



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:41 AM UTC

PDB ID : 1M72 / pdb_00001m72
Title : Crystal Structure of Caspase-1 from Spodoptera frugiperda
Authors : Forsyth, C.M.; Lemongello, D.; Friesen, P.D.; Fisher, A.J.
Deposited on : 2002-07-18
Resolution : 2.30 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

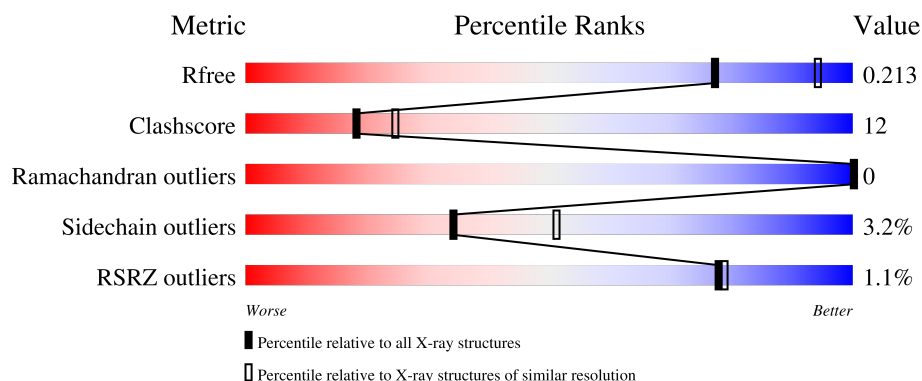
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	272	
1	B	272	
1	C	272	
2	D	6	
2	E	6	

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Mol	Chain	Length	Quality of chain
2	F	6	 67% 33%

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
3	EDO	B	503	-	-	X	-
3	EDO	C	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6433 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 Caspase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1974	1260	341	358	15			
1	B	248	Total	C	N	O	S	0	0	0
			1985	1267	343	360	15			
1	C	252	Total	C	N	O	S	0	0	0
			2016	1286	350	365	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	LEU	-	cloning artifact	UNP P89116
B	300	LEU	-	cloning artifact	UNP P89116
C	300	LEU	-	cloning artifact	UNP P89116

- Molecule 2 is a protein called Ace-Asp-Glu-Val-Asp-chloromethylketone.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	6	Total	C	N	O	0	0	1
			36	21	4	11			
2	E	6	Total	C	N	O	0	0	1
			36	21	4	11			
2	F	6	Total	C	N	O	0	0	1
			36	21	4	11			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	102	Total O 102 102	0	0
4	D	1	Total O 1 1	0	0
4	B	92	Total O 92 92	0	0
4	E	4	Total O 4 4	0	0

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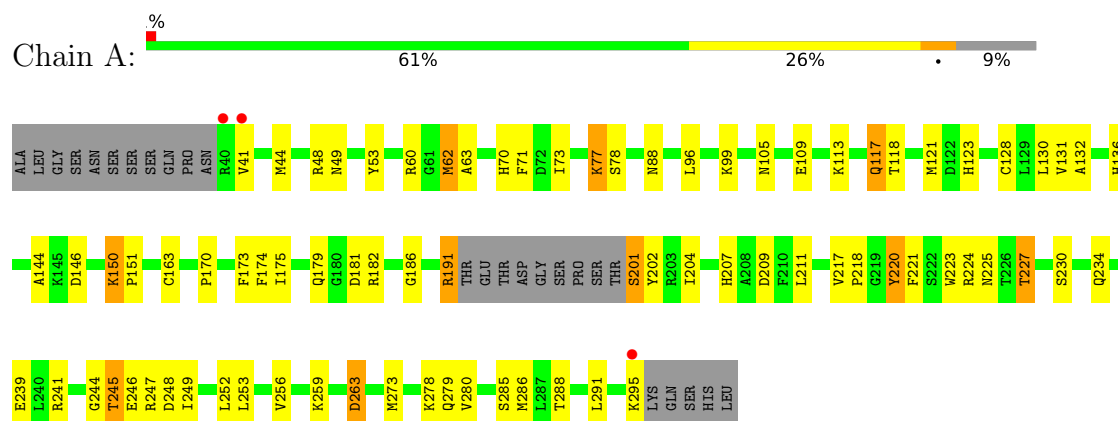
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	116	Total 116	O 116	0	0
4	F	3	Total 3	O 3	0	0

