Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2023 – 10:46 AM EDT

PDB ID	:	2Z8J
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 (i) 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 (i)) were used in the production of this report:

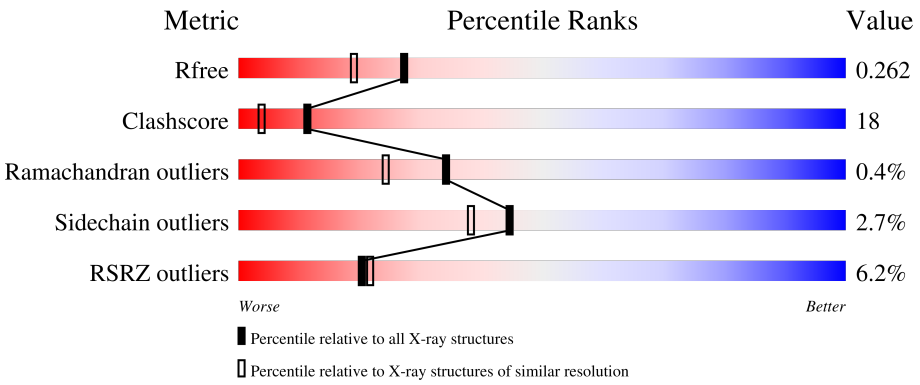
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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 <=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% 70% 25%
1	C	366	4% 72% 24%
2	B	190	11% 74% 24%
2	D	190	8% 67% 29%

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.

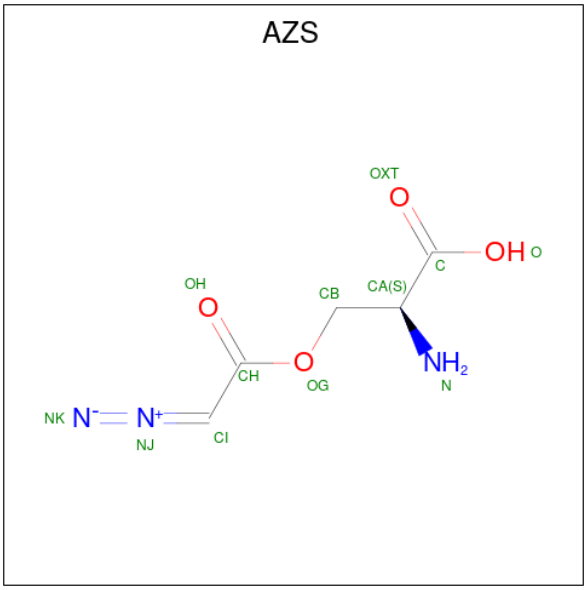
- Molecule 1 is a protein called Gamma-glutamyltranspeptidase.

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

- Molecule 2 is a protein called Gamma-glutamyltranspeptidase.

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

- Molecule 3 is O-DIAZOACETYL-L-SERINE (three-letter code: AZS) (formula: $C_5H_7N_3O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	12	5	3	4	0	0
			Total	C	N	O		
3	D	1	12	5	3	4	0	0

- Molecule 4 is water.

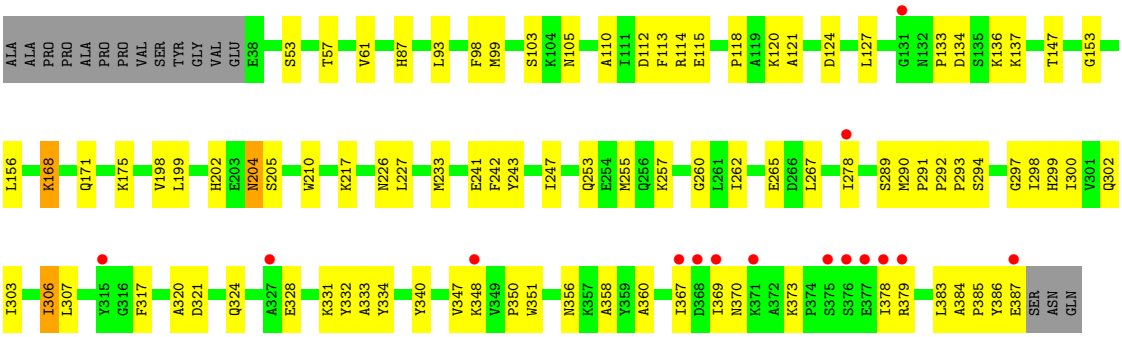
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	124	124	124	0	0
			Total	O		
4	B	70	70	70	0	0
			Total	O		
4	C	149	149	149	0	0
			Total	O		
4	D	70	70	70	0	0

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.

