



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:14 PM UTC

PDB ID : 1UEA / pdb_00001uea
Title : MMP-3/TIMP-1 COMPLEX
Authors : Bode, W.; Maskos, K.; Gomis-Rueth, F.-X.; Nagase, H.
Deposited on : 1997-06-06
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

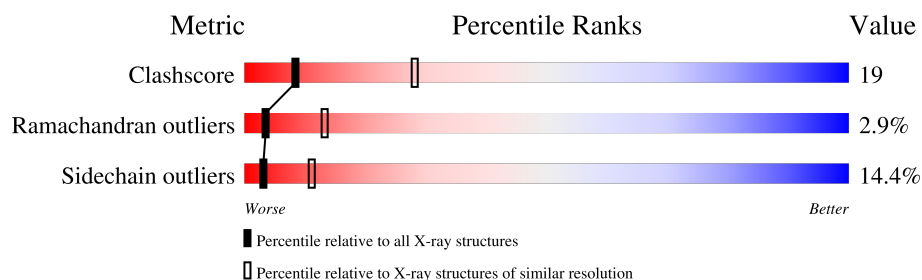
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	173	
1	C	173	
2	B	184	
2	D	184	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6039 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-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	Se	0	0	0
			1338	861	223	252	2			
1	C	168	Total	C	N	O	Se	43	0	0
			1338	861	223	252	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MSE	MET	engineered mutation	UNP P08254
A	219	MSE	MET	engineered mutation	UNP P08254
C	143	MSE	MET	engineered mutation	UNP P08254
C	219	MSE	MET	engineered mutation	UNP P08254

- Molecule 2 is a protein called TISSUE INHIBITOR OF METALLOPROTEINASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	33	0	0
			1421	902	247	257	15			
2	D	181	Total	C	N	O	S	30	0	0
			1421	902	247	257	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	30	ALA	ASN	engineered mutation	UNP P01033
B	78	ALA	ASN	engineered mutation	UNP P01033
D	30	ALA	ASN	engineered mutation	UNP P01033
D	78	ALA	ASN	engineered mutation	UNP P01033

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Zn 2	0	0
3	C	2	Total 2	Zn 2	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Ca 3	0	0
4	C	3	Total 3	Ca 3	0	0

- Molecule 5 is water.

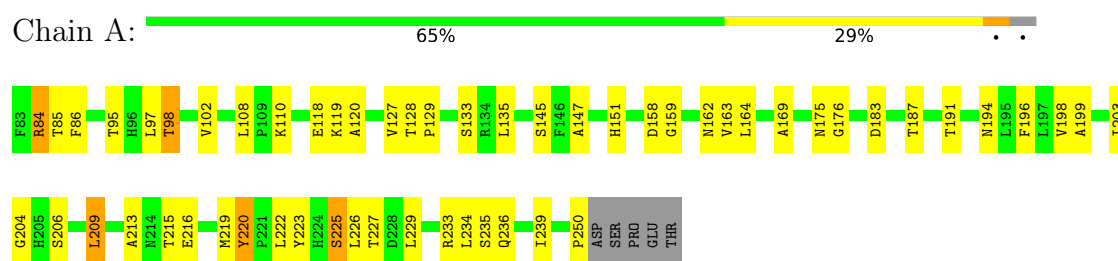
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total 127	O 127	0	0
5	B	117	Total 117	O 117	0	0
5	C	136	Total 136	O 136	0	0
5	D	131	Total 131	O 131	0	0