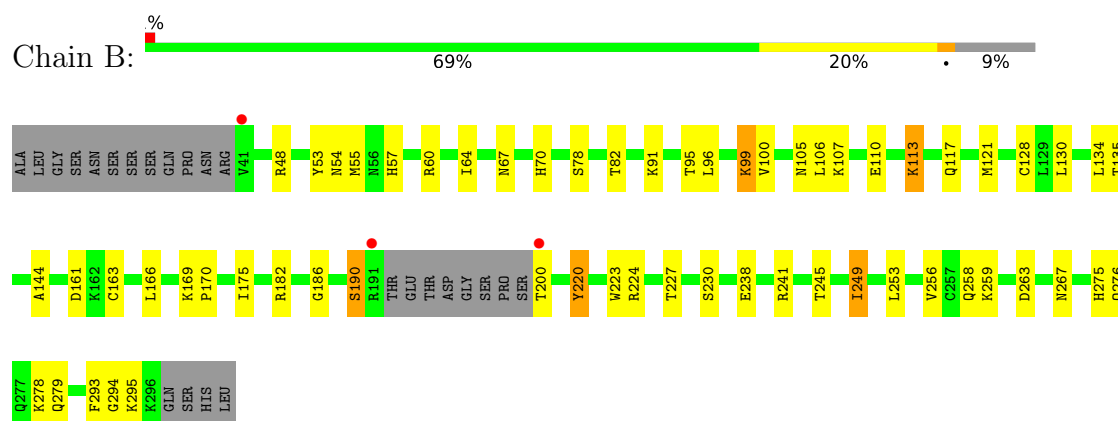
3 Residue-property plots [i](#)

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.

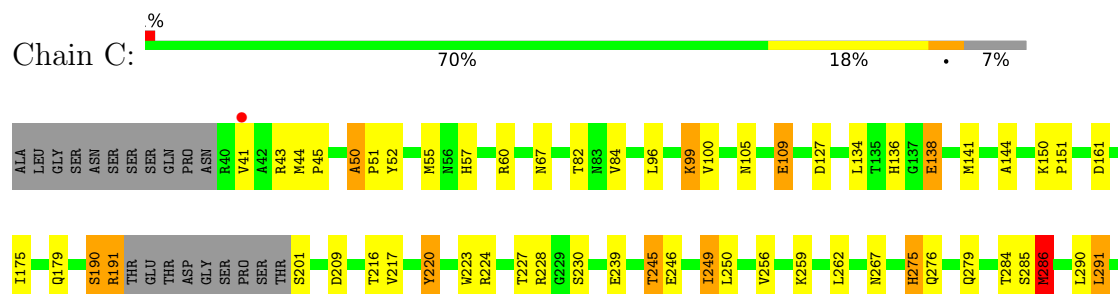
• Molecule 1: Caspase-1



• Molecule 1: Caspase-1



• Molecule 1: Caspase-1





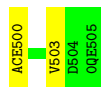
- Molecule 2: Ace-Asp-Glu-Val-Asp-chloromethylketone

Chain D:
67% 33%



- Molecule 2: Ace-Asp-Glu-Val-Asp-chloromethylketone

Chain E:
67% 33%



- Molecule 2: Ace-Asp-Glu-Val-Asp-chloromethylketone

Chain F:
67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.73Å 151.73Å 79.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.30) 97.6 (30.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.183 , 0.232 (Not available) , 0.213	Depositor DCC
R_{free} test set	2190 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6433	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: EDO, ACE, OQE

