



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:24 AM GMT

PDB ID : 3AMJ
Title : The crystal structure of the heterodimer of M16B peptidase from *Sphingomonas* sp. A1
Authors : Maruyama, Y.; Chuma, A.; Mikami, B.; Hashimoto, W.; Murata, K.
Deposited on : 2010-08-20
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

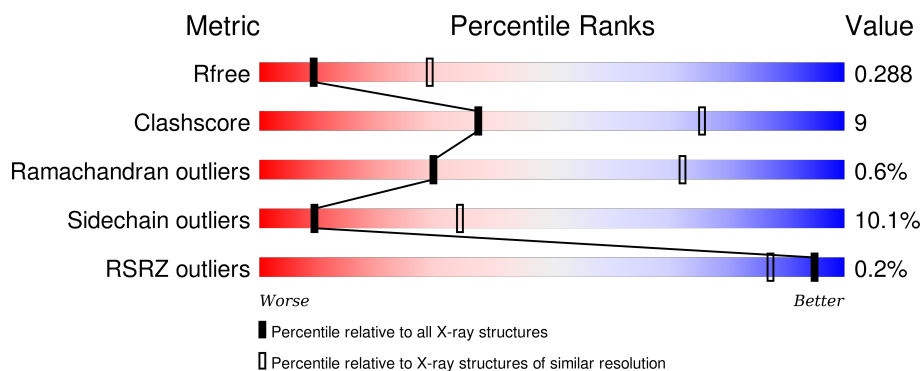
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	B	424	 68% 24% 5% .
1	D	424	 73% 21% . .
2	A	437	 73% 21% . .
2	C	437	 74% 21% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12891 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 zinc peptidase inactive subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	414	Total	C	N	O	S	0	0	0
			3145	1973	566	599	7			
1	D	411	Total	C	N	O	S	0	0	0
			3128	1963	562	596	7			

- Molecule 2 is a protein called zinc peptidase active subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	422	Total	C	N	O	S	0	0	0
			3278	2055	590	620	13			
2	A	422	Total	C	N	O	S	0	0	0
			3278	2055	590	620	13			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

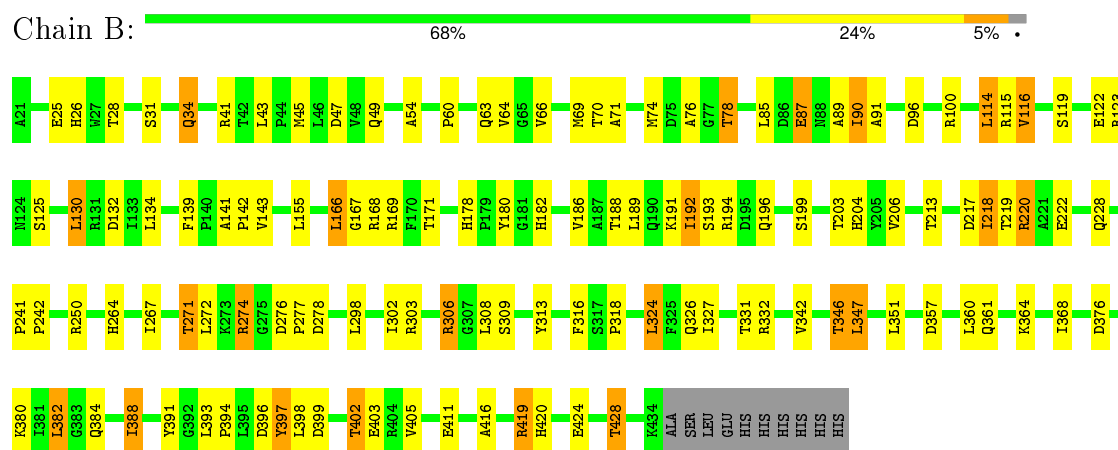
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	16	Total	O	0	0
			16	16		
4	C	15	Total	O	0	0
			15	15		
4	D	9	Total	O	0	0
			9	9		
4	A	20	Total	O	0	0
			20	20		

