



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:05 AM UTC

PDB ID : 4FU4 / pdb_00004fu4
Title : Human collagenase 3 (MMP-13) with peptide from pro-domain
Authors : Stura, E.A.; Vera, L.; Visse, R.; Nagase, H.; Dive, V.
Deposited on : 2012-06-28
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

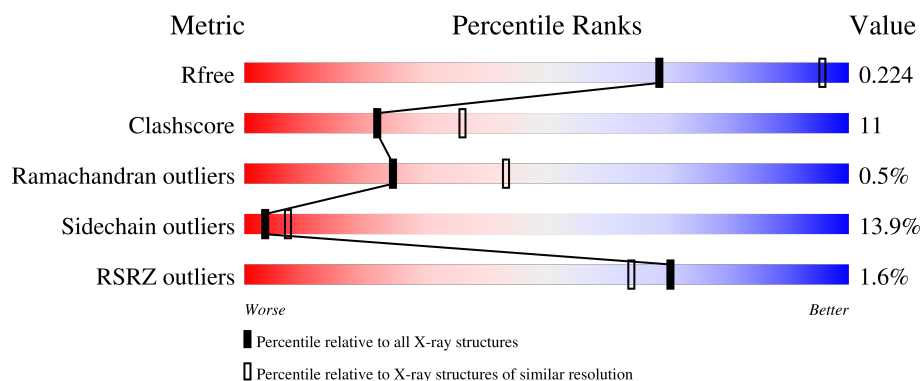
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	368	63% 30% 7%
1	B	368	69% 27% .
2	C	26	35% 58% 31% 12%
2	D	26	4% 58% 38% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6690 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 Collagenase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	1	0
			3005	1951	495	549	10			
1	B	368	Total	C	N	O	S	0	1	0
			3009	1956	494	549	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ALA	GLU	engineered mutation	UNP P45452
B	223	ALA	GLU	engineered mutation	UNP P45452

- Molecule 2 is a protein called Collagenase 3, pro-domain peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	26	Total	C	N	O	0	0	0
			220	135	35	50			
2	D	26	Total	C	N	O	0	1	0
			232	144	36	52			

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

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

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

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

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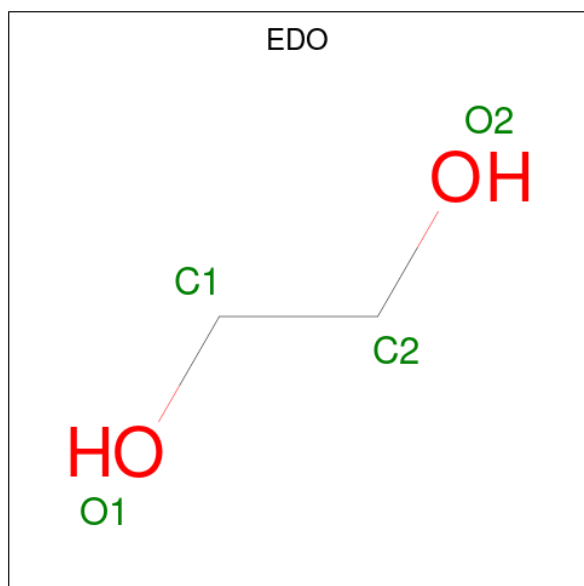
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total 4	Ca 4	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0
5	C	1	Total 1	Cl 1	0	0
5	D	1	Total 1	Cl 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	39	Total	O	0	0
			39	39		
7	B	58	Total	O	0	0
			58	58		
7	C	2	Total	O	0	0
			2	2		
7	D	5	Total	O	0	0
			5	5		