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	0.89	1/2022 (0.0%)	1.22	22/2735 (0.8%)
1	B	0.92	1/2033 (0.0%)	1.14	15/2749 (0.5%)
1	C	0.97	2/2065 (0.1%)	1.20	19/2792 (0.7%)
2	D	2.11	1/32 (3.1%)	0.76	0/43
2	E	2.10	1/32 (3.1%)	1.08	1/43 (2.3%)
2	F	2.25	1/32 (3.1%)	0.94	0/43
All	All	0.96	7/6216 (0.1%)	1.19	57/8405 (0.7%)

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	B	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	ACE	C-N	11.83	1.57	1.33
2	E	500	ACE	C-N	11.14	1.55	1.33
2	D	500	ACE	C-N	10.66	1.54	1.33
1	C	286	MET	SD-CE	-7.80	1.60	1.79
1	B	249	ILE	CA-CB	6.03	1.61	1.54
1	A	62	MET	SD-CE	-5.15	1.66	1.79
1	C	217	VAL	CA-C	5.14	1.58	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	TYR	N-CA-C	8.28	123.12	109.95
1	A	256	VAL	N-CA-C	-7.95	103.06	110.53
1	B	105	ASN	N-CA-C	7.39	121.59	111.39
1	C	209	ASP	N-CA-C	7.08	121.22	112.58
1	A	105	ASN	N-CA-C	7.07	121.14	111.39
1	C	100	VAL	N-CA-C	7.05	118.73	108.58
1	A	41	VAL	N-CA-C	6.88	118.03	108.12
1	A	179	GLN	N-CA-C	-6.72	103.67	112.41
1	B	190	SER	N-CA-C	6.64	119.82	109.52
1	C	246	GLU	N-CA-C	6.61	122.01	113.88
1	C	50	ALA	CA-C-N	6.61	126.20	119.19
1	C	50	ALA	C-N-CA	6.61	126.20	119.19
1	A	249	ILE	N-CA-C	6.53	118.06	110.62
1	B	166	LEU	N-CA-C	-6.45	103.84	112.94
1	C	220	TYR	N-CA-C	6.38	120.03	110.14
1	B	99	LYS	N-CA-C	-6.38	98.14	108.41
1	C	144	ALA	N-CA-C	-6.32	100.07	109.86
1	A	99	LYS	N-CA-C	-6.17	98.48	108.41
1	A	144	ALA	N-CA-C	-6.05	100.47	109.86
1	B	220	TYR	N-CA-C	5.97	119.67	110.42
1	C	84	VAL	N-CA-C	-5.97	104.69	110.42
1	A	150	LYS	CA-C-N	5.95	126.10	119.32
1	A	150	LYS	C-N-CA	5.95	126.10	119.32
1	A	163	CYS	CA-C-N	5.94	126.36	119.47
1	A	163	CYS	C-N-CA	5.94	126.36	119.47
1	B	100	VAL	N-CA-C	5.93	117.12	108.58
1	A	49	ASN	N-CA-C	5.84	119.38	112.72
1	C	105	ASN	N-CA-C	5.79	119.38	111.39
1	C	138	GLU	N-CA-C	-5.70	100.83	108.86
1	C	190	SER	N-CA-C	5.69	118.49	109.50
1	C	249	ILE	N-CA-C	5.67	117.09	110.62
1	B	293	PHE	N-CA-C	5.67	117.46	111.28
1	B	163	CYS	CA-C-N	5.66	125.78	119.32
1	B	163	CYS	C-N-CA	5.66	125.78	119.32
1	C	262	LEU	N-CA-C	5.66	120.19	113.12
1	A	248	ASP	N-CA-C	-5.52	102.72	110.50
1	A	71	PHE	N-CA-C	5.43	118.09	109.50
1	B	144	ALA	N-CA-C	-5.42	101.46	109.86
1	A	223	TRP	N-CA-C	5.41	118.63	109.76
1	A	209	ASP	N-CA-C	5.40	119.17	112.58
1	C	223	TRP	N-CA-C	5.39	118.60	109.76
1	A	204	ILE	N-CA-C	5.39	113.82	107.84
1	A	175	ILE	N-CA-C	5.38	115.60	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	256	VAL	N-CA-C	-5.31	105.32	110.42
1	B	256	VAL	N-CA-C	-5.29	105.38	110.72
1	A	263	ASP	N-CA-C	5.29	119.71	113.16
1	A	285	SER	N-CA-C	5.28	117.50	108.90
1	B	175	ILE	N-CA-C	5.25	115.41	107.75
1	C	41	VAL	N-CA-C	5.24	115.82	108.17
1	B	135	THR	N-CA-C	5.23	114.73	107.73
1	C	275	HIS	N-CA-C	5.15	118.20	109.76
2	E	503	VAL	N-CA-C	5.12	116.91	108.97
1	A	286	MET	N-CA-C	-5.06	106.42	112.59
1	B	223	TRP	N-CA-C	5.04	118.03	109.76
1	C	99	LYS	N-CA-C	-5.03	100.31	108.41
1	C	52	TYR	N-CA-C	5.02	117.75	109.72
1	B	64	ILE	CB-CA-C	-5.00	104.03	110.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	TYR	Sidechain
1	B	220	TYR	Sidechain