3 Residue-property plots

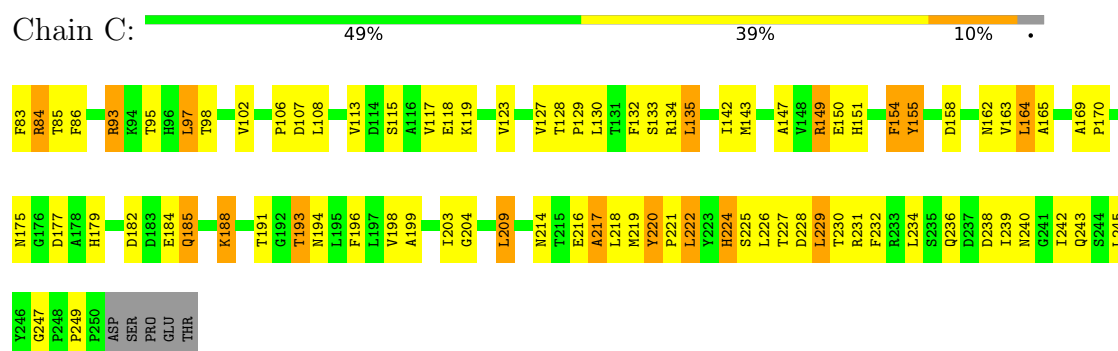
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

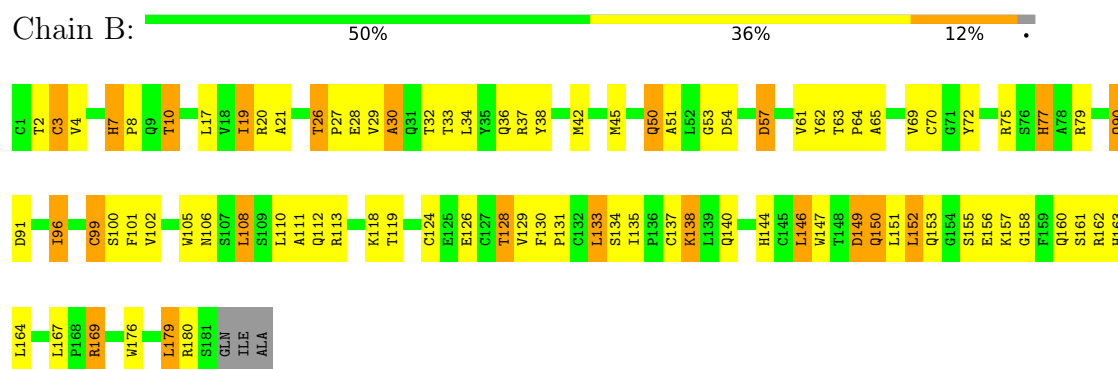
• Molecule 1: MATRIX METALLOPROTEINASE-3



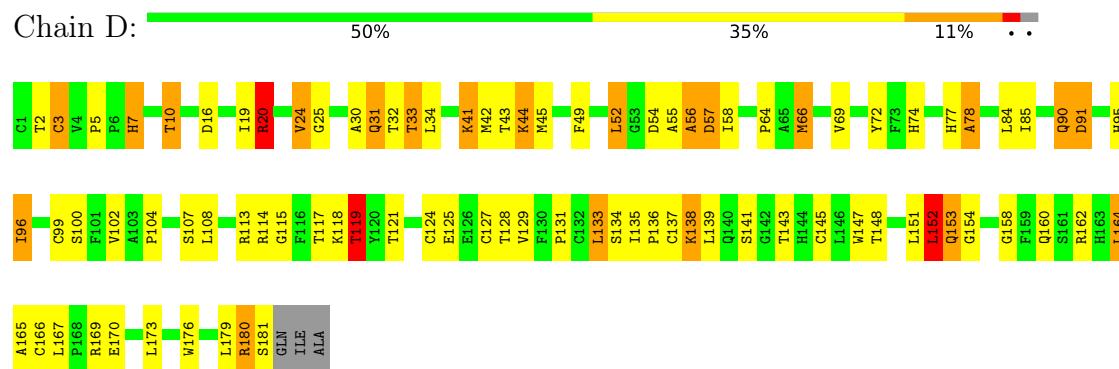
• Molecule 1: MATRIX METALLOPROTEINASE-3



