



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:30 PM UTC

PDB ID : 3MA2 / pdb_00003ma2
Title : Complex membrane type-1 matrix metalloproteinase (MT1-MMP) with tissue inhibitor of metalloproteinase-1 (TIMP-1)
Authors : Grossman, M.; Tworowski, D.; Dym, O.; Lee, M.-H.; Levy, Y.; Sagi, I.
Deposited on : 2010-03-23
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
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

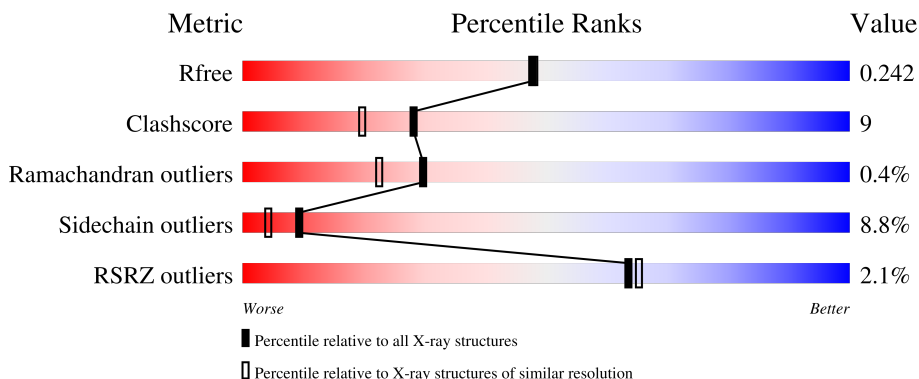
1 Overall quality at a glance

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	181	2% 70% 15% 6% • 7%
1	D	181	2% 64% 25% • • 6%
2	B	125	58% 27% 8% 6%
2	C	125	5% 69% 24% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4709 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 Matrix metalloproteinase-14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	171	Total	C	N	O	S	0	0	0
			1369	879	232	254	4			
1	A	168	Total	C	N	O	S	0	0	0
			1339	861	224	250	4			

- Molecule 2 is a protein called Metalloproteinase inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	S	0	0	0
			921	592	156	164	9			
2	C	119	Total	C	N	O	S	0	0	0
			927	591	158	169	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	304	ALA	VAL	engineered mutation	UNP P01033
B	306	VAL	PRO	engineered mutation	UNP P01033
B	398	LEU	THR	engineered mutation	UNP P01033
C	304	ALA	VAL	engineered mutation	UNP P01033
C	306	VAL	PRO	engineered mutation	UNP P01033
C	398	LEU	THR	engineered mutation	UNP P01033

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total 2	Zn 2	0	0
4	A	2	Total 2	Zn 2	0	0

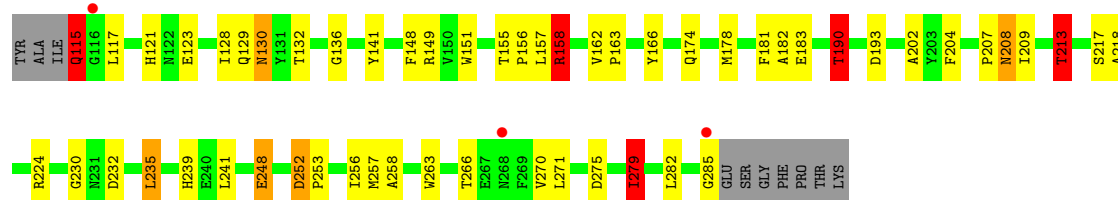
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	62	Total 62	O 62	0	0
5	A	35	Total 35	O 35	0	0
5	B	23	Total 23	O 23	0	0
5	C	25	Total 25	O 25	0	0