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	1974	0	1938	54	0
1	B	1985	0	1956	40	0
1	C	2016	0	1982	55	0
2	D	36	0	26	1	0
2	E	36	0	26	0	0
2	F	36	0	26	1	0
3	A	4	0	6	2	0
3	B	12	0	18	7	0
3	C	16	0	24	12	0
4	A	102	0	0	3	0
4	B	92	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	116	0	0	3	0
4	D	1	0	0	0	0
4	E	4	0	0	0	0
4	F	3	0	0	0	0
All	All	6433	0	6002	146	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 12.

All (146) 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:62:MET:HE2	1:A:123:HIS:HE1	1.27	0.97
1:A:62:MET:HE1	1:A:118:THR:HG23	1.55	0.89
1:A:62:MET:CE	1:A:118:THR:HG23	2.02	0.89
1:C:290:LEU:HD23	3:C:502:EDO:H22	1.57	0.86
1:A:62:MET:HE2	1:A:123:HIS:CE1	2.09	0.86
1:C:284:THR:HG22	1:C:286:MET:HE1	1.59	0.84
1:A:280:VAL:H	3:A:506:EDO:H21	1.39	0.83
1:C:275:HIS:CD2	1:C:276:GLN:HE21	1.96	0.83
1:A:77:LYS:HE3	1:A:224:ARG:HH22	1.44	0.82
1:A:191:ARG:HH11	1:A:191:ARG:CB	1.95	0.79
1:C:249:ILE:HG22	3:C:502:EDO:H12	1.65	0.76
1:C:179:GLN:HA	3:C:501:EDO:H11	1.66	0.76
1:C:267:ASN:HD22	1:C:275:HIS:HE1	1.35	0.75
1:C:228:ARG:HD2	4:C:1279:HOH:O	1.87	0.74
1:C:275:HIS:HD2	1:C:276:GLN:HE21	1.34	0.73
1:A:191:ARG:HH11	1:A:191:ARG:HB3	1.54	0.73
1:A:295:LYS:HG3	4:A:1220:HOH:O	1.90	0.72
1:C:43:ARG:HH12	1:C:57:HIS:HE1	1.38	0.72
1:C:60:ARG:HD2	1:C:96:LEU:O	1.90	0.71
1:A:77:LYS:HD2	1:A:78:SER:O	1.94	0.67
1:A:60:ARG:HD2	1:A:96:LEU:O	1.94	0.67
1:B:245:THR:HG21	1:B:295:LYS:HG2	1.78	0.66
1:B:117:GLN:O	1:B:121:MET:HG3	1.95	0.66
1:B:113:LYS:O	1:B:117:GLN:HG3	1.95	0.65
1:A:230:SER:O	1:A:234:GLN:HG2	1.96	0.65
1:C:285:SER:C	1:C:286:MET:HE3	2.23	0.64
1:C:224:ARG:HA	1:C:230:SER:HA	1.80	0.64
1:B:279:GLN:HA	3:B:507:EDO:H12	1.81	0.63
1:B:275:HIS:CD2	1:B:276:GLN:HG3	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ASN:HD22	1:C:275:HIS:CE1	2.18	0.62
1:C:245:THR:HB	4:C:1204:HOH:O	1.98	0.62