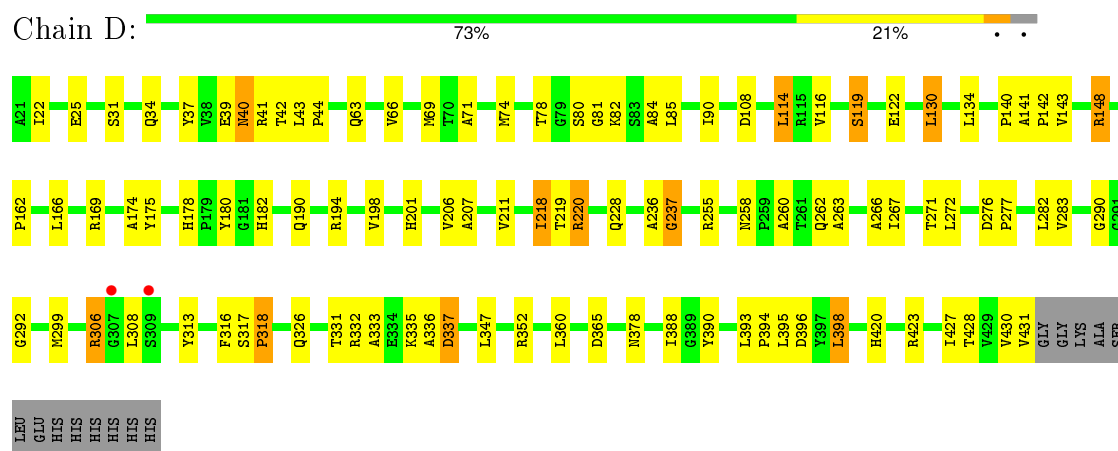
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

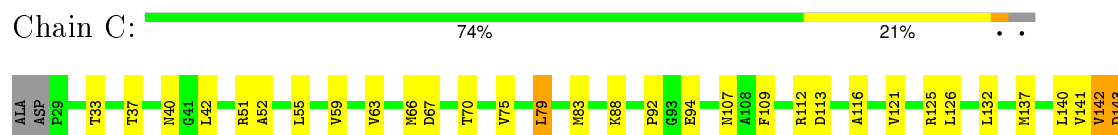
• Molecule 1: zinc peptidase inactive subunit



• Molecule 1: zinc peptidase inactive subunit



• Molecule 2: zinc peptidase active subunit





- Molecule 2: zinc peptidase active subunit

Chain A: 73% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.46Å 100.68Å 253.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.76 – 3.00 33.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.76-3.00) 99.9 (33.76-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.54 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.300 0.207 , 0.288	Depositor DCC
R_{free} test set	1778 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 16.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 35510 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12891	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN

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	B	0.47	0/3204	0.55	0/4350
1	D	0.44	0/3187	0.52	0/4329
2	A	0.49	0/3341	0.52	1/4534 (0.0%)
2	C	0.46	0/3341	0.51	0/4534
All	All	0.47	0/13073	0.53	1/17747 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	42	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	324	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3145	0	3138	78	0
1	D	3128	0	3119	61	0
2	A	3278	0	3261	60	0
2	C	3278	0	3261	47	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	20	0	0	2	0
4	B	16	0	0	0	0
4	C	15	0	0	0	0
4	D	9	0	0	0	0
All	All	12891	0	12779	239	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 9.