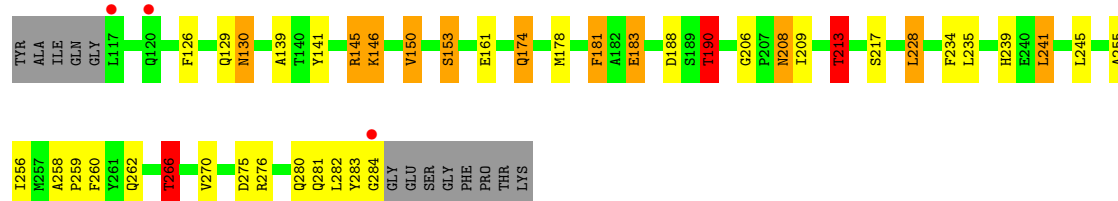
3 Residue-property plots [i](#)

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.

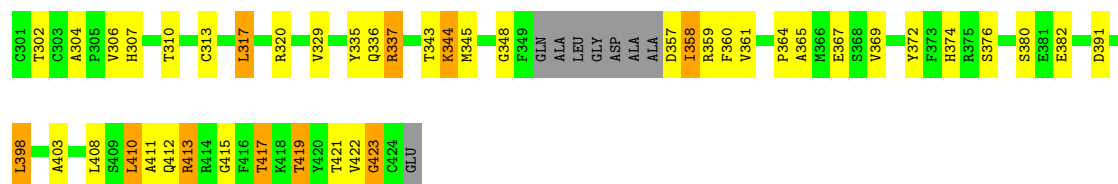
- Molecule 1: Matrix metalloproteinase-14



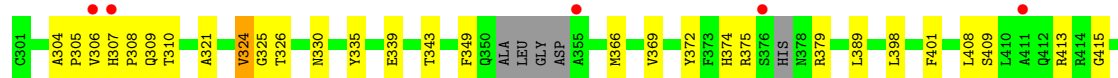
- Molecule 1: Matrix metalloproteinase-14

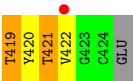


- Molecule 2: Metalloproteinase inhibitor 1



- Molecule 2: Metalloproteinase inhibitor 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.69Å 63.65Å 87.16Å 90.00° 105.86° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 50.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.05) 98.4 (50.00-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.196 , 0.247 0.199 , 0.242	Depositor DCC
R_{free} test set	1961 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4709	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