• Molecule 2: TISSUE INHIBITOR OF METALLOPROTEINASE-1



• Molecule 2: TISSUE INHIBITOR OF METALLOPROTEINASE-1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	80.62Å 80.62Å 157.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.80)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6039	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	A	0.52	0/1380	0.99	2/1882 (0.1%)
1	C	0.56	0/1380	1.17	16/1882 (0.9%)
2	B	0.55	0/1458	1.13	11/1977 (0.6%)
2	D	0.57	0/1458	1.14	14/1977 (0.7%)
All	All	0.55	0/5676	1.11	43/7718 (0.6%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	119	THR	N-CA-C	10.55	125.53	112.23
2	B	124	CYS	N-CA-C	9.20	121.25	111.03
2	D	55	ALA	N-CA-C	-8.37	101.22	112.26
1	C	217	ALA	N-CA-C	7.87	120.47	110.24
1	C	234	LEU	N-CA-C	-7.00	99.30	109.59
2	D	119	THR	N-CA-C	7.00	121.91	113.23
2	B	7	HIS	N-CA-C	-7.00	100.43	110.08
2	D	31	GLN	N-CA-C	-6.94	104.69	113.02
2	D	57	ASP	N-CA-C	6.90	125.49	110.80
1	C	155	TYR	CA-C-N	6.79	126.75	119.76
1	C	155	TYR	C-N-CA	6.79	126.75	119.76
1	C	227	THR	N-CA-C	-6.65	103.83	112.68
2	D	152	LEU	N-CA-C	-6.58	98.92	109.39
2	B	57	ASP	N-CA-C	-6.58	105.79	113.88
1	C	224	HIS	N-CA-C	6.58	118.14	110.97
1	C	188	LYS	N-CA-C	-6.57	105.14	113.02
1	A	220	TYR	N-CA-C	-6.43	100.05	109.50
2	B	3	CYS	N-CA-C	6.18	117.93	108.42
1	C	226	LEU	N-CA-C	6.13	117.84	108.52
2	D	7	HIS	N-CA-C	-6.09	101.68	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	220	TYR	N-CA-C	-5.93	102.17	109.65
2	D	3	CYS	N-CA-C	5.86	117.76	108.79
1	C	102	VAL	N-CA-C	5.78	117.21	110.62
2	D	136	PRO	N-CA-C	-5.76	107.29	114.20
1	C	247	GLY	CA-C-N	5.66	126.21	120.38
1	C	247	GLY	C-N-CA	5.66	126.21	120.38
1	A	213	ALA	N-CA-C	-5.60	106.61	113.50
2	B	90	GLN	N-CA-C	-5.58	100.10	108.96
2	B	50	GLN	N-CA-C	-5.57	105.14	112.72
2	D	16	ASP	N-CA-C	-5.55	106.64	113.41
2	D	125	GLU	N-CA-C	5.54	117.00	111.07
1	C	158	ASP	N-CA-C	5.48	119.70	112.25
1	C	221	PRO	N-CA-C	5.48	120.74	113.57
2	B	20	ARG	N-CA-C	-5.36	99.70	108.76
2	D	164	LEU	N-CA-C	5.28	118.60	110.42
2	B	70	CYS	N-CA-C	5.22	121.91	110.80
2	D	20	ARG	N-CA-C	-5.17	99.86	108.34
2	B	118	LYS	N-CA-C	5.17	121.81	110.80
2	D	135	ILE	N-CA-CB	5.09	114.42	110.45
2	D	124	CYS	N-CA-C	5.09	119.72	111.37
1	C	220	TYR	CA-C-N	5.07	124.57	119.19
1	C	220	TYR	C-N-CA	5.07	124.57	119.19
2	B	155	SER	N-CA-C	5.03	116.84	109.24

There are no chirality outliers.