All (239) 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:B:34:GLN:HE21	1:B:34:GLN:HA	1.33	0.91
1:D:71:ALA:HA	1:D:74:MET:HE3	1.51	0.88
1:B:71:ALA:HA	1:B:74:MET:HE2	1.61	0.83
1:B:342:VAL:O	1:B:346:THR:HG23	1.76	0.83
1:B:71:ALA:HA	1:B:74:MET:CE	2.08	0.83
1:B:31:SER:H	1:B:228:GLN:HE22	1.27	0.82
1:B:34:GLN:NE2	1:B:34:GLN:HA	1.94	0.82
1:D:262:GLN:HG2	1:D:332:ARG:HG2	1.64	0.80
2:C:273:LEU:HB2	2:C:350:ILE:HD11	1.64	0.80
1:B:306:ARG:HB2	1:B:308:LEU:HG	1.62	0.80
2:A:142:VAL:HG13	2:A:204:ARG:HG2	1.62	0.80
2:A:248:ARG:HH11	2:A:332:ARG:HH21	1.33	0.77
1:B:178:HIS:CD2	1:B:180:TYR:H	2.03	0.77
1:B:267:ILE:HG12	1:B:428:THR:HB	1.67	0.76
2:A:142:VAL:CG1	2:A:204:ARG:HG2	2.16	0.76
1:D:71:ALA:HA	1:D:74:MET:CE	2.17	0.74
2:C:55:LEU:HD21	2:C:126:LEU:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ARG:HH11	1:B:220:ARG:CG	2.01	0.73
1:B:278:ASP:OD2	1:B:419:ARG:NH1	2.22	0.72
2:A:47:ARG:HB3	2:A:221:VAL:HB	1.73	0.71
2:C:244:GLU:O	2:C:244:GLU:HG3	1.91	0.70
1:D:388:ILE:HG22	1:D:393:LEU:HD12	1.75	0.69
1:B:309:SER:HB2	1:B:331:THR:HG22	1.76	0.67
2:A:79:LEU:HD12	2:A:206:TRP:HD1	1.59	0.67
2:A:182:HIS:HD2	2:A:184:TYR:H	1.44	0.66
1:B:54:ALA:HB2	1:B:204:HIS:HB3	1.78	0.66
2:A:248:ARG:NH1	2:A:332:ARG:HH21	1.92	0.65
1:B:199:SER:O	1:B:203:THR:HG23	1.97	0.65
1:D:255:ARG:HH22	1:D:337:ASP:HA	1.63	0.64
1:D:220:ARG:HG2	1:D:220:ARG:HH11	1.63	0.64
2:A:248:ARG:NH1	2:A:332:ARG:NH2	2.46	0.63
1:B:364:LYS:O	1:B:368:ILE:HG12	1.97	0.62
1:B:376:ASP:HB2	1:B:380:LYS:HD2	1.81	0.62
2:A:430:ALA:O	2:A:433:ARG:HG2	2.00	0.62
1:B:219:THR:OG1	1:B:222:GLU:HG3	2.00	0.62
2:C:260:ARG:HG2	2:A:262:VAL:HG23	1.81	0.62
1:B:178:HIS:HD2	1:B:180:TYR:H	1.46	0.62
1:D:262:GLN:HA	1:D:332:ARG:HA	1.82	0.62
1:D:207:ALA:HB3	1:D:236:ALA:HB2	1.81	0.61
2:A:309:MET:HE3	2:A:360:GLN:HG3	1.82	0.61
2:C:309:MET:CE	2:C:360:GLN:HG3	2.31	0.61
2:C:221:VAL:CG1	2:C:396:ALA:HB2	2.31	0.61
2:C:142:VAL:CG1	2:C:204:ARG:HG2	2.31	0.61
2:A:327:TYR:CE2	2:A:329:SER:HB3	2.37	0.60
1:D:178:HIS:CD2	1:D:180:TYR:H	2.21	0.58
1:D:306:ARG:HG3	1:D:308:LEU:HG	1.83	0.58
2:A:99:VAL:HG11	2:A:106:ASP:HB3	1.86	0.58
1:D:308:LEU:HD23	1:D:335:LYS:HD3	1.86	0.57
2:C:251:GLN:HE22	2:A:70:THR:HG22	1.69	0.57
2:A:55:LEU:HD23	2:A:123:SER:HA	1.85	0.57
1:B:26:HIS:HE1	1:B:34:GLN:HG3	1.70	0.56
1:D:262:GLN:HG2	1:D:332:ARG:CG	2.34	0.56
2:A:143:ASP:HB3	2:A:146:LEU:HB2	1.87	0.56
1:D:175:TYR:HB3	1:D:178:HIS:HB3	1.87	0.55
1:D:178:HIS:HD2	1:D:180:TYR:H	1.55	0.55
2:A:309:MET:HE3	2:A:309:MET:HA	1.87	0.55
1:D:148:ARG:HH21	1:D:190:GLN:HA	1.70	0.55
2:C:79:LEU:HD12	2:C:206:TRP:HD1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:VAL:HG21	1:D:390:TYR:HA	1.88	0.55
1:B:49:GLN:HB2	1:B:382:LEU:HD11	1.89	0.55
1:B:384:GLN:O	1:B:388:ILE:HG23	2.06	0.55
