



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:53 AM UTC

PDB ID : 2XZ0 / pdb_00002xz0
Title : The Structure of the 2:1 (Partially Occupied) Complex Between Stearoyl Acyl Carrier Protein Desaturase from Ricinus Communis (Castor Bean) and Acyl Carrier Protein.
Authors : Moche, M.; Guy, J.E.; Whittle, E.; Lengqvist, J.; Shanklin, J.; Lindqvist, Y.
Deposited on : 2010-11-22
Resolution : 3.00 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

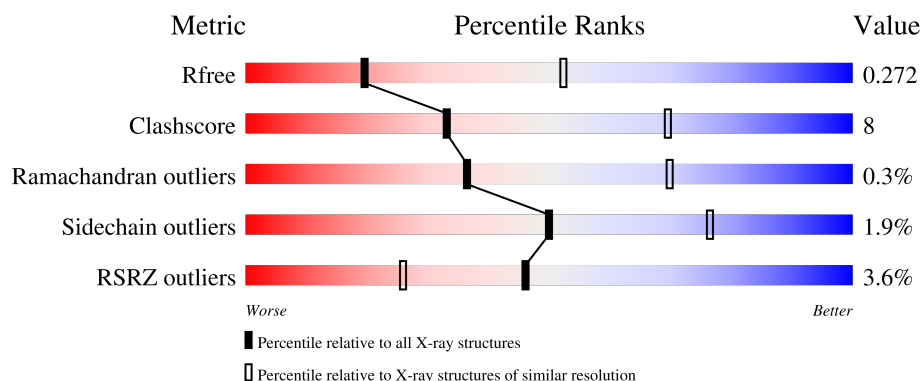
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	363	
1	B	363	
1	C	363	
2	D	82	

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
5	EDO	B	1367	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9080 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 ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2807	1780	487	526	14			
1	B	346	Total	C	N	O	S	0	0	0
			2807	1780	487	526	14			
1	C	346	Total	C	N	O	S	0	0	0
			2807	1780	487	526	14			

- Molecule 2 is a protein called ACYL CARRIER PROTEIN 1, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	82	Total	C	N	O	P	S	0	0
			623	385	96	140	1	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	10	SER	CYS	SEE REMARK 999	UNP P07854
D	76	GLY	SER	SEE REMARK 999	UNP P07854

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

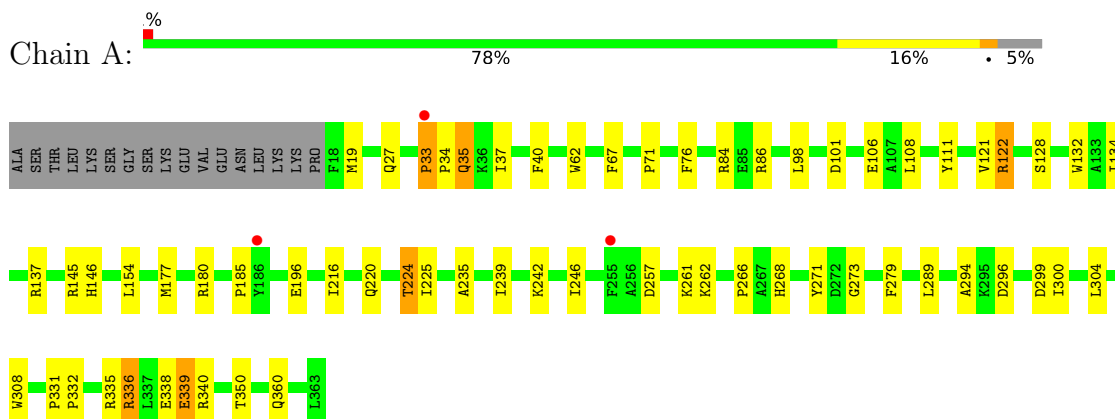
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	6	Total	O	0	0
			6	6		
6	C	8	Total	O	0	0
			8	8		

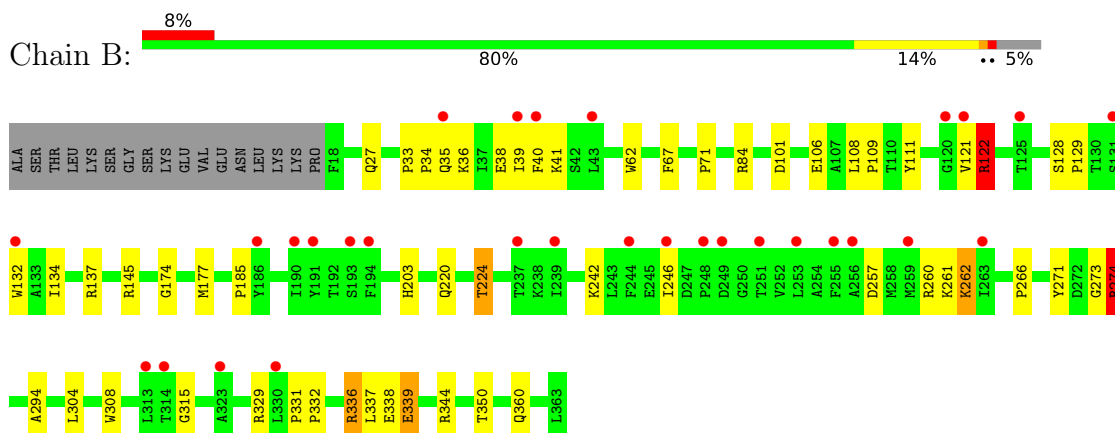
3 Residue-property plots

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.

