Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 02:44 AM EDT

PDB ID	:	4FU4
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

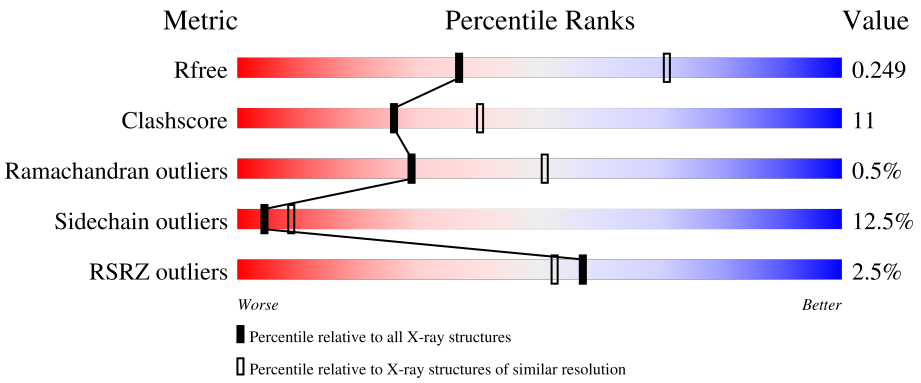
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (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 <=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	65% 29% 6%
1	B	368	% 72% 26% •
2	C	26	50% 62% 27% 12%
2	D	26	15% 58% 35% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	C	102	-	-	-	X

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
			Total	C	N	O	S			
1	A	368	3005	1951	495	549	10	0	1	0
1	B	368	3009	1956	494	549	10	0	1	0

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
			Total	C	N	O			
2	C	26	220	135	35	50	0	0	0
2	D	26	232	144	36	52	0	1	0

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

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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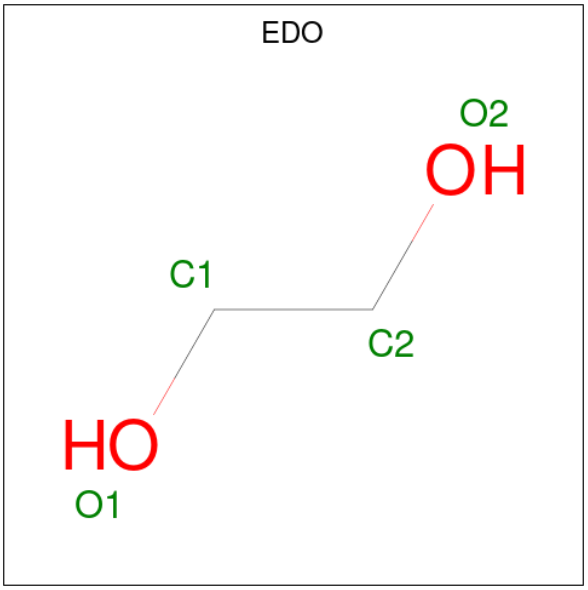
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	B	4	4	4	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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

- Molecule 7 is water.

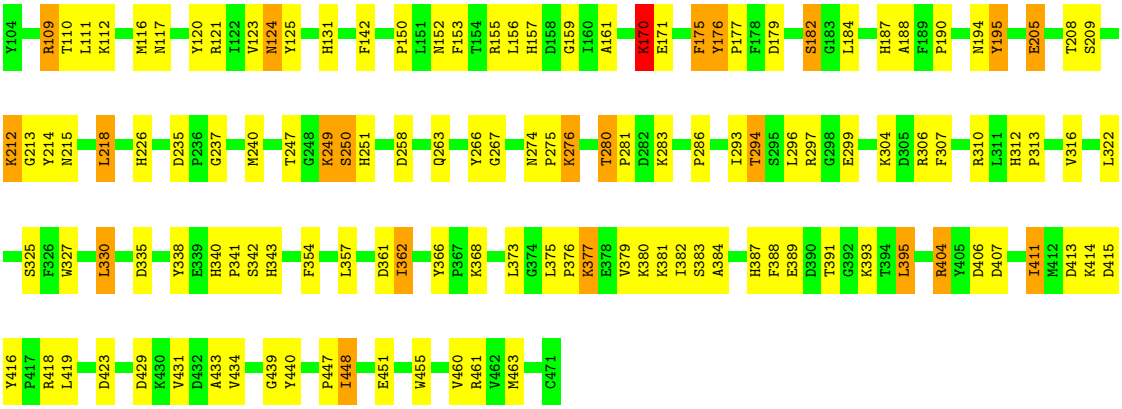
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	39	39	39	0	0
			Total	O		
7	B	58	58	58	0	0
			Total	O		
7	C	2	2	2	0	0
			Total	O		
7	D	5	5	5	0	0

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.