1:B:70:THR:HG22	1:B:74:MET:HE1	1.89	0.55
1:D:40:ASN:C	1:D:40:ASN:HD22	2.08	0.55
2:C:75:VAL:HA	2:C:198:MET:HE1	1.89	0.55
2:A:75:VAL:HA	2:A:198:MET:HE1	1.90	0.54
1:B:220:ARG:HG3	1:B:220:ARG:HH11	1.73	0.53
1:B:45:MET:HE3	1:B:115:ARG:NE	2.23	0.53
1:D:40:ASN:HD22	1:D:42:THR:H	1.56	0.53
1:B:402:THR:HG22	1:B:403:GLU:OE1	2.08	0.53
2:A:157:GLU:OE2	2:A:161:ARG:NH1	2.42	0.53
1:D:220:ARG:CG	1:D:220:ARG:HH11	2.20	0.53
1:B:220:ARG:HH11	1:B:220:ARG:HG2	1.73	0.53
1:D:162:PRO:HB3	1:D:431:VAL:HG11	1.89	0.53
2:C:231:ARG:NH2	2:C:234:GLU:OE2	2.42	0.53
2:C:142:VAL:HG13	2:C:204:ARG:HG2	1.90	0.53
1:B:41:ARG:HD2	1:B:217:ASP:HA	1.90	0.53
2:A:178:SER:O	2:A:278:HIS:NE2	2.42	0.52
1:B:316:PHE:O	1:B:318:PRO:HD3	2.09	0.52
1:D:166:LEU:HD21	1:D:266:ALA:HB2	1.91	0.52
1:B:71:ALA:HA	1:B:74:MET:HE3	1.90	0.52
1:B:60:PRO:HB2	1:B:63:GLN:HG2	1.91	0.52
1:B:166:LEU:HD12	1:B:264:HIS:HB3	1.92	0.52
2:C:182:HIS:HD2	2:C:184:TYR:H	1.58	0.51
2:C:282:ILE:HD12	2:C:329:SER:HB2	1.93	0.51
1:B:141:ALA:N	1:B:142:PRO:HD2	2.24	0.51
1:B:368:ILE:HD11	1:B:405:VAL:HB	1.92	0.50
1:D:40:ASN:HD21	1:D:42:THR:CB	2.23	0.50
2:A:107:ASN:HB3	2:A:118:TYR:CZ	2.47	0.50
1:B:272:LEU:HD12	1:B:316:PHE:HB3	1.93	0.50
2:C:317:ASN:O	2:C:319:HIS:HD2	1.95	0.50
1:D:333:ALA:HA	1:D:336:ALA:HB2	1.94	0.50
1:D:194:ARG:O	1:D:198:VAL:HG23	2.12	0.50
1:B:416:ALA:HA	1:B:419:ARG:HH12	1.77	0.49
1:D:174:ALA:HA	1:D:427:ILE:CD1	2.42	0.49
1:D:394:PRO:HB2	1:D:396:ASP:HB3	1.94	0.49
1:D:395:LEU:HD22	1:D:395:LEU:H	1.75	0.49
1:D:63:GLN:HB2	1:D:66:VAL:HG21	1.94	0.49
1:D:378:ASN:N	1:D:378:ASN:HD22	2.09	0.49
2:A:273:LEU:HB2	2:A:350:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ASP:HB3	1:B:382:LEU:HG	1.95	0.49
2:A:65:SER:OG	2:A:112:ARG:HA	2.13	0.49
2:A:201:GLN:NE2	2:A:204:ARG:HH11	2.10	0.49
2:A:182:HIS:CD2	2:A:183:PRO:HD2	2.48	0.49
1:D:40:ASN:HD21	1:D:42:THR:HB	1.78	0.49
2:C:221:VAL:HG11	2:C:396:ALA:HB2	1.95	0.49
2:C:182:HIS:CD2	2:C:184:TYR:H	2.31	0.49
2:A:201:GLN:NE2	2:A:204:ARG:NH1	2.61	0.48
2:C:113:ASP:O	2:C:332:ARG:NH1	2.45	0.48
1:D:41:ARG:HH12	1:D:219:THR:HG22	1.77	0.48
1:B:220:ARG:NH1	1:B:220:ARG:CG	2.69	0.48
2:C:66:MET:CE	2:C:332:ARG:HB3	2.44	0.48
2:A:282:ILE:CD1	2:A:415:PHE:HE1	2.26	0.48
2:C:221:VAL:HG12	2:C:396:ALA:HB2	1.94	0.48
1:D:394:PRO:C	1:D:396:ASP:H	2.16	0.48
2:C:432:ALA:HA	2:C:435:LEU:HD13	1.95	0.48
2:C:264:VAL:HG23	2:C:445:LEU:HD22	1.95	0.48
2:A:60:TRP:CE2	2:A:400:GLY:HA3	2.49	0.48
1:B:193:SER:OG	1:B:196:GLN:HG3	2.15	0.47
2:C:51:ARG:HB3	2:C:51:ARG:CZ	2.44	0.47
2:A:337:LEU:HD13	2:A:339:ILE:HD11	1.97	0.47
2:A:73:THR:HG21	2:A:186:VAL:HG11	1.96	0.46
2:A:48:GLU:OE1	2:A:226:HIS:CD2	2.69	0.46
1:D:22:ILE:HD11	1:D:398:LEU:HD23	1.95	0.46
1:B:271:THR:HG21	1:B:420:HIS:HA	1.97	0.46