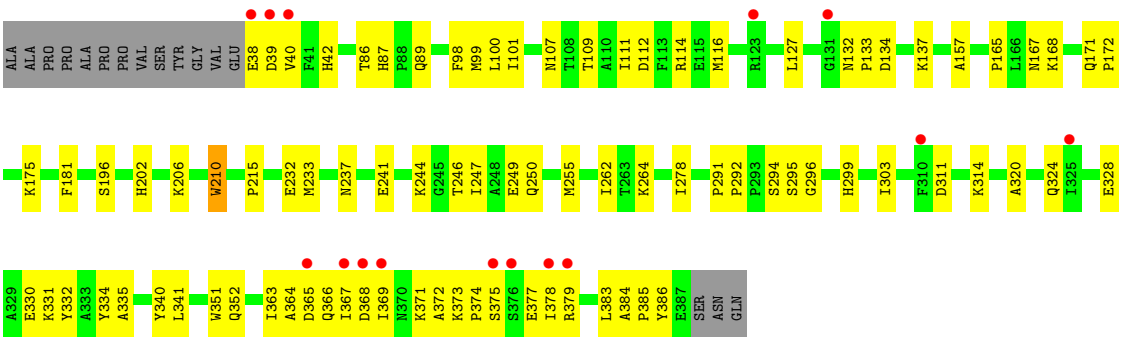
• Molecule 1: Gamma-glutamyltranspeptidase

Chain A:



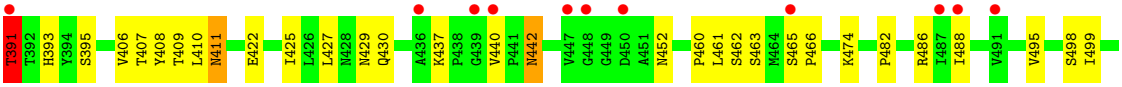
• Molecule 1: Gamma-glutamyltranspeptidase

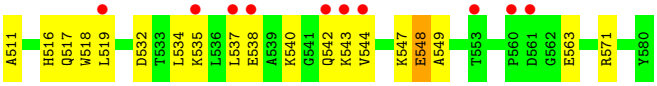
Chain C:



• Molecule 2: Gamma-glutamyltranspeptidase

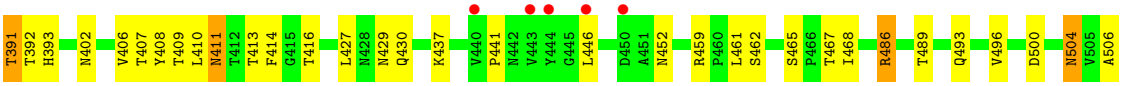
Chain B:

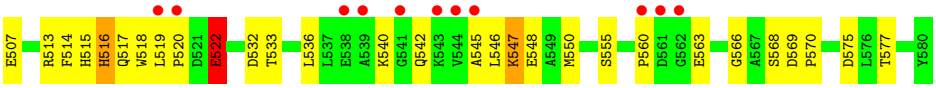




• Molecule 2: Gamma-glutamyltranspeptidase

Chain D:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	6.66 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.267 0.222 , 0.262	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 , 55.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.35	0/2705	0.59	0/3660
1	C	0.41	0/2705	0.64	0/3660
2	B	0.49	1/1434 (0.1%)	0.79	5/1952 (0.3%)
2	D	0.42	1/1434 (0.1%)	0.76	1/1952 (0.1%)
All	All	0.41	2/8278 (0.0%)	0.68	6/11224 (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
2	B	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	391	THR	C-O	10.36	1.43	1.23
2	D	391	THR	CA-CB	5.96	1.68	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	391	THR	CA-CB-CG2	-13.35	93.72	112.40
2	B	391	THR	CA-C-N	9.59	138.31	117.20
2	B	391	THR	N-CA-CB	6.89	123.39	110.30
2	B	391	THR	CA-C-O	-6.17	107.14	120.10
2	B	391	THR	N-CA-C	5.82	126.70	111.00
2	B	391	THR	O-C-N	-5.57	113.79	122.70

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2652	0	2620	101	0
1	C	2652	0	2620	91	0
2	B	1407	0	1391	62	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	288	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 18.