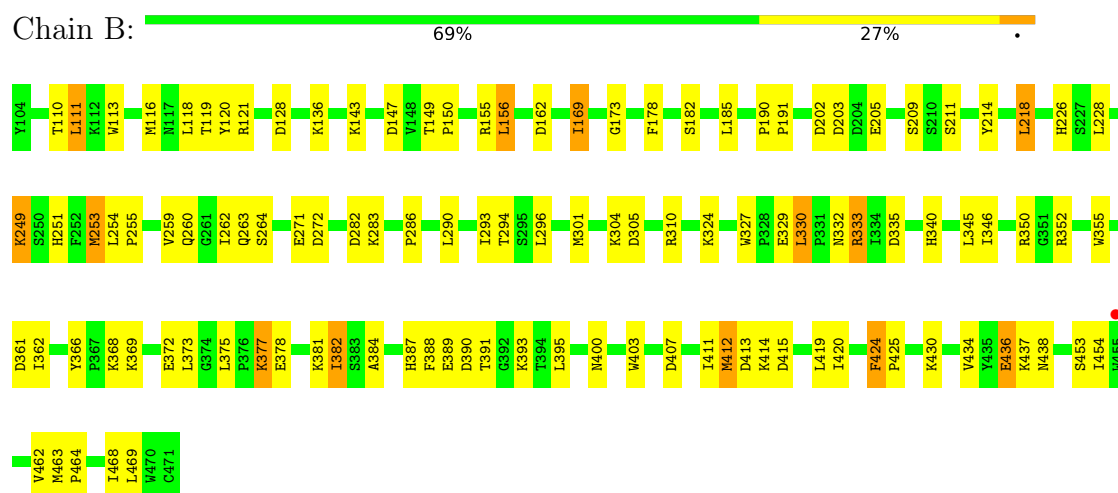
3 Residue-property plots

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 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: Collagenase 3



• Molecule 1: Collagenase 3

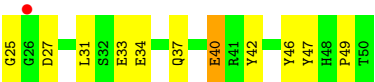


• Molecule 2: Collagenase 3, pro-domain peptide





● Molecule 2: Collagenase 3, pro-domain peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	127.08Å 156.58Å 106.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 2.85 49.34 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.34-2.85) 99.8 (49.34-2.85)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.178 , 0.247 (Not available) , 0.224	Depositor DCC
R_{free} test set	1255 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6690	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.54	0/3110	0.93	13/4225 (0.3%)
1	B	0.56	0/3115	0.91	5/4233 (0.1%)
2	C	0.55	0/225	0.97	0/302
2	D	0.54	0/238	0.90	0/320
All	All	0.55	0/6688	0.92	18/9080 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	LEU	CA-C-N	6.56	126.54	119.78
1	B	254	LEU	C-N-CA	6.56	126.54	119.78
1	A	280	THR	CB-CA-C	6.53	118.08	108.87
1	A	463	MET	N-CA-C	6.38	113.96	108.22
1	B	305	ASP	CB-CA-C	-6.18	109.47	116.63
1	A	192	GLY	CA-C-N	5.91	127.23	119.84
1	A	192	GLY	C-N-CA	5.91	127.23	119.84
1	A	274	ASN	CA-C-N	5.77	126.16	119.47
1	A	274	ASN	C-N-CA	5.77	126.16	119.47
1	B	424	PHE	CA-C-N	5.70	125.98	119.83
1	B	424	PHE	C-N-CA	5.70	125.98	119.83
1	A	312	HIS	CA-C-N	5.51	125.86	119.47
1	A	312	HIS	C-N-CA	5.51	125.86	119.47
1	A	305	ASP	CB-CA-C	-5.18	110.58	116.54
1	A	424	PHE	CA-C-N	-5.10	114.73	120.14
1	A	424	PHE	C-N-CA	-5.10	114.73	120.14
1	A	254	LEU	CA-C-N	5.08	125.01	119.78
1	A	254	LEU	C-N-CA	5.08	125.01	119.78

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	3005	0	2857	73	0
1	B	3009	0	2860	58	0
2	C	220	0	184	6	0
2	D	232	0	192	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	1	0
5	D	1	0	0	0	0
6	A	44	0	66	1	0
6	B	52	0	78	3	0
6	C	4	0	6	0	0
6	D	4	0	6	0	0
7	A	39	0	0	1	0
7	B	58	0	0	2	0
7	C	2	0	0	0	0
7	D	5	0	0	0	0
All	All	6690	0	6249	137	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 11.