1:B:220:ARG:HG3	1:B:220:ARG:NH1	2.30	0.46
2:A:315:ARG:HG3	2:A:315:ARG:HH11	1.81	0.46
1:B:393:LEU:HB3	1:B:394:PRO:CD	2.45	0.46
1:B:78:THR:CG2	1:B:132:ASP:HB3	2.46	0.46
2:A:411:ASP:O	2:A:415:PHE:HB2	2.15	0.46
1:B:396:ASP:O	1:B:398:LEU:N	2.48	0.46
2:C:231:ARG:HA	2:C:231:ARG:HE	1.81	0.46
2:A:145:GLU:HA	2:A:145:GLU:OE2	2.15	0.46
1:B:64:VAL:HG22	1:B:182:HIS:CD2	2.51	0.46
2:C:237:TYR:O	2:C:240:LEU:HB2	2.17	0.45
1:D:84:ALA:O	1:D:85:LEU:HD23	2.17	0.45
2:A:411:ASP:OD2	2:A:414:ARG:NH1	2.50	0.45
1:B:31:SER:N	1:B:228:GLN:HE22	2.05	0.45
1:D:40:ASN:ND2	1:D:42:THR:H	2.15	0.45
1:B:274:ARG:HG3	1:B:391:TYR:CD1	2.52	0.45
1:B:416:ALA:HA	1:B:419:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:HD13	1:B:318:PRO:HG3	1.98	0.45
1:D:63:GLN:HB2	1:D:66:VAL:CG2	2.46	0.45
1:B:100:ARG:NH1	2:A:387:TYR:HD1	2.15	0.45
2:C:292:TYR:HD1	2:C:419:LEU:HD13	1.82	0.45
2:A:130:MET:HE3	2:A:229:VAL:HG13	1.99	0.45
1:D:141:ALA:HB3	1:D:142:PRO:HD3	2.00	0.44
1:B:155:LEU:HD11	1:B:168:ARG:NH1	2.32	0.44
2:C:282:ILE:CD1	2:C:329:SER:HB2	2.46	0.44
1:D:43:LEU:HA	1:D:44:PRO:HD3	1.89	0.44
2:A:275:LEU:O	2:A:339:ILE:HA	2.18	0.44
1:B:396:ASP:O	1:B:399:ASP:N	2.49	0.44
1:D:258:ASN:HD22	1:D:260:ALA:HB2	1.82	0.44
1:B:130:LEU:HD22	1:B:134:LEU:HG	1.99	0.44
2:C:70:THR:H	2:A:69:THR:HG23	1.81	0.44
2:A:301:LEU:HA	2:A:308:ARG:HB2	1.98	0.44
1:D:394:PRO:C	1:D:396:ASP:N	2.71	0.44
1:B:76:ALA:HB1	1:B:143:VAL:HG11	1.99	0.44
2:A:142:VAL:HG13	2:A:204:ARG:CG	2.41	0.44
1:B:347:LEU:HD22	1:B:351:LEU:CD1	2.48	0.44
2:C:272:TYR:OH	2:C:341:GLU:OE2	2.26	0.44
1:D:119:SER:HB2	1:D:122:GLU:HG2	1.99	0.44
2:C:182:HIS:CD2	2:C:183:PRO:HD2	2.53	0.44
1:B:357:ASP:O	1:B:361:GLN:HG3	2.17	0.44
1:D:37:TYR:OH	1:D:39:GLU:HB2	2.18	0.44
2:C:271:PRO:HG2	2:C:344:PRO:HD2	2.00	0.43
1:B:87:GLU:OE2	2:A:315:ARG:NE	2.47	0.43
1:B:71:ALA:CA	1:B:74:MET:HE2	2.39	0.43
2:C:309:MET:HE1	2:C:360:GLN:HG3	2.00	0.43
2:A:112:ARG:HD3	4:A:24:HOH:O	2.19	0.43
2:C:137:MET:HG2	2:C:137:MET:O	2.19	0.43
2:C:337:LEU:HD23	2:C:337:LEU:HA	1.87	0.43
1:B:332:ARG:HG3	2:A:156:GLU:OE1	2.19	0.43
1:B:45:MET:HE1	1:B:115:ARG:NH2	2.33	0.43
1:D:263:ALA:N	1:D:331:THR:O	2.51	0.43
1:B:123:ARG:CZ	1:B:218:ILE:HD11	2.49	0.43
1:B:241:PRO:HA	1:B:242:PRO:HD2	1.75	0.43
1:B:396:ASP:O	1:B:397:TYR:C	2.57	0.43
2:A:289:ARG:HG2	4:A:22:HOH:O	2.18	0.43
2:C:52:ALA:O	2:C:223:ASP:HB2	2.19	0.43
1:D:430:VAL:HG12	1:D:431:VAL:N	2.34	0.42
1:D:218:ILE:HA	1:D:218:ILE:HD12	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:O	1:B:192:ILE:C	2.57	0.42
2:A:66:MET:HE3	2:A:332:ARG:HB3	2.00	0.42
1:D:266:ALA:C	1:D:267:ILE:HG13	2.40	0.42
2:C:430:ALA:O	2:C:433:ARG:HG2	2.20	0.42
1:D:206:VAL:HG13	1:D:237:GLY:H	1.84	0.42
1:B:90:ILE:HG13	1:B:91:ALA:N	2.34	0.42