1:B:54:ASN:HB3	3:B:503:EDO:H12	1.81	0.61
1:B:60:ARG:HD2	1:B:96:LEU:O	2.00	0.60
1:A:224:ARG:HA	1:A:230:SER:HA	1.82	0.60
1:A:88:ASN:OD1	1:A:241:ARG:NH2	2.34	0.60
1:B:267:ASN:HD22	1:B:275:HIS:HE1	1.50	0.60
1:C:295:LYS:NZ	1:C:299:HIS:HD2	2.00	0.60
1:C:99:LYS:HD3	4:C:1253:HOH:O	2.01	0.59
1:B:70:HIS:HD2	1:B:78:SER:OG	1.85	0.59
1:A:245:THR:HG22	1:A:246:GLU:HG3	1.84	0.59
1:A:44:MET:CE	1:A:201:SER:HB3	2.33	0.58
1:C:275:HIS:CD2	1:C:276:GLN:NE2	2.71	0.58
1:B:48:ARG:NH1	4:B:1236:HOH:O	2.37	0.58
1:B:106:LEU:HB3	1:B:110:GLU:HB2	1.86	0.57
1:B:245:THR:HG23	1:B:294:GLY:O	2.05	0.57
1:A:279:GLN:HG3	3:A:506:EDO:H22	1.88	0.56
1:C:249:ILE:HG22	3:C:502:EDO:C1	2.35	0.56
1:A:70:HIS:HD2	1:A:78:SER:OG	1.88	0.56
1:A:182:ARG:HH11	1:A:182:ARG:HG2	1.71	0.56
1:A:77:LYS:CE	1:A:224:ARG:HH22	2.17	0.56
1:C:267:ASN:ND2	1:C:275:HIS:HE1	2.01	0.55
1:A:62:MET:HE3	1:A:118:THR:HG23	1.82	0.55
1:C:179:GLN:HG2	3:C:501:EDO:H12	1.88	0.55
1:B:91:LYS:O	1:B:95:THR:HG23	2.05	0.55
1:B:267:ASN:ND2	1:B:275:HIS:HE1	2.05	0.54
1:A:217:VAL:HG13	1:A:218:PRO:HD2	1.89	0.54
1:A:48:ARG:NH2	1:B:263:ASP:OD1	2.41	0.54
1:C:179:GLN:HG2	3:C:501:EDO:C1	2.39	0.53
1:C:44:MET:CE	1:C:201:SER:HB2	2.39	0.53
1:A:62:MET:CE	1:A:123:HIS:HE1	2.10	0.52
1:A:136:HIS:HA	2:D:504:ASP:O	2.09	0.52
1:C:191:ARG:NH1	1:C:191:ARG:HG3	2.24	0.52
1:B:224:ARG:HA	1:B:230:SER:HA	1.92	0.51
1:C:191:ARG:CG	1:C:191:ARG:HH11	2.24	0.51
1:A:130:LEU:C	1:A:130:LEU:HD23	2.36	0.51
1:A:263:ASP:OD1	1:B:48:ARG:NH2	2.44	0.50
1:A:191:ARG:HH11	1:A:191:ARG:CG	2.25	0.50
1:B:53:TYR:HB3	3:B:503:EDO:H21	1.94	0.49
1:B:67:ASN:ND2	1:B:134:LEU:HD12	2.28	0.49
1:C:295:LYS:NZ	1:C:299:HIS:CD2	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLU:HG3	4:A:1267:HOH:O	2.12	0.49
1:B:182:ARG:HG2	1:B:182:ARG:HH11	1.78	0.49
1:B:99:LYS:HE3	4:B:1240:HOH:O	2.13	0.49
1:A:73:ILE:HD11	1:A:146:ASP:C	2.38	0.48