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	1338	0	1266	34	0
1	C	1338	0	1266	57	0
2	B	1421	0	1389	62	0
2	D	1421	0	1389	63	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	0	0	0
4	C	3	0	0	0	0
5	A	127	0	0	3	0
5	B	117	0	0	3	0
5	C	136	0	0	0	0
5	D	131	0	0	5	0
All	All	6039	0	5310	198	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 (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:GLY:HA2	2:B:57:ASP:HB3	1.47	0.96
2:B:96:ILE:HD11	2:B:102:VAL:HG21	1.51	0.92
1:C:86:PHE:HD2	2:D:66:MET:HE2	1.37	0.90
2:D:115:GLY:HA2	2:D:119:THR:HG23	1.59	0.85
2:D:10:THR:HG21	5:D:1045:HOH:O	1.79	0.83
1:C:84:ARG:HG2	1:C:85:THR:H	1.42	0.83
2:B:30:ALA:HB2	2:B:37:ARG:HD3	1.63	0.80
2:B:111:ALA:HB1	2:B:179:LEU:HD13	1.66	0.77
1:A:223:TYR:CE1	1:A:225:SER:HB3	2.21	0.76
1:C:214:ASN:HB3	1:C:216:GLU:HG2	1.69	0.75
1:C:84:ARG:HG2	1:C:85:THR:N	2.02	0.74
2:B:169:ARG:HG2	2:B:169:ARG:HH11	1.54	0.73
2:D:147:TRP:HD1	2:D:160:GLN:NE2	1.86	0.73
1:A:119:LYS:HE2	5:A:1219:HOH:O	1.89	0.73
2:B:110:LEU:HD12	2:B:110:LEU:H	1.52	0.72
2:B:32:THR:HG22	2:B:34:LEU:H	1.54	0.72
1:A:191:THR:HA	2:B:134:SER:OG	1.91	0.71
1:C:127:VAL:HG23	1:C:128:THR:HG23	1.73	0.71
2:D:90:GLN:HB2	2:D:95:HIS:CD2	2.26	0.70
2:D:66:MET:HE3	5:D:1115:HOH:O	1.91	0.70
2:B:53:GLY:HA2	2:B:57:ASP:CB	2.23	0.67
1:C:83:PHE:HB3	1:C:84:ARG:HH11	1.60	0.67
1:C:231:ARG:O	1:C:231:ARG:HG3	1.96	0.65
1:C:199:ALA:O	1:C:203:ILE:HG12	1.96	0.64
1:A:119:LYS:HG3	1:A:196:PHE:CE1	2.32	0.64
1:A:198:VAL:HG13	2:B:2:THR:HG21	1.79	0.64
1:C:86:PHE:CD2	2:D:66:MET:HE2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:HIS:HB3	2:D:10:THR:HG22	1.79	0.63
2:D:7:HIS:HB3	2:D:10:THR:CG2	2.29	0.62
1:C:198:VAL:HG13	2:D:2:THR:HG21	1.81	0.61
2:B:77:HIS:H	2:B:77:HIS:CD2	2.18	0.61
2:D:147:TRP:HD1	2:D:160:GLN:HE21	1.48	0.60
2:B:19:ILE:HD12	2:B:45:MET:HG3	1.83	0.60
1:C:154:PHE:HB3	2:D:34:LEU:HD13	1.84	0.60
1:A:158:ASP:OD2	1:A:162:ASN:HB3	2.02	0.59
1:A:120:ALA:HA	1:A:196:PHE:CE1	2.38	0.58
1:A:162:ASN:O	2:B:3:CYS:HB2	2.03	0.58
2:B:111:ALA:HB1	2:B:179:LEU:CD1	2.33	0.58
1:C:113:VAL:O	1:C:117:VAL:HG23	2.03	0.58
2:B:163:HIS:O	2:B:179:LEU:HD12	2.03	0.58
2:D:164:LEU:HB3	2:D:176:TRP:CE3	2.39	0.57
1:C:220:TYR:CE2	1:C:222:LEU:HB2	2.39	0.57
2:B:29:VAL:HG13	2:B:32:THR:O	2.04	0.57
1:A:159:GLY:HA2	1:A:183:ASP:OD2	2.05	0.56