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	1.70	12/1385 (0.9%)	1.36	6/1887 (0.3%)
1	D	1.86	19/1415 (1.3%)	1.41	8/1924 (0.4%)
2	B	1.73	13/944 (1.4%)	1.50	7/1278 (0.5%)
2	C	1.81	9/948 (0.9%)	1.46	11/1282 (0.9%)
All	All	1.78	53/4692 (1.1%)	1.42	32/6371 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	162	VAL	CA-CB	8.71	1.61	1.54
1	D	182	ALA	N-CA	7.79	1.55	1.46
2	C	307	HIS	CA-C	7.27	1.62	1.53
1	A	270	VAL	CA-CB	7.13	1.62	1.54
2	C	306	VAL	CA-CB	6.98	1.62	1.53
1	D	270	VAL	CA-CB	6.92	1.62	1.54
2	C	421	THR	CA-CB	6.54	1.65	1.53
2	C	321	ALA	C-O	-6.48	1.16	1.23
1	A	139	ALA	CA-C	6.46	1.61	1.52
1	D	163	PRO	C-O	6.42	1.30	1.23
1	A	228	LEU	C-O	-6.40	1.15	1.24
1	A	255	ALA	CA-CB	-6.30	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	258	ALA	C-O	-6.29	1.15	1.23
2	B	365	ALA	CA-CB	6.19	1.64	1.53
2	B	302	THR	CA-CB	6.17	1.63	1.53
1	D	263	TRP	N-CA	6.09	1.53	1.46
1	D	149	ARG	C-O	-6.06	1.17	1.24
2	B	307	HIS	CA-C	6.05	1.58	1.52
1	A	213	THR	CB-CG2	-6.01	1.32	1.52
1	A	183	GLU	C-O	-5.95	1.16	1.23
1	D	266	THR	CA-CB	-5.94	1.44	1.53
1	D	136	GLY	N-CA	5.89	1.51	1.45
1	A	146	LYS	C-O	-5.77	1.17	1.24
1	A	235	LEU	C-O	-5.73	1.17	1.24
2	C	349	PHE	N-CA	5.67	1.53	1.46
2	B	361	VAL	C-O	5.67	1.29	1.24
2	B	410	LEU	C-O	-5.66	1.17	1.24
1	D	207	PRO	C-O	5.65	1.30	1.23
1	A	260	PHE	CA-C	-5.61	1.45	1.52
1	D	218	ALA	C-O	-5.59	1.16	1.24
2	B	313	CYS	N-CA	5.48	1.53	1.46
1	D	252	ASP	C-O	-5.42	1.17	1.24
1	A	145	ARG	C-O	-5.39	1.17	1.24
2	C	413	ARG	CA-C	-5.35	1.45	1.52
1	D	162	VAL	CA-C	5.35	1.56	1.52
2	B	411	ALA	CA-CB	-5.34	1.44	1.53
2	B	412	GLN	N-CA	5.31	1.52	1.46
1	D	230	GLY	N-CA	5.26	1.50	1.45
1	A	150	VAL	CA-CB	5.26	1.60	1.54
1	A	181	PHE	C-O	-5.17	1.17	1.24
1	D	158	ARG	C-O	-5.17	1.18	1.24
2	C	330	ASN	CA-C	5.14	1.59	1.52
2	C	369	VAL	CA-CB	5.13	1.61	1.54
2	B	358	ILE	N-CA	5.11	1.52	1.46
1	D	148	PHE	C-O	-5.09	1.18	1.24
2	B	403	ALA	CA-CB	5.09	1.61	1.54
1	D	257	MET	N-CA	5.08	1.52	1.46
1	D	190	THR	C-O	-5.07	1.17	1.25
1	D	224	ARG	C-O	5.05	1.30	1.23
2	B	306	VAL	CA-C	5.03	1.58	1.52
2	B	359	ARG	CA-C	5.03	1.59	1.52
2	B	304	ALA	CA-CB	-5.01	1.46	1.53
2	C	343	THR	CA-CB	-5.00	1.47	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	422	VAL	N-CA-C	-7.74	105.15	111.81
2	B	380	SER	N-CA-C	7.46	120.29	111.71
2	C	307	HIS	CA-C-N	7.13	127.45	119.32
2	C	307	HIS	C-N-CA	7.13	127.45	119.32
2	B	391	ASP	CB-CA-C	-6.68	101.93	111.95
1	A	258	ALA	CA-C-N	6.45	126.16	119.64
1	A	258	ALA	C-N-CA	6.45	126.16	119.64
1	D	155	THR	CA-C-N	-6.44	113.30	120.45
1	D	155	THR	C-N-CA	-6.44	113.30	120.45
1	A	266	THR	N-CA-CB	-6.35	102.14	110.59
2	B	403	ALA	CA-C-N	-6.16	113.60	119.76
2	B	403	ALA	C-N-CA	-6.16	113.60	119.76