2:C:121:VAL:HG13	2:C:125:ARG:HB2	2.01	0.42
1:B:368:ILE:CD1	1:B:405:VAL:HB	2.50	0.42
1:D:317:SER:HA	1:D:318:PRO:HD3	1.82	0.42
1:D:220:ARG:NH1	1:D:220:ARG:CG	2.82	0.42
2:C:42:LEU:HD23	2:C:213:PRO:HA	2.01	0.42
2:A:264:VAL:HG23	2:A:445:LEU:HA	2.00	0.42
1:D:430:VAL:HG12	1:D:431:VAL:H	1.85	0.42
2:A:165:LYS:HA	2:A:166:PRO:HD2	1.90	0.42
1:D:25:GLU:HB3	1:D:220:ARG:HH12	1.85	0.42
1:B:66:VAL:HG22	1:B:192:ILE:HD13	2.01	0.42
2:A:42:LEU:HD21	2:A:218:VAL:HG23	2.01	0.42
1:D:276:ASP:HA	1:D:277:PRO:HD2	1.89	0.42
1:D:114:LEU:HD12	1:D:130:LEU:HD12	2.02	0.42
1:D:108:ASP:OD2	1:D:108:ASP:N	2.52	0.41
2:A:276:ALA:HB1	2:A:337:LEU:HD21	2.02	0.41
2:A:121:VAL:HG13	2:A:125:ARG:HB2	2.02	0.41
1:D:282:LEU:HD11	1:D:420:HIS:CD2	2.55	0.41
1:D:80:SER:O	1:D:82:LYS:N	2.53	0.41
1:D:140:PRO:HB2	1:D:143:VAL:HG23	2.02	0.41
1:B:85:LEU:HD22	1:B:89:ALA:HB1	2.03	0.41
2:C:313:LEU:HD22	2:C:356:ASP:HB3	2.02	0.41
2:C:302:ASP:HB2	2:C:309:MET:HG3	2.02	0.41
1:B:114:LEU:HD22	1:B:116:VAL:HG22	2.03	0.41
1:B:96:ASP:OD1	2:A:376:ARG:HG2	2.20	0.41
2:A:221:VAL:HG13	2:A:396:ALA:HB2	2.01	0.41
2:C:109:PHE:CE1	2:C:116:ALA:HB3	2.55	0.41
1:B:25:GLU:OE2	1:B:220:ARG:NH1	2.54	0.41
1:B:139:PHE:O	1:B:194:ARG:HD2	2.20	0.41
2:C:67:ASP:CG	2:C:332:ARG:HH22	2.24	0.41
2:C:66:MET:HE1	2:C:332:ARG:HB3	2.03	0.41
2:A:48:GLU:HG2	2:A:224:VAL:O	2.20	0.41
1:D:82:LYS:HD2	1:D:82:LYS:N	2.35	0.41
2:A:381:MET:HB3	2:A:416:TYR:HE2	1.85	0.41
2:C:92:PRO:C	2:C:94:GLU:H	2.24	0.41
2:A:309:MET:CE	2:A:309:MET:HA	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:407:LEU:HB3	2:A:411:ASP:OD1	2.21	0.41
1:B:276:ASP:HA	1:B:277:PRO:HD3	1.99	0.41
1:B:298:LEU:HD13	1:B:327:ILE:HG23	2.02	0.41
2:A:176:ALA:HA	2:A:185:ARG:HB2	2.03	0.41
2:C:304:TYR:CE2	2:C:306:GLY:HA3	2.56	0.41
1:D:207:ALA:HB3	1:D:236:ALA:CB	2.49	0.40
1:B:78:THR:HG23	1:B:132:ASP:HB3	2.03	0.40
1:B:139:PHE:H	1:B:194:ARG:NH1	2.20	0.40
2:A:98:ARG:O	2:A:102:MET:HG3	2.21	0.40
1:D:31:SER:HB3	1:D:228:GLN:HE22	1.87	0.40
2:A:68:GLU:OE1	2:A:74:GLY:N	2.46	0.40
1:B:302:ILE:HG23	1:B:308:LEU:HB2	2.03	0.40
1:B:267:ILE:O	1:B:326:GLN:HA	2.21	0.40
1:B:167:GLY:O	1:B:171:THR:HG23	2.22	0.40
2:C:83:MET:SD	2:C:140:LEU:HD22	2.62	0.40
1:D:134:LEU:O	1:D:201:HIS:HE1	2.04	0.40
2:C:143:ASP:OD1	2:C:146:LEU:HG	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	B	412/424 (97%)	387 (94%)	23 (6%)	2 (0%)	34	76
1	D	409/424 (96%)	371 (91%)	34 (8%)	4 (1%)	19	61
2	A	420/437 (96%)	398 (95%)	21 (5%)	1 (0%)	52	88
2	C	420/437 (96%)	385 (92%)	32 (8%)	3 (1%)	26	70
All	All	1661/1722 (96%)	1541 (93%)	110 (7%)	10 (1%)	30	72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	292	GLY
1	B	397	TYR
2	C	315	ARG
1	D	81	GLY
2	A	306	GLY
2	C	287	LYS
1	D	237	GLY
1	B	192	ILE
1	D	290	GLY
2	C	63	VAL