2:D:96:ILE:HG13	2:D:100:SER:HB2	1.86	0.56
2:D:165:ALA:HB2	2:D:179:LEU:HD21	1.87	0.56
2:B:7:HIS:HB3	2:B:10:THR:HG22	1.88	0.56
2:D:114:ARG:NH2	2:D:117:THR:HG21	2.20	0.55
2:D:84:LEU:HD13	2:D:85:ILE:N	2.22	0.55
1:A:129:PRO:HB3	1:A:250:PRO:HD3	1.89	0.55
1:C:238:ASP:O	1:C:242:ILE:HG22	2.07	0.55
1:A:199:ALA:O	1:A:203:ILE:HG12	2.08	0.54
1:C:155:TYR:CD2	2:D:69:VAL:HG21	2.42	0.54
1:A:120:ALA:HA	1:A:196:PHE:HE1	1.72	0.54
2:B:160:GLN:HA	2:B:164:LEU:HB2	1.89	0.54
2:D:24:VAL:HG12	2:D:25:GLY:N	2.21	0.54
1:C:188:LYS:HG2	1:C:188:LYS:O	2.08	0.53
1:C:194:ASN:OD1	1:C:196:PHE:HB3	2.08	0.53
2:B:17:LEU:HD23	2:B:19:ILE:HD13	1.90	0.53
1:A:163:VAL:HA	2:B:3:CYS:HB3	1.91	0.52
1:C:128:THR:HB	1:C:129:PRO:HD2	1.92	0.52
2:B:156:GLU:H	2:B:156:GLU:CD	2.17	0.52
2:D:152:LEU:O	2:D:154:GLY:N	2.43	0.52
2:D:96:ILE:HG13	2:D:100:SER:CB	2.39	0.52
1:A:187:THR:HG21	1:A:191:THR:O	2.10	0.52
1:C:164:LEU:HB2	2:D:2:THR:HG23	1.92	0.52
2:D:19:ILE:O	2:D:84:LEU:HD22	2.10	0.52
2:D:170:GLU:CG	2:D:173:LEU:HB3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:VAL:HA	2:D:3:CYS:HB3	1.91	0.51
2:D:128:THR:HG22	5:D:1283:HOH:O	2.11	0.51
1:C:209:LEU:HB3	1:C:219:MSE:HE2	1.93	0.51
2:D:133:LEU:HD23	5:D:1116:HOH:O	2.10	0.51
2:B:19:ILE:CD1	2:B:45:MET:HG3	2.40	0.51
1:C:143:MSE:HB2	1:C:177:ASP:CG	2.35	0.51
2:B:10:THR:HB	5:B:1047:HOH:O	2.11	0.51
2:B:128:THR:O	2:B:144:HIS:HA	2.10	0.51
1:C:214:ASN:HB3	1:C:216:GLU:CG	2.38	0.51
2:D:145:CYS:HB3	2:D:176:TRP:CE2	2.45	0.51
2:D:148:THR:H	2:D:160:GLN:HE22	1.57	0.50
1:C:85:THR:HB	2:D:33:THR:HG22	1.93	0.50
1:C:97:LEU:CD2	1:C:130:LEU:HD22	2.41	0.50
1:C:165:ALA:HB1	1:C:179:HIS:O	2.11	0.50
2:D:133:LEU:HD23	2:D:133:LEU:N	2.26	0.50
2:D:158:GLY:O	2:D:162:ARG:HG3	2.11	0.50
2:D:147:TRP:HA	2:D:160:GLN:HE22	1.77	0.50
2:D:148:THR:N	2:D:160:GLN:HE22	2.10	0.50
1:A:147:ALA:HB1	1:A:151:HIS:HB3	1.94	0.50
2:B:72:TYR:HE1	5:B:1367:HOH:O	1.95	0.50
2:B:164:LEU:HB3	2:B:176:TRP:CE3	2.47	0.49
2:B:36:GLN:HG3	2:B:65:ALA:HA	1.93	0.49
2:B:106:ASN:HA	2:B:113:ARG:HH21	1.76	0.49
1:C:222:LEU:HG	2:D:5:PRO:HB3	1.94	0.49
1:C:95:THR:HA	1:C:130:LEU:HD23	1.95	0.49
2:D:170:GLU:HG2	2:D:173:LEU:HB3	1.95	0.49
2:B:62:TYR:O	2:B:96:ILE:HG22	2.13	0.48
2:D:131:PRO:HA	2:D:147:TRP:HB3	1.95	0.48
2:D:169:ARG:HH11	2:D:169:ARG:HG2	1.78	0.48