All (137) 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:175:PHE:N	1:A:175:PHE:HD2	1.60	0.94
1:A:175:PHE:N	1:A:175:PHE:CD2	2.30	0.90
1:A:175:PHE:HD2	1:A:175:PHE:H	0.89	0.87
2:C:43:LEU:H	2:C:43:LEU:HD13	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:TRP:HB3	1:B:412:MET:HE2	1.63	0.81
1:B:414:LYS:HD3	1:B:415:ASP:H	1.50	0.75
1:A:299:GLU:OE1	1:A:310:ARG:HD3	1.91	0.70
1:A:448:ILE:HB	1:B:462:VAL:HG11	1.73	0.69
1:B:384:ALA:HB1	1:B:434:VAL:HG12	1.73	0.69
1:B:388:PHE:HE1	1:B:395:LEU:HD13	1.60	0.67
1:A:150:PRO:HD3	1:A:267:GLY:HA2	1.76	0.66
2:D:47[B]:TYR:HD2	2:D:49:PRO:HD3	1.62	0.65
1:A:121:ARG:NH1	1:A:159:GLY:O	2.29	0.65
1:A:286:PRO:HG2	1:B:286:PRO:O	1.98	0.62
1:B:110:THR:HB	1:B:111:LEU:HD13	1.82	0.62
1:B:116:MET:HE3	1:B:150:PRO:HB2	1.81	0.62
1:A:299:GLU:HG2	1:A:312:HIS:HA	1.82	0.61
1:B:264:SER:HA	6:B:515:EDO:H21	1.83	0.60
1:B:327:TRP:HB2	1:B:330:LEU:HD22	1.83	0.60
1:B:143:LYS:NZ	1:B:147:ASP:OD2	2.35	0.59
1:A:194:ASN:OD1	1:A:195:TYR:N	2.30	0.59
1:A:330:LEU:HD21	1:A:357:LEU:HD11	1.85	0.59
1:B:333:ARG:O	1:B:350:ARG:HD2	2.03	0.59
1:B:173:GLY:HA3	2:D:25:GLY:HA3	1.84	0.59
1:A:123:VAL:HG12	1:A:124:ASN:HD22	1.69	0.58
1:A:375:LEU:HB3	1:A:379:VAL:HG11	1.85	0.58
2:D:33:GLU:O	2:D:37:GLN:HB2	2.03	0.57
1:B:113:TRP:CE2	1:B:191:PRO:HB3	2.40	0.56
1:B:437:LYS:HG2	1:B:438:ASN:OD1	2.06	0.56
1:B:377:LYS:HD3	1:B:377:LYS:H	1.72	0.55
1:B:393:LYS:NZ	1:B:413:ASP:OD2	2.34	0.55
1:B:436:GLU:HG2	7:B:651:HOH:O	2.06	0.54
1:B:255:PRO:O	1:B:259:VAL:HG23	2.07	0.54
1:A:117:ASN:OD1	1:A:152:ASN:HB3	2.08	0.54
1:B:182:SER:OG	1:B:214:TYR:OH	2.23	0.54
1:B:393:LYS:HZ2	1:B:413:ASP:CG	2.16	0.53
1:A:451:GLU:OE1	1:A:461:ARG:NH1	2.42	0.53
1:A:263:GLN:HA	1:A:267:GLY:H	1.72	0.53
1:A:388:PHE:HE1	1:A:395:LEU:HD22	1.74	0.52
1:B:190:PRO:HG3	2:D:42:TYR:HB3	1.92	0.52
1:B:324:LYS:HE2	1:B:332:ASN:OD1	2.10	0.52
1:A:377:LYS:N	1:A:377:LYS:HE2	2.25	0.51
1:A:205:GLU:HG3	1:A:214:TYR:HD2	1.74	0.51
1:B:249:LYS:HE3	1:B:249:LYS:HA	1.93	0.51
1:A:322:LEU:O	1:A:325:SER:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLY:HA3	1:A:280:THR:HG21	1.92	0.51
1:A:176:TYR:N	1:A:176:TYR:CD1	2.77	0.51