All (288) 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
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:A:289:SER:HB3	1:A:297:GLY:HA2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:MET:HE3	1:A:291:PRO:HD2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:467:THR:C	2:D:468:ILE:HD12	2.23	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: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
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
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: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
2:B:391:THR:N	2:B:409:THR:HG1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:CZ	2:B:462:SER:HB2	2.35	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:C:255:MET:HE3	1:C:262:ILE:HD12	1.87	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
1:A:113:PHE:HB3	1:A:153:GLY:HA3	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:A:156:LEU:C	1:A:156:LEU:HD23	2.28	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
1:C:232:GLU:HG2	1:C:233:MET:HE3	1.91	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:C:368:ASP:CG	1:C:371:LYS:HB3	2.30	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
1:A:334:TYR:CD2	2:B:517:GLN:HA	2.46	0.51
1:A:204:ASN:N	1:A:204:ASN:ND2	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:136:LYS:HD3	1:A:136:LYS:C	2.31	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
2:B:549:ALA:CB	1:C:40:VAL:CG2	2.90	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:255:MET:HE1	2:D:427:LEU:HD13	1.95	0.49
1:C:332:TYR:OH	1:C:366:GLN:HB2	2.12	0.48
2:D:519:LEU:HA	2:D:520:PRO:C	2.33	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
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:D:546:LEU:C	2:D:546:LEU:HD13	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:112:ASP:OD1	1:C:112:ASP:C	2.52	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
1:C:295:SER:O	1:C:299:HIS:HD2	1.98	0.47
1:C:365:ASP:C	1:C:367:ILE:H	2.18	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:C:311:ASP:CG	1:C:314:LYS:HG3	2.35	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
1:C:383:LEU:C	1:C:385:PRO:HD2	2.36	0.45
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
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
2:D:504:ASN:HD22	2:D:504:ASN:C	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASN:HD22	1:A:205:SER:N	2.14	0.44
1:A:303:ILE:CD1	1:A:333:ALA:HB2	2.41	0.44
1:A:324:GLN:CD	4:A:485:HOH:O	2.56	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: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: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
2:B:465:SER:O	2:B:466:PRO:C	2.55	0.43
1:C:206:LYS:HE2	4:C:452:HOH:O	2.19	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:C:373:LYS:HB2	1:C:373:LYS:HZ3	1.79	0.42
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
1:C:299:HIS:O	1:C:303:ILE:HG12	2.19	0.42
2:D:515:HIS:HE2	2:D:517:GLN:HB3	1.84	0.42
2:B:474:LYS:HE3	2:B:474:LYS:HB2	1.75	0.42
2:B:442:ASN:C	2:B:442:ASN:HD22	2.23	0.42
2:B:442:ASN:C	2:B:442:ASN:ND2	2.73	0.42
1:C:373:LYS:NZ	1:C:373:LYS:CB	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:255:MET:CE	1:C:262:ILE:HD12	2.50	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: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
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
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: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

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%)	29	18
2	D	188/190 (99%)	174 (93%)	11 (6%)	3 (2%)	9	2
All	All	1072/1112 (96%)	1009 (94%)	59 (6%)	4 (0%)	34	24

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 (i)

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%)	268 (98%)	7 (2%)	47	40
1	C	275/287 (96%)	272 (99%)	3 (1%)	73	73
2	B	154/154 (100%)	148 (96%)	6 (4%)	32	25
2	D	154/154 (100%)	147 (96%)	7 (4%)	27	20
All	All	858/882 (97%)	835 (97%)	23 (3%)	44	38

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

Mol	Chain	Res	Type
1	A	53	SER
1	A	112	ASP
1	A	120	LYS
1	A	168	LYS
1	A	204	ASN
1	A	210	TRP
1	A	306	ILE
2	B	391	THR
2	B	408	TYR
2	B	430	GLN
2	B	442	ASN
2	B	486	ARG
2	B	548	GLU
1	C	107	ASN
1	C	210	TRP
1	C	379	ARG
2	D	408	TYR
2	D	430	GLN
2	D	486	ARG
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 (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
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
2	B	393	HIS
2	B	442	ASN
2	B	452	ASN
2	B	515	HIS
2	B	542	GLN