2:D:84:LEU:HD13	2:D:84:LEU:C	2.39	0.48
2:B:131:PRO:HA	2:B:147:TRP:HB3	1.95	0.48
1:A:215:THR:HG22	1:A:220:TYR:CZ	2.49	0.48
1:A:234:LEU:HD23	1:A:239:ILE:HG12	1.96	0.48
1:C:236:GLN:O	1:C:240:ASN:ND2	2.47	0.47
2:D:69:VAL:O	2:D:69:VAL:HG13	2.14	0.47
1:A:220:TYR:CE2	1:A:222:LEU:HB2	2.49	0.47
2:B:7:HIS:O	2:B:10:THR:HG23	2.15	0.47
1:C:106:PRO:O	1:C:107:ASP:C	2.57	0.47
2:D:133:LEU:HD23	2:D:133:LEU:H	1.79	0.47
1:C:98:THR:OG1	1:C:135:LEU:HD13	2.14	0.47
1:C:185:GLN:HA	1:C:185:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:HG23	2:B:99:CYS:SG	2.54	0.47
2:B:90:GLN:O	2:B:91:ASP:HB2	2.15	0.46
2:B:160:GLN:HG2	2:B:164:LEU:HD22	1.97	0.46
1:C:162:ASN:O	1:C:164:LEU:HD13	2.16	0.46
1:C:169:ALA:O	1:C:175:ASN:HB3	2.15	0.46
2:B:169:ARG:HG2	2:B:169:ARG:NH1	2.25	0.46
2:B:105:TRP:O	2:B:108:LEU:HB2	2.16	0.46
2:B:19:ILE:HD11	2:B:45:MET:HE3	1.97	0.46
1:A:128:THR:HB	1:A:129:PRO:HD2	1.98	0.46
2:D:45:MET:HG2	2:D:49:PHE:CZ	2.51	0.45
1:C:149:ARG:O	1:C:151:HIS:N	2.49	0.45
1:C:83:PHE:HE2	2:D:66:MET:HE1	1.81	0.45
2:D:179:LEU:O	2:D:180:ARG:O	2.34	0.45
1:A:85:THR:HG22	2:B:33:THR:HG23	1.98	0.45
2:B:130:PHE:HA	2:B:131:PRO:HD3	1.76	0.45
1:A:127:VAL:HG23	1:A:128:THR:HG23	1.97	0.45
2:B:110:LEU:HD12	2:B:110:LEU:N	2.26	0.45
2:D:114:ARG:HH21	2:D:117:THR:HG21	1.81	0.45
1:C:83:PHE:HB3	1:C:84:ARG:NH1	2.29	0.45
1:A:204:GLY:O	1:A:209:LEU:HB2	2.17	0.45
2:B:79:ARG:HH11	2:B:79:ARG:HG3	1.80	0.45
2:D:90:GLN:O	2:D:91:ASP:HB2	2.17	0.45
2:B:30:ALA:HB2	2:B:37:ARG:CD	2.41	0.45
1:A:84:ARG:HH11	1:A:84:ARG:HG2	1.81	0.44
2:B:26:THR:HG22	2:B:27:PRO:HD2	2.00	0.44
1:C:83:PHE:HB2	1:C:86:PHE:O	2.17	0.44
1:C:193:THR:HG22	1:C:198:VAL:HG21	2.00	0.44
1:C:220:TYR:HE2	1:C:222:LEU:HB2	1.79	0.44
2:B:61:VAL:O	2:B:61:VAL:HG13	2.17	0.44
1:C:93:ARG:H	1:C:93:ARG:HG2	1.72	0.44
2:D:72:TYR:CE2	2:D:74:HIS:HB2	2.53	0.44
2:B:63:THR:HB	2:B:96:ILE:CG2	2.48	0.44
2:B:137:CYS:SG	2:B:146:LEU:HG	2.57	0.44
2:D:127:CYS:HB3	2:D:166:CYS:SG	2.57	0.44
1:A:102:VAL:HB	1:A:145:SER:HB3	1.99	0.44
2:D:20:ARG:HG2	2:D:43:THR:OG1	2.18	0.44
1:C:127:VAL:O	1:C:249:PRO:HD3	2.18	0.43
1:C:169:ALA:HB1	1:C:170:PRO:HD2	1.99	0.43
2:B:149:ASP:O	2:B:151:LEU:N	2.52	0.43
2:D:56:ALA:O	2:D:58:ILE:N	2.51	0.43
2:B:21:ALA:HB2	2:B:42:MET:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:GLN:NE2	2:B:161:SER:O	2.52	0.43