1:A:296:LEU:HG	1:A:297:ARG:HG3	1.93	0.51
2:C:43:LEU:H	2:C:43:LEU:CD1	2.18	0.50
1:A:391:THR:HG23	1:A:393:LYS:HG3	1.94	0.50
1:A:280:THR:HB	1:A:307:PHE:CZ	2.47	0.49
1:A:354:PHE:CE1	1:A:368:LYS:HB2	2.47	0.49
1:A:249:LYS:HD2	1:A:250:SER:H	1.78	0.49
1:A:294:THR:HG23	1:A:338:TYR:HA	1.95	0.49
1:B:388:PHE:CE1	1:B:395:LEU:HD13	2.46	0.48
1:B:149:THR:HG21	1:B:262:ILE:HG13	1.94	0.48
1:B:271:GLU:CD	1:B:272:ASP:H	2.22	0.48
1:B:355:TRP:HD1	1:B:362:ILE:HD13	1.78	0.47
1:A:338:TYR:CD1	1:A:387:HIS:HB2	2.49	0.47
1:A:406:ASP:HB3	1:A:411:ILE:HD12	1.95	0.47
1:A:418:ARG:HE	1:A:423:ASP:CG	2.22	0.47
1:A:361:ASP:OD2	2:C:48:HIS:HA	2.14	0.47
1:A:440:TYR:HE1	1:A:460:VAL:HG21	1.80	0.47
1:A:235:ASP:OD1	1:A:280:THR:HG21	2.16	0.47
6:B:520:EDO:H11	7:B:641:HOH:O	2.15	0.46
1:A:175:PHE:O	1:A:177:PRO:HD3	2.16	0.46
1:A:384:ALA:HB1	1:A:434:VAL:HG12	1.97	0.46
1:A:448:ILE:HD13	1:A:463:MET:O	2.16	0.46
1:A:404:ARG:HB2	1:A:416:TYR:CZ	2.51	0.46
1:A:366:TYR:CZ	1:A:368:LYS:HE2	2.51	0.46
1:A:116:MET:SD	1:A:150:PRO:HB2	2.55	0.46
1:B:283:LYS:HB2	1:B:469:LEU:HD13	1.98	0.45
1:A:109:ARG:O	1:A:110:THR:HG22	2.16	0.45
1:B:169:ILE:HG13	1:B:203:ASP:HB3	1.98	0.45
1:B:387:HIS:ND1	1:B:407:ASP:OD1	2.50	0.45
2:D:40:GLU:O	2:D:40:GLU:HG2	2.17	0.45
1:B:290:LEU:CD1	1:B:293:ILE:HD11	2.47	0.45
1:A:306:ARG:NH1	6:A:513:EDO:H11	2.32	0.45
1:A:205:GLU:HG3	1:A:214:TYR:CD2	2.50	0.45
1:A:414:LYS:O	1:A:415:ASP:HB2	2.17	0.45
1:B:382:ILE:HD13	1:B:382:ILE:N	2.33	0.44
1:B:403:TRP:HB3	1:B:412:MET:CE	2.42	0.44
1:A:170:LYS:HB3	1:A:171:GLU:H	1.51	0.44
1:A:293:ILE:HG13	1:A:433:ALA:HB1	2.00	0.44
1:B:202:ASP:HB3	1:B:205:GLU:HG2	1.98	0.44
1:A:142:PHE:HB3	1:A:153:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLN:HG2	1:A:267:GLY:HA3	2.00	0.44
1:A:182:SER:N	1:A:205:GLU:OE1	2.49	0.43
1:A:447:PRO:HG3	1:B:464:PRO:HD3	2.00	0.43
1:B:355:TRP:CD1	1:B:362:ILE:HD13	2.54	0.43
1:A:240:MET:HG2	1:A:258:ASP:OD1	2.18	0.43
1:B:378:GLU:OE2	1:B:378:GLU:HA	2.18	0.43
1:A:439:GLY:HA3	1:A:455:TRP:NE1	2.33	0.43
1:B:119:THR:O	1:B:162:ASP:HB2	2.19	0.43
1:B:468:ILE:HG23	1:B:469:LEU:HG	2.01	0.43
1:B:400:ASN:C	1:B:420:ILE:HG13	2.43	0.43
1:B:118:LEU:HA	1:B:118:LEU:HD23	1.73	0.43