2	C	304	ALA	CA-C-N	-6.12	113.46	119.76
2	C	304	ALA	C-N-CA	-6.12	113.46	119.76
2	B	419	THR	N-CA-C	6.04	120.93	113.50
2	C	375	ARG	N-CA-C	5.96	121.29	113.30
2	C	339	GLU	N-CA-C	-5.94	100.82	110.20
2	C	306	VAL	N-CA-C	5.79	116.49	107.28
2	C	305	PRO	CA-C-N	-5.65	115.56	123.13
2	C	305	PRO	C-N-CA	-5.65	115.56	123.13
2	C	325	GLY	N-CA-C	5.40	118.47	110.42
1	D	279	ILE	CB-CA-C	-5.37	103.40	112.16
1	A	241	LEU	N-CA-C	-5.35	105.61	111.82
1	A	190	THR	CA-CB-CG2	5.19	119.33	110.50
1	D	213	THR	OG1-CB-CG2	5.15	119.60	109.30
1	A	206	GLY	N-CA-C	-5.15	101.83	112.34
2	B	413	ARG	N-CA-C	-5.14	105.68	111.28
2	B	337	ARG	CB-CG-CD	-5.13	99.50	111.30
1	D	271	LEU	CA-C-N	-5.08	114.48	119.92
1	D	271	LEU	C-N-CA	-5.08	114.48	119.92
1	D	213	THR	CA-CB-CG2	5.03	119.06	110.50
1	D	117	LEU	N-CA-C	5.00	117.49	110.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	TYR	Peptide
1	D	115	GLN	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	A	1339	0	1207	25	0
1	D	1369	0	1252	32	0
2	B	921	0	890	21	0
2	C	927	0	877	6	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	35	0	0	2	0
5	B	23	0	0	1	0
5	C	25	0	0	0	0
5	D	62	0	0	2	0
All	All	4709	0	4226	78	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 (78) 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:D:115:GLN:HB3	2:B:367:GLU:OE1	1.45	1.16
1:D:208:ASN:HD22	1:D:209:ILE:H	1.05	0.99
1:A:130:ASN:HD21	1:A:181:PHE:H	1.11	0.94
1:D:130:ASN:HD21	1:D:181:PHE:H	1.13	0.94
2:B:372:TYR:OH	2:B:374:HIS:HD2	1.58	0.86
1:A:183:GLU:HG3	1:A:217:SER:HB2	1.59	0.85
1:D:121:HIS:HD2	1:D:123:GLU:O	1.60	0.84
1:D:115:GLN:CB	2:B:367:GLU:OE1	2.28	0.81
1:D:208:ASN:ND2	1:D:209:ILE:H	1.80	0.79
1:A:280:GLN:HA	1:A:284:GLY:HA3	1.68	0.76
2:C:372:TYR:OH	2:C:374:HIS:HD2	1.71	0.71
1:A:208:ASN:HD22	1:A:209:ILE:H	1.39	0.69
2:C:415:GLY:HA2	2:C:419:THR:HB	1.75	0.67
1:D:157:LEU:C	1:D:158:ARG:HD2	2.20	0.66
1:A:129:GLN:HE21	1:A:178:MET:HE3	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:GLN:CD	1:D:115:GLN:N	2.55	0.65
1:D:208:ASN:HD22	1:D:209:ILE:N	1.88	0.61
2:B:320:ARG:HD2	2:B:382:GLU:HB3	1.81	0.61
2:B:329:VAL:HG22	2:B:336:GLN:HG2	1.81	0.61
2:B:369:VAL:HG12	2:B:369:VAL:O	2.02	0.60
1:D:157:LEU:O	1:D:158:ARG:HD2	2.03	0.58
1:A:190:THR:HG21	2:B:364:PRO:HG3	1.86	0.58
1:A:208:ASN:ND2	1:A:209:ILE:H	2.01	0.58
2:B:422:VAL:C	2:B:423:GLY:O	2.46	0.58
1:A:146:LYS:HD3	1:A:234:PHE:CD1	2.39	0.57
1:A:266:THR:HG21	5:A:74:HOH:O	2.02	0.57
2:B:413:ARG:O	2:B:417:THR:HB	2.06	0.56
1:A:145:ARG:HD3	1:A:161:GLU:OE2	2.07	0.55
1:D:151:TRP:CZ3	1:D:279:ILE:HG12	2.41	0.55
1:A:150:VAL:O	1:A:153:SER:HB2	2.07	0.53
1:D:121:HIS:CD2	1:D:123:GLU:O	2.51	0.53
1:D:183:GLU:HG2	1:D:217:SER:HB2	1.91	0.53
1:A:276:ARG:O	1:A:280:GLN:HG3	2.08	0.53