1:A:207:HIS:HE1	4:A:1225:HOH:O	1.97	0.48
1:C:138:GLU:HB2	1:C:141:MET:HG2	1.94	0.48
1:C:190:SER:O	1:C:191:ARG:HB2	2.13	0.48
1:A:239:GLU:OE2	1:A:247:ARG:NH1	2.47	0.48
1:C:299:HIS:O	1:C:300:LEU:HB2	2.13	0.47
1:C:239:GLU:OE1	1:C:259:LYS:HD2	2.15	0.47
1:C:109:GLU:H	1:C:109:GLU:CD	2.22	0.47
1:C:286:MET:HE3	1:C:286:MET:N	2.29	0.47
1:B:53:TYR:HB3	3:B:503:EDO:C2	2.44	0.47
1:C:55:MET:HE3	1:C:60:ARG:HH21	1.80	0.47
1:C:284:THR:CG2	1:C:286:MET:HE1	2.39	0.47
1:B:128:CYS:HB3	1:B:170:PRO:HG2	1.98	0.46
1:B:245:THR:CG2	1:B:295:LYS:HG2	2.45	0.46
1:B:57:HIS:CE1	1:B:169:LYS:HE2	2.51	0.46
1:B:238:GLU:HA	1:B:241:ARG:NH1	2.30	0.46
1:C:67:ASN:ND2	1:C:134:LEU:HD12	2.30	0.46
1:A:211:LEU:HD21	1:A:253:LEU:CD1	2.46	0.45
1:C:175:ILE:HD12	1:C:175:ILE:N	2.32	0.45
1:A:77:LYS:HE2	1:A:136:HIS:HE1	1.80	0.45
1:A:288:THR:O	1:B:258:GLN:HB2	2.17	0.45
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.83	0.45
1:C:191:ARG:HG3	1:C:191:ARG:HH11	1.82	0.45
1:A:132:ALA:HA	1:A:174:PHE:O	2.17	0.45
1:C:279:GLN:HA	3:C:504:EDO:H12	1.99	0.44
1:A:44:MET:HE1	1:A:201:SER:HB3	1.99	0.44
1:C:220:TYR:CD1	1:C:220:TYR:N	2.85	0.44
1:B:54:ASN:H	3:B:503:EDO:C1	2.30	0.44
1:C:295:LYS:HZ3	1:C:299:HIS:HD2	1.65	0.44
1:A:191:ARG:CG	1:A:191:ARG:NH1	2.81	0.44
1:B:54:ASN:N	3:B:503:EDO:H21	2.33	0.44
1:B:186:GLY:HA3	1:B:278:LYS:HG3	2.00	0.44
1:C:150:LYS:HA	1:C:151:PRO:HD3	1.87	0.44
1:A:131:VAL:O	1:A:173:PHE:HA	2.18	0.43
1:A:77:LYS:HD2	1:A:77:LYS:C	2.44	0.43
1:C:43:ARG:HH12	1:C:57:HIS:CE1	2.26	0.43
1:C:161:ASP:OD1	1:C:161:ASP:N	2.49	0.43
1:C:291:LEU:H	3:C:502:EDO:H11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:HIS:CD2	1:C:127:ASP:HA	2.53	0.43
1:C:249:ILE:CG2	3:C:502:EDO:H12	2.43	0.43
1:A:225:ASN:OD1	1:A:227:THR:HG23	2.17	0.43
1:B:55:MET:HB3	1:B:60:ARG:HH21	1.83	0.43
1:C:67:ASN:ND2	1:C:82:THR:OG1	2.49	0.43
1:B:107:LYS:HB2	1:B:110:GLU:HG3	2.00	0.43
