D	450	ASP	2.8
1	A	383	LEU	2.8
2	B	534	LEU	2.8
1	A	373	LYS	2.8
1	C	377	GLU	2.8
2	B	518	TRP	2.8
1	A	338	SER	2.7
2	B	545	ALA	2.7
1	A	374	PRO	2.7
1	C	324	GLN	2.7
1	C	314	LYS	2.7
1	C	327	ALA	2.7
2	D	538	GLU	2.7
1	A	376	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	311	ASP	2.7
2	B	543	LYS	2.7
1	A	316	GLY	2.7
1	C	337	ARG	2.7
1	C	330	GLU	2.6
1	A	121	ALA	2.6
1	A	341	LEU	2.6
2	D	438	PRO	2.6
1	A	136	LYS	2.6
1	C	382	LYS	2.6
2	B	488	ILE	2.6
1	A	329	ALA	2.6
1	A	324	GLN	2.6
2	D	525	VAL	2.6
1	A	364	ALA	2.6
1	A	278	ILE	2.5
1	C	318	GLY	2.5
1	A	366	GLN	2.5
2	B	523	LEU	2.5
1	A	377	GLU	2.5
1	A	334	TYR	2.5
1	C	359	TYR	2.5
2	B	438	PRO	2.5
1	A	332	TYR	2.5
1	A	117	ALA	2.5
1	A	320	ALA	2.5
1	C	371	LYS	2.5
1	C	168	LYS	2.4
1	C	383	LEU	2.4
1	A	131	GLY	2.4
2	B	455	GLY	2.4
1	A	292	PRO	2.4
2	D	531	PRO	2.4
1	A	303	ILE	2.4
1	A	293	PRO	2.4
1	A	340	TYR	2.4
1	A	335	ALA	2.4
2	D	449	GLY	2.4
1	A	331	LYS	2.4
1	C	340	TYR	2.3
2	B	535	LYS	2.3
1	A	130	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	448	GLY	2.3
2	B	541	GLY	2.3
1	A	330	GLU	2.3
1	A	259	GLY	2.3
1	A	387	GLU	2.2
1	A	262	ILE	2.2
2	D	560	PRO	2.2
2	B	561	ASP	2.2
1	A	269	ALA	2.2
1	C	316	GLY	2.2
1	C	381	GLY	2.2
1	A	38	GLU	2.2
1	A	107	ASN	2.2
1	A	298	ILE	2.2
1	C	313	LYS	2.2
2	D	533	THR	2.2
2	B	542	GLN	2.2
2	D	535	LYS	2.2
1	C	347	VAL	2.2
2	B	525	VAL	2.2
1	A	328	GLU	2.2
1	C	336	ASP	2.2
1	C	385	PRO	2.1
1	A	381	GLY	2.1
1	A	380	PRO	2.1
1	A	346	PHE	2.1
2	D	436	ALA	2.1
2	B	533	THR	2.1
1	A	337	ARG	2.1
2	D	448	GLY	2.1
1	A	333	ALA	2.1
1	A	145	SER	2.1
1	A	267	LEU	2.1
2	D	530	SER	2.1
2	B	450	ASP	2.1
1	A	132	ASN	2.0
1	C	123	ARG	2.0
2	B	560	PRO	2.0
1	A	306	ILE	2.0
2	D	485	SER	2.0
1	C	356	ASN	2.0
1	C	341	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	266	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AZS	D	390	12/12	0.65	0.24	35,48,59,63	0
3	AZS	B	390	12/12	0.68	0.22	38,56,63,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.