1:B:290:LEU:HD13	1:B:293:ILE:HD11	2.00	0.43
1:B:301:MET:HE3	1:B:301:MET:HB3	1.70	0.43
1:A:120:TYR:CZ	1:A:155:ARG:HB2	2.54	0.42
1:A:280:THR:HA	1:A:281:PRO:HD3	1.91	0.42
1:A:342:SER:HB3	1:A:389:GLU:OE1	2.18	0.42
1:A:112:LYS:HG3	1:A:266:TYR:CE1	2.55	0.42
1:B:366:TYR:CE2	1:B:368:LYS:HE3	2.54	0.42
1:A:187:HIS:HA	5:C:101:CL:CL	2.56	0.42
1:A:212:LYS:HD3	1:A:213:GLY:H	1.84	0.42
1:A:404:ARG:HD2	1:A:413:ASP:OD2	2.19	0.42
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.96	0.42
2:C:29:ASP:O	2:C:32:SER:OG	2.25	0.42
2:C:47:TYR:HB3	2:C:48:HIS:ND1	2.34	0.42
1:A:125:TYR:CD2	1:A:131:HIS:HA	2.55	0.42
1:A:327:TRP:CB	1:A:330:LEU:HD22	2.50	0.42
1:A:156:LEU:HD12	1:A:161:ALA:HB2	2.02	0.42
1:A:335:ASP:HB3	1:A:382:ILE:O	2.20	0.42
2:C:35:ASP:OD1	2:C:35:ASP:N	2.53	0.41
1:B:335:ASP:OD1	1:B:350:ARG:NH2	2.53	0.41
1:A:338:TYR:HB2	7:A:635:HOH:O	2.20	0.41
1:B:119:THR:HB	1:B:156:LEU:HD22	2.02	0.41
1:A:111:LEU:HD13	1:A:190:PRO:HB2	2.03	0.41
1:A:195:TYR:HD1	1:A:195:TYR:HA	1.79	0.41
1:A:274:ASN:HA	1:A:275:PRO:HD3	1.85	0.41
1:A:357:LEU:HD23	1:A:362:ILE:HA	2.02	0.41
1:B:253:MET:HE2	1:B:253:MET:HB3	1.69	0.41
1:B:120:TYR:CE1	1:B:155:ARG:HG3	2.56	0.41
1:B:121:ARG:HG3	1:B:156:LEU:O	2.19	0.41
1:A:215:ASN:HB3	1:A:218:LEU:HB2	2.01	0.41
1:A:312:HIS:CG	1:A:313:PRO:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ASP:OD1	6:B:509:EDO:H22	2.21	0.41
1:B:411:ILE:HG13	1:B:412:MET:O	2.21	0.41
1:A:179:ASP:OD2	1:A:184:LEU:N	2.49	0.41
1:B:178:PHE:HB3	1:B:202:ASP:OD2	2.22	0.40
1:B:259:VAL:O	1:B:263:GLN:HG3	2.21	0.40
1:B:190:PRO:HA	1:B:226:HIS:O	2.22	0.40
1:B:228:LEU:HA	1:B:228:LEU:HD23	1.84	0.40
1:A:276:LYS:H	1:A:276:LYS:HG2	1.39	0.40
1:A:188:ALA:HB3	1:A:226:HIS:HB2	2.04	0.40
1:B:424:PHE:HA	1:B:425:PRO:HD2	1.85	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	A	367/368 (100%)	335 (91%)	28 (8%)	4 (1%)	11	23
1	B	367/368 (100%)	344 (94%)	23 (6%)	0	100	100
2	C	24/26 (92%)	19 (79%)	5 (21%)	0	100	100
2	D	25/26 (96%)	23 (92%)	2 (8%)	0	100	100
All	All	783/788 (99%)	721 (92%)	58 (7%)	4 (0%)	24	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	182	SER
1	A	376	PRO
1	A	341	PRO