1:C:136:HIS:HA	2:F:504:ASP:O	2.19	0.43
1:C:279:GLN:HA	3:C:504:EDO:C2	2.49	0.43
1:B:130:LEU:C	1:B:130:LEU:HD23	2.44	0.43
1:A:186:GLY:HA3	1:A:278:LYS:HG3	2.01	0.43
1:A:113:LYS:HE2	1:A:113:LYS:HB3	1.79	0.42
1:B:161:ASP:N	1:B:161:ASP:OD1	2.52	0.42
1:A:128:CYS:HB2	1:A:170:PRO:O	2.19	0.42
1:B:54:ASN:H	3:B:503:EDO:H12	1.84	0.42
1:B:67:ASN:ND2	1:B:82:THR:OG1	2.51	0.42
1:C:50:ALA:HA	1:C:51:PRO:HD3	1.83	0.42
1:C:191:ARG:NH1	1:C:191:ARG:CG	2.80	0.42
1:A:117:GLN:O	1:A:121:MET:HG3	2.20	0.41
1:A:181:ASP:O	1:A:221:PHE:CE1	2.73	0.41
1:A:182:ARG:HG2	1:A:182:ARG:NH1	2.34	0.41
1:A:239:GLU:OE1	1:A:259:LYS:HE3	2.19	0.41
1:B:253:LEU:HD23	1:B:253:LEU:HA	1.84	0.41
1:B:249:ILE:HD12	1:B:249:ILE:HA	1.87	0.41
1:C:291:LEU:HD12	1:C:291:LEU:C	2.46	0.41
1:A:53:TYR:CD1	1:A:170:PRO:HD3	2.56	0.41
1:B:55:MET:HB3	1:B:60:ARG:NH2	2.35	0.41
1:A:44:MET:HE2	1:A:202:TYR:CD2	2.56	0.41
1:A:63:ALA:HA	1:A:130:LEU:O	2.20	0.41
1:C:250:LEU:HG	3:C:502:EDO:H21	2.03	0.41
1:B:245:THR:HG23	1:B:294:GLY:C	2.45	0.40
1:C:67:ASN:HD22	1:C:134:LEU:HD12	1.85	0.40
1:C:275:HIS:CD2	1:C:276:GLN:HG3	2.57	0.40
1:A:150:LYS:HA	1:A:151:PRO:HD3	1.90	0.40
1:A:244:GLY:HA2	1:A:252:LEU:HD11	2.02	0.40
1:C:290:LEU:HA	3:C:502:EDO:C2	2.52	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	243/272 (89%)	234 (96%)	9 (4%)	0	100	100
1	B	244/272 (90%)	238 (98%)	6 (2%)	0	100	100
1	C	248/272 (91%)	241 (97%)	7 (3%)	0	100	100
2	D	3/6 (50%)	3 (100%)	0	0	100	100
2	E	3/6 (50%)	3 (100%)	0	0	100	100
2	F	3/6 (50%)	3 (100%)	0	0	100	100
All	All	744/834 (89%)	722 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	215/239 (90%)	207 (96%)	8 (4%)	30	45
1	B	217/239 (91%)	212 (98%)	5 (2%)	44	63
1	C	220/239 (92%)	212 (96%)	8 (4%)	31	47
2	D	4/4 (100%)	4 (100%)	0	100	100
2	E	4/4 (100%)	4 (100%)	0	100	100
2	F	4/4 (100%)	4 (100%)	0	100	100
All	All	664/729 (91%)	643 (97%)	21 (3%)	34	51