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Mol	Chain	Res	Type
1	C	42	HIS
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	299	HIS
1	C	309	ASN
1	C	366	GLN
2	D	393	HIS
2	D	452	ASN
2	D	493	GLN
2	D	497	ASN
2	D	504	ASN
2	D	542	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 monosaccharides 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	4.71	4 (44%)	9,13,13	3.24	3 (33%)
3	AZS	B	390	2	9,11,11	4.96	4 (44%)	9,13,13	3.20	3 (33%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	390	AZS	OH-CH	10.83	1.43	1.21
3	D	390	AZS	OH-CH	10.30	1.42	1.21
3	B	390	AZS	CI-NJ	8.97	1.48	1.32
3	D	390	AZS	CI-NJ	8.31	1.47	1.32
3	B	390	AZS	OG-CH	3.73	1.43	1.34
3	D	390	AZS	OG-CH	3.67	1.43	1.34
3	D	390	AZS	CI-CH	2.62	1.53	1.47
3	B	390	AZS	CI-CH	2.34	1.53	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	390	AZS	OG-CH-OH	-6.26	109.18	122.93
3	D	390	AZS	OG-CH-OH	-5.99	109.76	122.93
3	D	390	AZS	OH-CH-CI	-5.65	109.38	124.90
3	B	390	AZS	OH-CH-CI	-5.59	109.55	124.90
3	D	390	AZS	CB-OG-CH	-4.22	109.42	116.60
3	B	390	AZS	CB-OG-CH	-3.92	109.93	116.60

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

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Mol	Chain	Res	Type	Atoms
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 (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	350/366 (95%)	0.18	15 (4%)	35	38	20, 37, 60, 75	0
1	C	350/366 (95%)	0.09	15 (4%)	35	38	17, 31, 68, 85	0
2	B	190/190 (100%)	0.49	21 (11%)	5	5	19, 32, 59, 68	0
2	D	190/190 (100%)	0.36	16 (8%)	11	11	17, 29, 66, 78	0
All	All	1080/1112 (97%)	0.24	67 (6%)	20	22	17, 34, 63, 85	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	367	ILE	6.8
1	C	376	SER	6.1
2	D	440	VAL	5.3
1	C	368	ASP	5.2
1	C	40	VAL	5.2
1	A	369	ILE	5.0
2	D	560	PRO	5.0
2	B	436	ALA	4.4
2	B	440	VAL	4.3
1	A	367	ILE	4.1
2	B	439	GLY	3.8
2	B	519	LEU	3.7
2	B	491	VAL	3.7
1	C	39	ASP	3.6
2	B	543	LYS	3.5
2	B	448	GLY	3.5
1	A	131	GLY	3.5
1	A	375	SER	3.5
1	A	378	ILE	3.5
2	B	537	LEU	3.5
2	B	487	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	391	THR	3.3
1	C	369	ILE	3.2
2	B	447	VAL	3.2
1	C	375	SER	3.2
2	D	446	LEU	3.2
1	C	379	ARG	3.2
1	C	378	ILE	3.2
1	C	325	ILE	3.0
1	A	379	ARG	3.0
2	B	488	ILE	3.0
2	D	538	GLU	3.0
2	B	560	PRO	3.0
2	D	561	ASP	2.9
2	D	539	ALA	2.9
1	A	315	TYR	2.8
2	D	543	LYS	2.8
1	C	38	GLU	2.8
1	A	368	ASP	2.7
2	D	519	LEU	2.7
1	A	377	GLU	2.6
2	B	544	VAL	2.6
1	A	376	SER	2.5
2	D	545	ALA	2.5
1	A	327	ALA	2.5
2	D	541	GLY	2.5
1	C	131	GLY	2.5
1	A	387	GLU	2.4
1	A	371	LYS	2.4
2	D	520	PRO	2.4
2	B	561	ASP	2.4
1	C	365	ASP	2.4
2	D	443	VAL	2.3
2	B	553	THR	2.3
2	B	535	LYS	2.3
2	D	544	VAL	2.3
2	D	450	ASP	2.3
1	A	348	LYS	2.2
1	C	310	PHE	2.1
2	B	465	SER	2.1
2	B	538	GLU	2.1
2	B	450	ASP	2.1
2	D	562	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	444	TYR	2.1
1	A	278	ILE	2.0
1	C	123	ARG	2.0
2	B	542	GLN	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 monosaccharides 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	0.68	0.33	35,48,59,63	0
3	AZS	B	390	12/12	0.71	0.31	38,56,63,68	0

6.5 Other polymers (i)

There are no such residues in this entry.