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	323/322 (100%)	282 (87%)	41 (13%)	4	8
1	B	323/322 (100%)	281 (87%)	42 (13%)	4	8
2	C	23/23 (100%)	15 (65%)	8 (35%)	0	0
2	D	24/23 (104%)	19 (79%)	5 (21%)	1	1
All	All	693/690 (100%)	597 (86%)	96 (14%)	3	7

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	124	ASN
1	A	130	THR
1	A	154	THR
1	A	157	HIS
1	A	175	PHE
1	A	195	TYR
1	A	205	GLU
1	A	208	THR
1	A	209	SER
1	A	212	LYS
1	A	218	LEU
1	A	247	THR
1	A	249	LYS
1	A	250	SER
1	A	251	HIS
1	A	276	LYS
1	A	280	THR
1	A	283	LYS
1	A	294	THR
1	A	304	LYS
1	A	316	VAL
1	A	330	LEU
1	A	340	HIS

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Mol	Chain	Res	Type
1	A	346	ILE
1	A	362	ILE
1	A	373	LEU
1	A	377	LYS
1	A	379	VAL
1	A	380	LYS
1	A	381	LYS
1	A	386	VAL
1	A	395	LEU
1	A	404	ARG
1	A	407	ASP
1	A	411	ILE
1	A	419	LEU
1	A	430	LYS
1	A	448	ILE
1	A	456	SER
1	A	462	VAL
1	B	111	LEU
1	B	136	LYS
1	B	156	LEU
1	B	169	ILE
1	B	185	LEU
1	B	209	SER
1	B	211	SER
1	B	218	LEU
1	B	249	LYS
1	B	251	HIS
1	B	253	MET
1	B	260	GLN
1	B	282	ASP
1	B	294	THR
1	B	296	LEU
1	B	304	LYS
1	B	310	ARG
1	B	329	GLU
1	B	330	LEU
1	B	333	ARG
1	B	340	HIS
1	B	345	LEU
1	B	346	ILE
1	B	352	ARG
1	B	361	ASP

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Mol	Chain	Res	Type
1	B	369	LYS
1	B	372	GLU
1	B	373	LEU
1	B	375	LEU
1	B	377	LYS
1	B	381	LYS
1	B	382	ILE
1	B	389	GLU
1	B	390	ASP
1	B	391	THR
1	B	412	MET
1	B	419	LEU
1	B	430	LYS
1	B	436	GLU
1	B	453	SER
1	B	454	ILE
1	B	463	MET
2	C	33	GLU
2	C	37	GLN
2	C	43	LEU
2	C	44	ARG
2	C	46	TYR
2	C	47	TYR
2	C	48	HIS
2	C	50	THR
2	D	27	ASP
2	D	31	LEU
2	D	34	GLU
2	D	40	GLU
2	D	46	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	401	GLN
1	A	409	ASN
1	A	438	ASN
1	B	157	HIS
1	B	274	ASN
1	B	314	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 16 are monoatomic - leaving 26 for Mogul analysis.