1:A:169:ALA:O	1:A:175:ASN:HB3	2.18	0.43
2:B:106:ASN:HA	2:B:113:ARG:NH2	2.33	0.43
1:C:95:THR:O	1:C:130:LEU:HA	2.19	0.43
1:C:216:GLU:HG3	1:C:217:ALA:N	2.34	0.43
1:A:235:SER:O	1:A:236:GLN:C	2.61	0.43
1:C:182:ASP:C	1:C:184:GLU:H	2.27	0.43
1:A:98:THR:HG21	5:A:1419:HOH:O	2.19	0.42
2:D:49:PHE:O	2:D:52:LEU:HG	2.19	0.42
1:C:97:LEU:O	1:C:132:PHE:HA	2.19	0.42
2:B:38:TYR:HB2	2:B:61:VAL:CG1	2.50	0.42
2:B:57:ASP:HA	5:B:1080:HOH:O	2.20	0.42
1:A:209:LEU:HB3	1:A:219:MSE:HE2	2.02	0.42
1:C:147:ALA:HB1	1:C:151:HIS:HB3	2.01	0.42
1:A:194:ASN:OD1	1:A:196:PHE:HB3	2.19	0.42
2:B:158:GLY:O	2:B:162:ARG:HG3	2.20	0.42
2:D:41:LYS:NZ	2:D:42:MET:O	2.52	0.42
2:D:147:TRP:HA	2:D:160:GLN:NE2	2.35	0.42
2:D:152:LEU:O	2:D:153:GLN:C	2.62	0.42
1:C:119:LYS:O	1:C:123:VAL:HG23	2.19	0.42
1:C:218:LEU:HD22	1:C:232:PHE:HZ	1.85	0.42
1:A:135:LEU:HD11	1:C:135:LEU:HD11	2.02	0.42
2:B:77:HIS:H	2:B:77:HIS:HD2	1.67	0.42
2:B:150:GLN:C	2:B:152:LEU:N	2.75	0.42
2:D:160:GLN:HG2	2:D:164:LEU:HD22	2.02	0.42
1:C:204:GLY:O	1:C:209:LEU:HB2	2.20	0.41
2:D:104:PRO:HG2	2:D:107:SER:OG	2.20	0.41
2:D:137:CYS:O	2:D:138:LYS:HB2	2.20	0.41
2:B:99:CYS:O	2:B:100:SER:C	2.63	0.41
2:B:110:LEU:H	2:B:110:LEU:CD1	2.25	0.41
2:B:8:PRO:HG3	2:B:101:PHE:CE2	2.55	0.41
1:C:142:ILE:O	1:C:142:ILE:HG22	2.21	0.41
1:A:110:LYS:HE2	5:A:1216:HOH:O	2.21	0.41
1:A:133:SER:HB3	1:C:134:ARG:O	2.21	0.41
1:A:176:GLY:O	1:A:206:SER:HB3	2.20	0.41
2:B:77:HIS:CD2	2:B:77:HIS:N	2.85	0.41
2:B:133:LEU:HD12	2:B:133:LEU:HA	1.90	0.41
2:D:145:CYS:HB3	2:D:176:TRP:NE1	2.36	0.41
1:C:239:ILE:O	1:C:243:GLN:HB2	2.20	0.41
2:D:31:GLN:HB3	5:D:1398:HOH:O	2.21	0.41
2:D:43:THR:OG1	2:D:44:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:HIS:O	2:D:78:ALA:HB2	2.20	0.41
2:B:152:LEU:HD22	2:B:152:LEU:HA	1.80	0.40
2:B:138:LYS:HG3	2:B:140:GLN:HE21	1.87	0.40
1:C:224:HIS:O	1:C:225:SER:HB2	2.21	0.40
2:D:84:LEU:O	2:D:102:VAL:HA	2.21	0.40
2:D:114:ARG:O	2:D:119:THR:HG22	2.22	0.40
1:C:218:LEU:C	1:C:220:TYR:H	2.29	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	166/173 (96%)	148 (89%)	16 (10%)	2 (1%)	10	34
1	C	166/173 (96%)	142 (86%)	21 (13%)	3 (2%)	6	23
2	B	179/184 (97%)	152 (85%)	22 (12%)	5 (3%)	4	14
2	D	179/184 (97%)	150 (84%)	19 (11%)	10 (6%)	1	4
All	All	690/714 (97%)	592 (86%)	78 (11%)	20 (3%)	3	13