1:A:126:PHE:CZ	1:A:161:GLU:HB2	2.44	0.53
2:B:374:HIS:HE1	5:B:49:HOH:O	1.91	0.53
2:B:337:ARG:HD2	2:B:360:PHE:CD1	2.44	0.52
1:A:141:TYR:O	1:A:145:ARG:HG3	2.09	0.52
1:D:204:PHE:HZ	1:D:248:GLU:HG3	1.74	0.51
1:A:190:THR:CG2	5:A:43:HOH:O	2.58	0.51
1:A:190:THR:HB	2:B:335:TYR:OH	2.11	0.51
2:C:309:GLN:HE22	2:C:420:TYR:HA	1.77	0.50
1:D:256:ILE:HG22	1:D:275:ASP:CG	2.38	0.49
2:B:317:LEU:HD12	2:B:348:GLY:HA3	1.94	0.49
2:B:422:VAL:O	2:B:423:GLY:O	2.31	0.48
2:B:415:GLY:HA2	2:B:419:THR:OG1	2.14	0.48
1:D:130:ASN:HD21	1:D:181:PHE:N	1.96	0.48
1:D:213:THR:HG21	1:D:241:LEU:HD23	1.96	0.47
1:D:190:THR:HB	2:C:335:TYR:OH	2.15	0.47
2:B:343:THR:O	2:B:344:LYS:HD3	2.15	0.46
1:D:130:ASN:ND2	1:D:181:PHE:H	1.97	0.46
1:D:158:ARG:HD2	1:D:158:ARG:N	2.20	0.46
2:B:320:ARG:NH1	2:B:382:GLU:OE2	2.39	0.45
1:A:146:LYS:HD3	1:A:234:PHE:CE1	2.52	0.44
2:B:372:TYR:OH	2:B:374:HIS:CD2	2.51	0.44
1:D:190:THR:CG2	5:D:25:HOH:O	2.65	0.44
1:D:190:THR:HG22	5:D:25:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASP:HB2	1:A:209:ILE:HD11	1.99	0.43
1:D:202:ALA:HB2	1:D:213:THR:HB	2.00	0.42
1:A:174:GLN:HE21	1:A:174:GLN:HA	1.84	0.42
1:A:213:THR:HG21	1:A:241:LEU:HD23	2.01	0.42
1:A:256:ILE:HG22	1:A:275:ASP:CG	2.44	0.42
1:D:239:HIS:CD2	1:D:239:HIS:C	2.98	0.42
1:D:128:ILE:HB	1:D:141:TYR:CE2	2.54	0.42
1:D:129:GLN:HE21	1:D:178:MET:HE3	1.85	0.41
1:A:239:HIS:CD2	1:A:239:HIS:C	2.97	0.41
2:B:345:MET:HE3	2:B:345:MET:HB2	1.93	0.41
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.85	0.41
1:D:252:ASP:HA	1:D:253:PRO:HD3	1.75	0.41
1:D:193:ASP:OD1	1:D:193:ASP:N	2.47	0.41
2:B:357:ASP:OD1	2:B:357:ASP:C	2.63	0.41
1:D:156:PRO:HD3	1:D:285:GLY:C	2.46	0.41
1:D:232:ASP:HB3	1:D:235:LEU:HD22	2.03	0.41
1:A:259:PRO:HB3	2:B:398:LEU:HD11	2.03	0.41
1:D:166:TYR:CD1	1:D:166:TYR:N	2.87	0.40
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.92	0.40
2:C:308:PRO:HG3	2:C:401:PHE:CE2	2.56	0.40
2:C:324:VAL:HA	2:C:379:ARG:HG3	2.03	0.40
1:D:279:ILE:H	1:D:279:ILE:HG13	1.66	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	166/181 (92%)	157 (95%)	8 (5%)	1 (1%)	21	13
1	D	169/181 (93%)	165 (98%)	4 (2%)	0	100	100
2	B	113/125 (90%)	108 (96%)	4 (4%)	1 (1%)	14	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	113/125 (90%)	109 (96%)	4 (4%)	0	100	100
All	All	561/612 (92%)	539 (96%)	20 (4%)	2 (0%)	30	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	423	GLY
1	A	208	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	133/148 (90%)	124 (93%)	9 (7%)	14	8
1	D	137/148 (93%)	125 (91%)	12 (9%)	9	4
2	B	99/107 (92%)	89 (90%)	10 (10%)	7	3
2	C	97/107 (91%)	87 (90%)	10 (10%)	7	2
All	All	466/510 (91%)	425 (91%)	41 (9%)	9	4