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	B	322/331 (97%)	283 (88%)	39 (12%)	6	25
1	D	321/331 (97%)	290 (90%)	31 (10%)	10	37
2	A	339/352 (96%)	311 (92%)	28 (8%)	14	46
2	C	339/352 (96%)	303 (89%)	36 (11%)	8	31
All	All	1321/1366 (97%)	1187 (90%)	134 (10%)	9	34

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	28	THR
1	B	34	GLN
1	B	43	LEU
1	B	69	MET
1	B	78	THR
1	B	87	GLU
1	B	90	ILE
1	B	114	LEU
1	B	116	VAL
1	B	119	SER
1	B	122	GLU
1	B	125	SER

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Mol	Chain	Res	Type
1	B	130	LEU
1	B	166	LEU
1	B	169	ARG
1	B	186	VAL
1	B	188	THR
1	B	189	LEU
1	B	206	VAL
1	B	213	THR
1	B	218	ILE
1	B	220	ARG
1	B	250	ARG
1	B	271	THR
1	B	274	ARG
1	B	303	ARG
1	B	306	ARG
1	B	313	TYR
1	B	324	LEU
1	B	346	THR
1	B	347	LEU
1	B	360	LEU
1	B	382	LEU
1	B	388	ILE
1	B	402	THR
1	B	411	GLU
1	B	419	ARG
1	B	424	GLU
1	B	428	THR
2	C	33	THR
2	C	37	THR
2	C	40	ASN
2	C	59	VAL
2	C	79	LEU
2	C	88	LYS
2	C	107	ASN
2	C	112	ARG
2	C	132	LEU
2	C	141	VAL
2	C	142	VAL
2	C	143	ASP
2	C	151	ILE
2	C	156	GLU
2	C	165	LYS