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	$\# Z > 2$
6	EDO	B	516	-	3,3,3	0.44	0	2,2,2	0.51	0
6	EDO	B	508	-	3,3,3	0.55	0	2,2,2	0.43	0
6	EDO	B	520	-	3,3,3	0.46	0	2,2,2	0.78	0
6	EDO	B	510	-	3,3,3	0.42	0	2,2,2	0.58	0
6	EDO	C	102	-	3,3,3	0.56	0	2,2,2	0.07	0
6	EDO	B	517	-	3,3,3	0.53	0	2,2,2	0.13	0
6	EDO	B	514	-	3,3,3	0.52	0	2,2,2	0.31	0
6	EDO	A	510	-	3,3,3	0.40	0	2,2,2	0.46	0
6	EDO	B	518	-	3,3,3	0.47	0	2,2,2	0.43	0
6	EDO	A	516	-	3,3,3	0.41	0	2,2,2	0.50	0
6	EDO	A	518	-	3,3,3	0.49	0	2,2,2	0.25	0
6	EDO	A	508	-	3,3,3	0.52	0	2,2,2	0.44	0
6	EDO	A	515	-	3,3,3	0.39	0	2,2,2	0.66	0
6	EDO	B	519	-	3,3,3	0.46	0	2,2,2	0.32	0
6	EDO	D	102	-	3,3,3	0.51	0	2,2,2	0.29	0
6	EDO	B	515	-	3,3,3	0.56	0	2,2,2	0.13	0
6	EDO	A	509	-	3,3,3	0.46	0	2,2,2	0.47	0
6	EDO	A	514	-	3,3,3	0.55	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	B	512	-	3,3,3	0.48	0	2,2,2	0.38	0
6	EDO	B	509	-	3,3,3	0.31	0	2,2,2	0.71	0
6	EDO	A	517	-	3,3,3	0.38	0	2,2,2	0.52	0
6	EDO	A	512	-	3,3,3	0.46	0	2,2,2	0.30	0
6	EDO	B	513	-	3,3,3	0.39	0	2,2,2	0.53	0
6	EDO	B	511	-	3,3,3	0.60	0	2,2,2	0.04	0
6	EDO	A	513	-	3,3,3	0.42	0	2,2,2	0.49	0
6	EDO	A	511	-	3,3,3	0.50	0	2,2,2	0.28	0