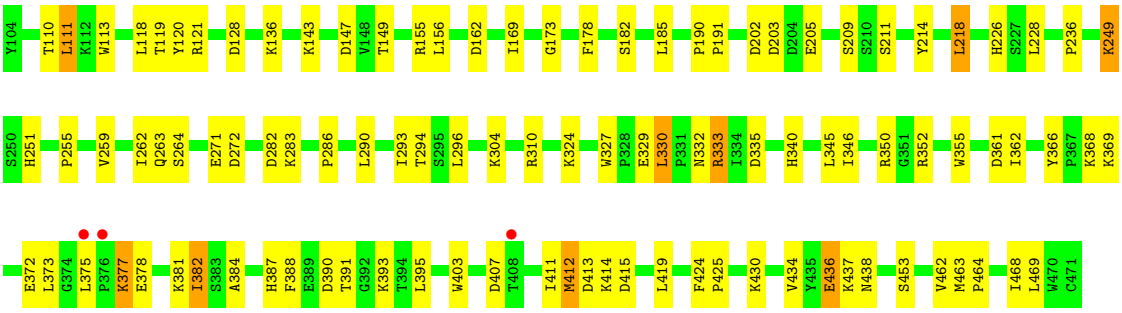
• Molecule 1: Collagenase 3

Chain A:



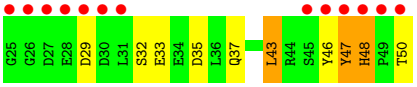
• Molecule 1: Collagenase 3

Chain B:



• Molecule 2: Collagenase 3, pro-domain peptide

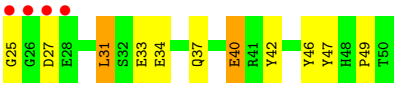
Chain C:



• Molecule 2: Collagenase 3, pro-domain peptide

Chain D:

15%
58%
35%
8%


G25
G26
D27
E28
L31
S32
E33
E34
Q37
E40
R41
Y42
Y46
Y47
H48
P49
T50

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.95 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.178 , 0.247 0.182 , 0.249	Depositor DCC
R_{free} test set	1255 reflections (5.00%)	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)	0.33 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, 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	0.44	0/3110	0.61	0/4225
1	B	0.45	0/3115	0.62	0/4233
2	C	0.44	0/225	0.66	0/302
2	D	0.47	0/238	0.75	1/320 (0.3%)
All	All	0.44	0/6688	0.62	1/9080 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	31	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3005	0	2857	75	0
1	B	3009	0	2860	54	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	135	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 (135) 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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:143:LYS:NZ	1:B:147:ASP:OD2	2.35	0.56
1:B:437:LYS:HG2	1:B:438:ASN:OD1	2.06	0.56
1:B:393:LYS:NZ	1:B:413:ASP:OD2	2.34	0.56
1:B:377:LYS:HD3	1:B:377:LYS:H	1.72	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: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
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:B:403:TRP:HB3	1:B:412:MET:CE	2.42	0.49
1:B:182:SER:OG	1:B:214:TYR:OH	2.23	0.49
1:A:354:PHE:CE1	1:A:368:LYS:HB2	2.47	0.49
1:B:403:TRP:HB3	1:B:412:MET:HE2	1.94	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:A:383:SER:OG	1:A:431:VAL:O	2.28	0.48
1:A:393:LYS:NZ	1:A:413:ASP:OD2	2.46	0.47
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:B:143:LYS:HZ2	1:B:147:ASP:CG	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASP:HB3	1:A:411:ILE:HD12	1.95	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: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
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:271:GLU:CD	1:B:272:ASP:H	2.22	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: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: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:418:ARG:HE	1:A:423:ASP:CG	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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 (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	367/368 (100%)	335 (91%)	28 (8%)	4 (1%)	14	30
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%)	29	51

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/322 (100%)	285 (88%)	38 (12%)	5	10
1	B	323/322 (100%)	286 (88%)	37 (12%)	5	11
2	C	23/23 (100%)	16 (70%)	7 (30%)	0	0
2	D	24/23 (104%)	19 (79%)	5 (21%)	1	1
All	All	693/690 (100%)	606 (87%)	87 (13%)	4	8

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	124	ASN
1	A	157	HIS
1	A	170	LYS
1	A	175	PHE
1	A	176	TYR
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
1	A	343[A]	HIS
1	A	343[B]	HIS
1	A	362	ILE
1	A	373	LEU
1	A	377	LYS
1	A	380	LYS
1	A	381	LYS
1	A	395	LEU
1	A	404	ARG
1	A	407	ASP
1	A	411	ILE
1	A	419	LEU
1	A	429	ASP
1	A	448	ILE
1	B	111	LEU
1	B	136	LYS
1	B	185	LEU
1	B	209	SER