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	117	GLN
1	A	191	ARG
1	A	201	SER
1	A	227	THR
1	A	245	THR
1	A	273	MET
1	A	291	LEU
1	B	113	LYS
1	B	190	SER
1	B	200	THR
1	B	227	THR
1	B	259	LYS
1	C	45	PRO
1	C	109	GLU
1	C	191	ARG
1	C	216	THR
1	C	227	THR
1	C	245	THR
1	C	286	MET
1	C	291	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	67	ASN
1	A	70	HIS
1	A	123	HIS
1	A	153	ASN
1	A	234	GLN
1	A	267	ASN
1	A	276	GLN
1	B	57	HIS
1	B	67	ASN
1	B	70	HIS
1	B	83	ASN
1	B	153	ASN
1	B	267	ASN
1	B	276	GLN
1	C	56	ASN

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Mol	Chain	Res	Type
1	C	57	HIS
1	C	59	HIS
1	C	67	ASN
1	C	83	ASN
1	C	153	ASN
1	C	267	ASN
1	C	275	HIS
1	C	299	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](#)

8 ligands are modelled in this entry.

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	$\# Z > 2$
3	EDO	A	506	-	3,3,3	0.41	0	2,2,2	0.39	0
3	EDO	C	508	-	3,3,3	0.63	0	2,2,2	0.33	0
3	EDO	B	507	-	3,3,3	0.37	0	2,2,2	0.60	0
3	EDO	C	501	-	3,3,3	0.63	0	2,2,2	0.68	0
3	EDO	C	502	-	3,3,3	0.23	0	2,2,2	0.46	0
3	EDO	C	504	-	3,3,3	0.42	0	2,2,2	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	503	-	3,3,3	0.20	0	2,2,2	0.50	0
3	EDO	B	505	-	3,3,3	0.68	0	2,2,2	0.26	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
3	EDO	A	506	-	-	0/1/1/1	-
3	EDO	C	508	-	-	0/1/1/1	-
3	EDO	B	507	-	-	0/1/1/1	-
3	EDO	C	501	-	-	0/1/1/1	-
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	C	504	-	-	0/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	505	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2
3	C	502	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	506	EDO	2	0
3	B	507	EDO	1	0
3	C	501	EDO	3	0
3	C	502	EDO	7	0
3	C	504	EDO	2	0
3	B	503	EDO	6	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	247/272 (90%)	-0.31	3 (1%) 76 77	18, 29, 46, 62	0
1	B	248/272 (91%)	-0.39	3 (1%) 76 77	16, 28, 45, 67	0
1	C	252/272 (92%)	-0.54	2 (0%) 82 83	13, 24, 40, 60	0
2	D	4/6 (66%)	-0.02	0 100 100	34, 37, 39, 41	0
2	E	4/6 (66%)	-0.20	0 100 100	29, 36, 40, 40	0
2	F	4/6 (66%)	-0.10	0 100 100	30, 32, 37, 40	0
All	All	759/834 (91%)	-0.41	8 (1%) 78 79	13, 27, 45, 67	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	300	LEU	3.8
1	A	40	ARG	2.9
1	B	41	VAL	2.9
1	B	191	ARG	2.7
1	A	295	LYS	2.7
1	B	200	THR	2.4
1	A	41	VAL	2.1
1	C	41	VAL	2.1

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(Å ²)	Q<0.9
3	EDO	B	505	4/4	0.92	0.11	33,41,42,42	0
3	EDO	B	507	4/4	0.93	0.15	35,35,36,37	0
3	EDO	C	501	4/4	0.93	0.14	24,27,29,32	0
3	EDO	C	508	4/4	0.93	0.11	45,48,48,48	0
3	EDO	A	506	4/4	0.94	0.13	31,34,35,36	0
3	EDO	C	504	4/4	0.95	0.12	37,40,40,42	0
3	EDO	B	503	4/4	0.96	0.15	24,27,30,30	0
3	EDO	C	502	4/4	0.97	0.09	28,29,30,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.