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
6	EDO	B	516	-	-	1/1/1/1	-
6	EDO	B	508	-	-	0/1/1/1	-
6	EDO	B	520	-	-	0/1/1/1	-
6	EDO	B	510	-	-	1/1/1/1	-
6	EDO	C	102	-	-	0/1/1/1	-
6	EDO	B	517	-	-	1/1/1/1	-
6	EDO	B	514	-	-	1/1/1/1	-
6	EDO	A	510	-	-	1/1/1/1	-
6	EDO	B	518	-	-	1/1/1/1	-
6	EDO	A	516	-	-	0/1/1/1	-
6	EDO	A	518	-	-	0/1/1/1	-
6	EDO	A	508	-	-	0/1/1/1	-
6	EDO	A	515	-	-	1/1/1/1	-
6	EDO	B	519	-	-	0/1/1/1	-
6	EDO	D	102	-	-	0/1/1/1	-
6	EDO	B	515	-	-	0/1/1/1	-
6	EDO	A	509	-	-	1/1/1/1	-
6	EDO	A	514	-	-	0/1/1/1	-
6	EDO	B	512	-	-	1/1/1/1	-
6	EDO	B	509	-	-	0/1/1/1	-
6	EDO	A	517	-	-	0/1/1/1	-
6	EDO	A	512	-	-	0/1/1/1	-
6	EDO	B	513	-	-	0/1/1/1	-
6	EDO	B	511	-	-	0/1/1/1	-
6	EDO	A	513	-	-	0/1/1/1	-
6	EDO	A	511	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	509	EDO	O1-C1-C2-O2
6	A	511	EDO	O1-C1-C2-O2
6	B	512	EDO	O1-C1-C2-O2
6	B	518	EDO	O1-C1-C2-O2
6	B	510	EDO	O1-C1-C2-O2
6	B	514	EDO	O1-C1-C2-O2
6	B	516	EDO	O1-C1-C2-O2
6	B	517	EDO	O1-C1-C2-O2
6	A	515	EDO	O1-C1-C2-O2
6	A	510	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	520	EDO	1	0
6	B	515	EDO	1	0
6	B	509	EDO	1	0
6	A	513	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	368/368 (100%)	-0.52	2 (0%) 87 85	9, 27, 50, 67	1 (0%)
1	B	368/368 (100%)	-0.54	1 (0%) 90 89	9, 21, 57, 78	1 (0%)
2	C	26/26 (100%)	1.44	9 (34%) 1 0	19, 85, 111, 118	0
2	D	26/26 (100%)	0.13	1 (3%) 44 35	10, 47, 82, 89	1 (3%)
All	All	788/788 (100%)	-0.45	13 (1%) 70 64	9, 26, 60, 118	3 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	455[A]	TRP	3.9
2	C	47	TYR	3.9
2	C	46	TYR	3.5
1	A	343[A]	HIS	3.1
2	C	49	PRO	3.1
2	C	48	HIS	2.9
2	C	50	THR	2.9
2	C	31	LEU	2.8
1	A	175	PHE	2.4
2	D	26	GLY	2.3
2	C	25	GLY	2.2
2	C	26	GLY	2.1
2	C	28	GLU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
6	EDO	C	102	4/4	0.75	0.20	48,65,67,69	0
6	EDO	B	518	4/4	0.81	0.12	27,31,34,35	0
6	EDO	A	517	4/4	0.83	0.12	40,40,40,41	0
6	EDO	A	512	4/4	0.85	0.15	39,53,61,63	0
6	EDO	A	509	4/4	0.85	0.14	22,28,43,53	0
6	EDO	B	520	4/4	0.86	0.11	21,29,40,42	0
6	EDO	A	508	4/4	0.87	0.13	17,20,30,33	0
6	EDO	A	514	4/4	0.87	0.15	35,39,40,44	0
6	EDO	B	517	4/4	0.88	0.15	38,48,50,50	0
6	EDO	B	508	4/4	0.88	0.13	31,33,34,44	0
6	EDO	B	513	4/4	0.89	0.11	28,32,32,38	0
6	EDO	B	515	4/4	0.89	0.15	28,30,37,38	0
6	EDO	B	510	4/4	0.90	0.12	22,30,30,33	0
6	EDO	B	516	4/4	0.90	0.09	24,29,30,35	0
6	EDO	B	509	4/4	0.90	0.12	23,25,28,34	0
6	EDO	A	516	4/4	0.91	0.08	26,32,40,40	0
6	EDO	A	515	4/4	0.91	0.10	26,32,33,37	0
6	EDO	A	518	4/4	0.92	0.11	33,41,42,54	0
6	EDO	D	102	4/4	0.93	0.11	33,33,41,42	0
6	EDO	B	514	4/4	0.94	0.07	16,17,31,33	0
6	EDO	A	511	4/4	0.94	0.09	31,32,36,38	0
6	EDO	B	511	4/4	0.95	0.13	17,20,23,24	0
6	EDO	A	513	4/4	0.95	0.08	34,38,41,42	0
6	EDO	A	510	4/4	0.96	0.08	22,32,39,48	0
5	CL	C	101	1/1	0.97	0.11	25,25,25,25	0
6	EDO	B	512	4/4	0.97	0.07	28,29,34,40	0
6	EDO	B	519	4/4	0.97	0.07	23,27,30,38	0
5	CL	D	101	1/1	0.98	0.05	27,27,27,27	0
4	CA	B	506	1/1	0.98	0.13	41,41,41,41	0
4	CA	A	506	1/1	0.98	0.08	42,42,42,42	0
4	CA	A	505	1/1	0.99	0.02	15,15,15,15	0
3	ZN	A	502	1/1	0.99	0.01	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	B	503	1/1	0.99	0.01	17,17,17,17	0
4	CA	B	504	1/1	0.99	0.03	32,32,32,32	0
4	CA	B	505	1/1	0.99	0.02	16,16,16,16	0
4	CA	A	503	1/1	0.99	0.02	33,33,33,33	0
5	CL	A	507	1/1	0.99	0.02	16,16,16,16	0
5	CL	B	507	1/1	0.99	0.03	19,19,19,19	0
4	CA	A	504	1/1	0.99	0.04	50,50,50,50	0
3	ZN	B	502	1/1	1.00	0.02	14,14,14,14	0
3	ZN	A	501	1/1	1.00	0.01	17,17,17,17	0
3	ZN	B	501	1/1	1.00	0.03	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.