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Mol	Chain	Res	Type
1	B	211	SER
1	B	218	LEU
1	B	236	PRO
1	B	249	LYS
1	B	251	HIS
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
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	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	463	MET
2	C	33	GLU
2	C	37	GLN
2	C	43	LEU
2	C	46	TYR
2	C	47	TYR
2	C	48	HIS
2	C	50	THR
2	D	27	ASP
2	D	31	LEU

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Mol	Chain	Res	Type
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	509	-	3,3,3	0.33	0	2,2,2	0.69	0
6	EDO	A	512	-	3,3,3	0.50	0	2,2,2	0.26	0
6	EDO	A	518	-	3,3,3	0.53	0	2,2,2	0.20	0
6	EDO	B	510	-	3,3,3	0.45	0	2,2,2	0.55	0
6	EDO	A	513	-	3,3,3	0.45	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	B	516	-	3,3,3	0.47	0	2,2,2	0.48	0
6	EDO	B	517	-	3,3,3	0.57	0	2,2,2	0.07	0
6	EDO	B	518	-	3,3,3	0.50	0	2,2,2	0.39	0
6	EDO	C	102	-	3,3,3	0.59	0	2,2,2	0.07	0
6	EDO	B	511	-	3,3,3	0.63	0	2,2,2	0.03	0
6	EDO	B	519	-	3,3,3	0.49	0	2,2,2	0.28	0
6	EDO	A	510	-	3,3,3	0.43	0	2,2,2	0.43	0
6	EDO	B	508	-	3,3,3	0.59	0	2,2,2	0.43	0
6	EDO	A	515	-	3,3,3	0.42	0	2,2,2	0.64	0
6	EDO	B	514	-	3,3,3	0.55	0	2,2,2	0.27	0
6	EDO	A	511	-	3,3,3	0.54	0	2,2,2	0.23	0
6	EDO	B	512	-	3,3,3	0.51	0	2,2,2	0.34	0
6	EDO	A	517	-	3,3,3	0.41	0	2,2,2	0.49	0
6	EDO	A	509	-	3,3,3	0.49	0	2,2,2	0.44	0
6	EDO	B	515	-	3,3,3	0.59	0	2,2,2	0.08	0
6	EDO	B	520	-	3,3,3	0.49	0	2,2,2	0.80	0
6	EDO	A	508	-	3,3,3	0.55	0	2,2,2	0.43	0
6	EDO	B	513	-	3,3,3	0.41	0	2,2,2	0.49	0
6	EDO	A	514	-	3,3,3	0.59	0	2,2,2	0.12	0
6	EDO	A	516	-	3,3,3	0.44	0	2,2,2	0.47	0
6	EDO	D	102	-	3,3,3	0.54	0	2,2,2	0.24	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	509	-	-	0/1/1/1	-
6	EDO	A	512	-	-	0/1/1/1	-
6	EDO	A	518	-	-	0/1/1/1	-
6	EDO	B	510	-	-	1/1/1/1	-
6	EDO	A	513	-	-	0/1/1/1	-
6	EDO	B	516	-	-	1/1/1/1	-
6	EDO	B	517	-	-	1/1/1/1	-
6	EDO	B	518	-	-	1/1/1/1	-
6	EDO	C	102	-	-	0/1/1/1	-
6	EDO	B	511	-	-	0/1/1/1	-
6	EDO	B	519	-	-	0/1/1/1	-
6	EDO	A	510	-	-	0/1/1/1	-
6	EDO	B	508	-	-	0/1/1/1	-
6	EDO	A	515	-	-	1/1/1/1	-
6	EDO	B	514	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	511	-	-	1/1/1/1	-
6	EDO	B	512	-	-	1/1/1/1	-
6	EDO	A	517	-	-	0/1/1/1	-
6	EDO	A	509	-	-	1/1/1/1	-
6	EDO	B	515	-	-	0/1/1/1	-
6	EDO	B	520	-	-	0/1/1/1	-
6	EDO	A	508	-	-	0/1/1/1	-
6	EDO	B	513	-	-	0/1/1/1	-
6	EDO	A	514	-	-	0/1/1/1	-
6	EDO	A	516	-	-	0/1/1/1	-
6	EDO	D	102	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	509	EDO	O1-C1-C2-O2
6	B	518	EDO	O1-C1-C2-O2
6	A	511	EDO	O1-C1-C2-O2
6	B	512	EDO	O1-C1-C2-O2
6	B	510	EDO	O1-C1-C2-O2
6	B	514	EDO	O1-C1-C2-O2
6	B	517	EDO	O1-C1-C2-O2
6	B	516	EDO	O1-C1-C2-O2