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	SER
1	A	227	THR
2	B	54	ASP
2	B	150	GLN
1	C	229	LEU
2	D	30	ALA
2	D	52	LEU
2	D	56	ALA

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Mol	Chain	Res	Type
2	D	57	ASP
2	D	153	GLN
2	D	180	ARG
2	B	30	ALA
1	C	150	GLU
1	C	228	ASP
2	D	24	VAL
2	D	138	LYS
2	D	78	ALA
2	D	91	ASP
2	B	149	ASP
2	B	51	ALA

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	142/145 (98%)	129 (91%)	13 (9%)	8	27
1	C	142/145 (98%)	123 (87%)	19 (13%)	4	13
2	B	157/159 (99%)	130 (83%)	27 (17%)	2	7
2	D	157/159 (99%)	130 (83%)	27 (17%)	2	7
All	All	598/608 (98%)	512 (86%)	86 (14%)	3	11

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	86	PHE
1	A	95	THR
1	A	97	LEU
1	A	98	THR
1	A	108	LEU
1	A	118	GLU
1	A	164	LEU
1	A	209	LEU

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Mol	Chain	Res	Type
1	A	216	GLU
1	A	226	LEU
1	A	229	LEU
1	A	233	ARG
2	B	4	VAL
2	B	10	THR
2	B	19	ILE
2	B	26	THR
2	B	28	GLU
2	B	50	GLN
2	B	64	PRO
2	B	69	VAL
2	B	75	ARG
2	B	77	HIS
2	B	96	ILE
2	B	99	CYS
2	B	108	LEU
2	B	126	GLU
2	B	128	THR
2	B	129	VAL
2	B	133	LEU
2	B	135	ILE
2	B	138	LYS
2	B	146	LEU
2	B	152	LEU
2	B	153	GLN
2	B	157	LYS
2	B	167	LEU
2	B	169	ARG
2	B	179	LEU
2	B	180	ARG
1	C	84	ARG
1	C	93	ARG
1	C	97	LEU
1	C	108	LEU
1	C	115	SER
1	C	118	GLU
1	C	133	SER
1	C	135	LEU
1	C	149	ARG
1	C	154	PHE
1	C	164	LEU

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Mol	Chain	Res	Type
1	C	185	GLN
1	C	191	THR
1	C	193	THR
1	C	209	LEU
1	C	222	LEU
1	C	229	LEU
1	C	230	THR
1	C	245	LEU
2	D	10	THR
2	D	20	ARG
2	D	32	THR
2	D	33	THR
2	D	41	LYS
2	D	44	LYS
2	D	54	ASP
2	D	64	PRO
2	D	66	MET
2	D	90	GLN
2	D	96	ILE
2	D	99	CYS
2	D	108	LEU
2	D	113	ARG
2	D	118	LYS
2	D	119	THR
2	D	121	THR
2	D	129	VAL
2	D	133	LEU
2	D	134	SER
2	D	139	LEU
2	D	141	SER
2	D	143	THR
2	D	151	LEU
2	D	152	LEU
2	D	167	LEU
2	D	181	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	HIS
2	B	74	HIS
2	B	77	HIS

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Mol	Chain	Res	Type
2	B	140	GLN
2	B	150	GLN
2	B	177	GLN
1	C	162	ASN
2	D	50	GLN
2	D	77	HIS
2	D	106	ASN
2	D	160	GLN
2	D	163	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.