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	115	GLN
1	D	130	ASN
1	D	132	THR
1	D	158	ARG
1	D	174	GLN
1	D	190	THR
1	D	208	ASN
1	D	213	THR
1	D	235	LEU
1	D	248	GLU
1	D	279	ILE
1	D	282	LEU

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Mol	Chain	Res	Type
1	A	130	ASN
1	A	153	SER
1	A	174	GLN
1	A	190	THR
1	A	213	THR
1	A	262	GLN
1	A	266	THR
1	A	281	GLN
1	A	282	LEU
2	B	310	THR
2	B	317	LEU
2	B	344	LYS
2	B	358	ILE
2	B	376	SER
2	B	398	LEU
2	B	408	LEU
2	B	410	LEU
2	B	417	THR
2	B	421	THR
2	C	310	THR
2	C	324	VAL
2	C	326	THR
2	C	366	MET
2	C	389	LEU
2	C	398	LEU
2	C	408	LEU
2	C	409	SER
2	C	419	THR
2	C	421	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	115	GLN
1	D	129	GLN
1	D	130	ASN
1	D	174	GLN
1	D	208	ASN
1	D	262	GLN
1	D	280	GLN
1	D	281	GLN
1	A	122	ASN

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Mol	Chain	Res	Type
1	A	129	GLN
1	A	130	ASN
1	A	174	GLN
1	A	208	ASN
1	A	262	GLN
1	A	281	GLN
2	B	307	HIS
2	B	336	GLN
2	B	374	HIS
2	B	406	ASN
2	C	309	GLN
2	C	374	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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	A	168/181 (92%)	-0.18	3 (1%) 67 69	16, 24, 40, 53	0
1	D	171/181 (94%)	-0.42	3 (1%) 67 69	12, 18, 34, 41	0
2	B	117/125 (93%)	-0.21	0 100 100	17, 24, 41, 46	0
2	C	119/125 (95%)	0.09	6 (5%) 34 34	16, 26, 47, 56	0
All	All	575/612 (93%)	-0.20	12 (2%) 63 65	12, 22, 42, 56	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	355	ALA	3.4
2	C	307	HIS	3.2
2	C	422	VAL	3.1
1	A	117	LEU	2.9
1	D	116	GLY	2.9
2	C	376	SER	2.7
1	D	268	ASN	2.6
1	A	284	GLY	2.5
2	C	306	VAL	2.5
1	D	285	GLY	2.2
2	C	411	ALA	2.1
1	A	120	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 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($\text{\AA}^2$)	Q<0.9
3	CA	D	296	1/1	0.98	0.02	19,19,19,19	0
3	CA	D	293	1/1	0.99	0.01	17,17,17,17	0
3	CA	A	296	1/1	0.99	0.02	21,21,21,21	0
3	CA	A	293	1/1	1.00	0.02	21,21,21,21	0
4	ZN	D	294	1/1	1.00	0.01	16,16,16,16	0
4	ZN	D	295	1/1	1.00	0.01	16,16,16,16	0
4	ZN	A	294	1/1	1.00	0.02	20,20,20,20	0
4	ZN	A	295	1/1	1.00	0.01	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.