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Mol	Chain	Res	Type
2	C	167	ARG
2	C	169	LYS
2	C	193	ASN
2	C	231	ARG
2	C	242	ARG
2	C	243	VAL
2	C	244	GLU
2	C	250	GLN
2	C	269	GLU
2	C	287	LYS
2	C	297	LEU
2	C	310	THR
2	C	337	LEU
2	C	353	LEU
2	C	381	MET
2	C	405	LEU
2	C	417	GLN
2	C	434	LEU
2	C	437	ASP
2	C	444	ASN
2	C	445	LEU
1	D	34	GLN
1	D	40	ASN
1	D	69	MET
1	D	78	THR
1	D	90	ILE
1	D	114	LEU
1	D	116	VAL
1	D	119	SER
1	D	130	LEU
1	D	148	ARG
1	D	169	ARG
1	D	182	HIS
1	D	218	ILE
1	D	220	ARG
1	D	271	THR
1	D	272	LEU
1	D	283	VAL
1	D	299	MET
1	D	306	ARG
1	D	313	TYR
1	D	316	PHE

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Mol	Chain	Res	Type
1	D	318	PRO
1	D	326	GLN
1	D	337	ASP
1	D	347	LEU
1	D	352	ARG
1	D	360	LEU
1	D	365	ASP
1	D	398	LEU
1	D	423	ARG
1	D	428	THR
2	A	37	THR
2	A	40	ASN
2	A	47	ARG
2	A	66	MET
2	A	79	LEU
2	A	88	LYS
2	A	132	LEU
2	A	141	VAL
2	A	142	VAL
2	A	152	GLN
2	A	169	LYS
2	A	221	VAL
2	A	231	ARG
2	A	232	LEU
2	A	250	GLN
2	A	264	VAL
2	A	297	LEU
2	A	309	MET
2	A	310	THR
2	A	312	GLN
2	A	337	LEU
2	A	346	LYS
2	A	353	LEU
2	A	385	LYS
2	A	419	LEU
2	A	434	LEU
2	A	444	ASN
2	A	445	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	GLN
1	B	40	ASN
1	B	178	HIS
1	B	182	HIS
1	B	204	HIS
1	B	228	GLN
1	B	264	HIS
1	B	286	ASN
1	B	378	ASN
1	B	400	HIS
2	C	40	ASN
2	C	120	GLN
2	C	182	HIS
2	C	193	ASN
2	C	197	ASN
2	C	201	GLN
2	C	226	HIS
2	C	251	GLN
2	C	319	HIS
1	D	40	ASN
1	D	178	HIS
1	D	182	HIS
1	D	201	HIS
1	D	204	HIS
1	D	228	GLN
1	D	258	ASN
1	D	326	GLN
1	D	378	ASN
2	A	40	ASN
2	A	120	GLN
2	A	182	HIS
2	A	193	ASN
2	A	201	GLN
2	A	226	HIS
2	A	251	GLN
2	A	335	GLN
2	A	395	GLN
2	A	444	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	B	414/424 (97%)	-0.60	0 100 100	10, 20, 32, 44	0
1	D	411/424 (96%)	-0.16	2 (0%) 91 76	13, 39, 83, 89	0
2	A	422/437 (96%)	-0.66	0 100 100	7, 16, 26, 39	0
2	C	422/437 (96%)	-0.55	1 (0%) 95 87	9, 23, 37, 49	0
All	All	1669/1722 (96%)	-0.49	3 (0%) 95 87	7, 21, 71, 89	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	307	GLY	3.2
2	C	450	PRO	2.7
1	D	309	SER	2.5

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	A	2	1/1	0.96	0.09	-1.94	20,20,20,20	0
3	ZN	C	1	1/1	0.93	0.18	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.