6	A	515	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	509	EDO	1	0
6	A	513	EDO	1	0
6	B	515	EDO	1	0
6	B	520	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 (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	368/368 (100%)	-0.46	0 100 100	9, 27, 50, 67	0
1	B	368/368 (100%)	-0.36	3 (0%) 86 85	9, 22, 57, 78	0
2	C	26/26 (100%)	2.45	13 (50%) 0 0	19, 85, 111, 118	0
2	D	26/26 (100%)	0.29	4 (15%) 2 1	15, 47, 82, 89	0
All	All	788/788 (100%)	-0.29	20 (2%) 57 52	9, 26, 60, 118	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	47	TYR	7.1
2	C	25	GLY	6.3
2	C	49	PRO	5.9
2	C	27	ASP	5.7
2	C	48	HIS	5.7
2	C	46	TYR	5.5
2	C	28	GLU	4.6
2	C	50	THR	4.5
2	C	29	ASP	4.3
2	C	30	ASP	4.1
2	C	31	LEU	3.3
2	C	26	GLY	3.2
2	D	25	GLY	2.9
1	B	375	LEU	2.7
2	C	45	SER	2.6
2	D	27	ASP	2.6
1	B	408	THR	2.5
2	D	26	GLY	2.5
1	B	376	PRO	2.2
2	D	28	GLU	2.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	C	102	4/4	0.60	0.42	48,65,67,69	0
6	EDO	B	508	4/4	0.76	0.29	31,33,34,44	0
6	EDO	B	515	4/4	0.88	0.41	28,30,37,38	0
6	EDO	A	511	4/4	0.90	0.17	31,32,36,38	0
6	EDO	B	517	4/4	0.90	0.31	38,48,50,50	0
6	EDO	B	518	4/4	0.90	0.16	27,31,34,35	0
6	EDO	A	508	4/4	0.90	0.21	17,20,30,33	0
6	EDO	A	509	4/4	0.91	0.22	22,28,43,53	0
6	EDO	B	513	4/4	0.91	0.27	28,32,32,38	0
6	EDO	A	512	4/4	0.91	0.27	39,53,61,63	0
6	EDO	A	513	4/4	0.91	0.20	34,38,41,42	0
6	EDO	A	514	4/4	0.91	0.18	35,39,40,44	0
6	EDO	B	520	4/4	0.91	0.21	21,29,40,42	0
6	EDO	A	518	4/4	0.91	0.18	33,41,42,54	0
6	EDO	B	511	4/4	0.93	0.18	17,20,23,24	0
6	EDO	B	512	4/4	0.93	0.21	28,29,34,40	0
6	EDO	B	516	4/4	0.94	0.28	24,29,30,35	0
6	EDO	B	510	4/4	0.95	0.32	22,30,30,33	0
6	EDO	B	514	4/4	0.95	0.13	16,17,31,33	0
6	EDO	B	519	4/4	0.95	0.16	23,27,30,38	0
4	CA	B	504	1/1	0.95	0.07	32,32,32,32	0
6	EDO	A	517	4/4	0.95	0.13	40,40,40,41	0
6	EDO	D	102	4/4	0.95	0.24	33,33,41,42	0
6	EDO	A	515	4/4	0.96	0.16	26,32,33,37	0
6	EDO	A	516	4/4	0.96	0.21	26,32,40,40	0
6	EDO	B	509	4/4	0.96	0.18	23,25,28,34	0
5	CL	D	101	1/1	0.96	0.11	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	510	4/4	0.97	0.19	22,32,39,48	0
4	CA	A	506	1/1	0.97	0.09	42,42,42,42	0
4	CA	A	504	1/1	0.97	0.06	50,50,50,50	0
5	CL	C	101	1/1	0.97	0.13	25,25,25,25	0
4	CA	B	505	1/1	0.98	0.10	16,16,16,16	0
4	CA	B	506	1/1	0.98	0.15	41,41,41,41	0
4	CA	A	503	1/1	0.98	0.10	33,33,33,33	0
5	CL	A	507	1/1	0.99	0.10	16,16,16,16	0
5	CL	B	507	1/1	0.99	0.08	19,19,19,19	0
4	CA	B	503	1/1	0.99	0.12	17,17,17,17	0
3	ZN	A	502	1/1	0.99	0.09	36,36,36,36	0
4	CA	A	505	1/1	0.99	0.12	15,15,15,15	0
3	ZN	A	501	1/1	0.99	0.08	17,17,17,17	0
3	ZN	B	501	1/1	1.00	0.11	12,12,12,12	0
3	ZN	B	502	1/1	1.00	0.11	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.