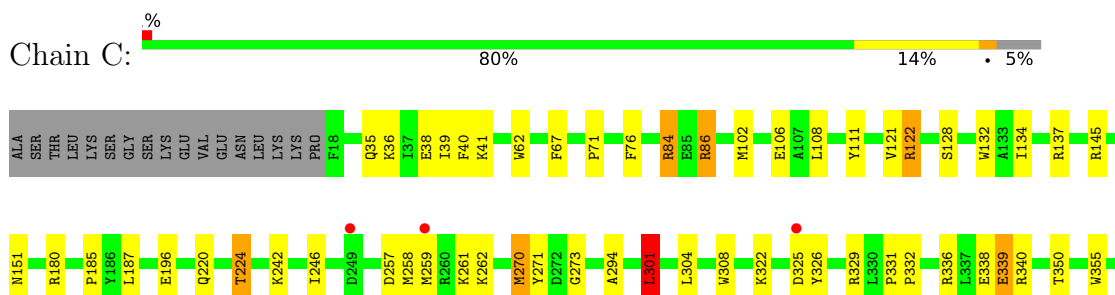
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE, CHLOROPLASTIC



• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE, CHLOROPLASTIC

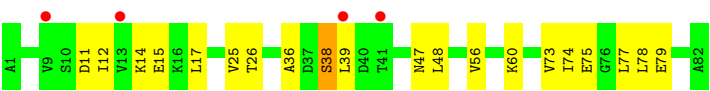
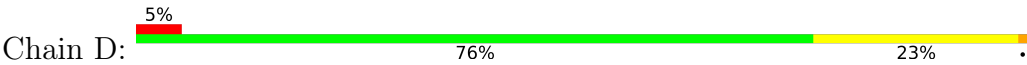


• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE, CHLOROPLASTIC





- Molecule 2: ACYL CARRIER PROTEIN 1, CHLOROPLASTIC



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.27Å 188.27Å 81.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.28 – 3.00 29.28 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.28-3.00) 99.8 (29.28-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.243 , 0.277 0.237 , 0.272	Depositor DCC
R_{free} test set	1363 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9080	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: SEP, EDO, ZN, FE

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	0.63	0/2875	0.94	6/3892 (0.2%)
1	B	0.71	4/2875 (0.1%)	1.00	6/3892 (0.2%)
1	C	0.69	3/2875 (0.1%)	0.98	8/3892 (0.2%)
2	D	0.56	0/613	0.84	0/822
All	All	0.67	7/9238 (0.1%)	0.96	20/12498 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	ARG	CZ-NH1	-8.57	1.20	1.32
1	C	122	ARG	CZ-NH2	8.37	1.44	1.33
1	B	122	ARG	CZ-NH1	-7.29	1.22	1.32
1	B	27	GLN	CD-OE1	-6.99	1.10	1.23
1	C	122	ARG	CD-NE	6.10	1.54	1.46
1	B	260	ARG	CZ-NH1	-5.75	1.24	1.32
1	C	84	ARG	CZ-NH1	-5.50	1.25	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ARG	NE-CZ-NH2	9.52	127.77	119.20
1	C	122	ARG	NE-CZ-NH2	9.21	127.49	119.20
1	B	122	ARG	NE-CZ-NH2	8.99	127.30	119.20
1	C	122	ARG	NE-CZ-NH1	-7.79	113.71	121.50
1	C	301	LEU	CD1-CG-CD2	-7.70	93.87	110.80
1	A	336	ARG	CG-CD-NE	-6.72	97.22	112.00
1	B	336	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	A	122	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	B	260	ARG	NH1-CZ-NH2	-5.90	111.63	119.30
1	C	86	ARG	NE-CZ-NH1	5.81	127.31	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	C	86	ARG	CB-CG-CD	5.68	124.38	111.30
1	C	86	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	A	33	PRO	CA-C-N	5.39	125.03	119.05
1	A	33	PRO	C-N-CA	5.39	125.03	119.05
1	C	270	MET	CB-CG-SD	-5.34	96.67	112.70
1	A	336	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	19	MET	N-CA-C	5.13	117.04	109.50
1	C	84	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	B	274	ARG	NH1-CZ-NH2	-5.03	112.76	119.30

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	2807	0	2748	41	0
1	B	2807	0	2748	54	1
1	C	2807	0	2748	53	1
2	D	623	0	626	19	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	4	0	6	0	0
6	A	9	0	0	0	0
6	B	6	0	0	0	0
6	C	8	0	0	0	0
All	All	9080	0	8876	140	2

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 8.

All (140) 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:B:336:ARG:NH2	1:C:322:LYS:HG3	1.52	1.22
1:B:336:ARG:NH1	1:C:322:LYS:O	1.74	1.18
1:B:336:ARG:CZ	1:C:322:LYS:HG3	1.76	1.15
1:B:122:ARG:HG2	1:B:122:ARG:HH11	1.27	0.96
1:A:34:PRO:O	1:A:37:ILE:HG12	1.75	0.87
1:B:336:ARG:NH2	1:C:322:LYS:CG	2.40	0.83
1:C:294:ALA:HB3	1:C:338:GLU:HG3	1.66	0.78
1:B:294:ALA:HB3	1:B:338:GLU:HG3	1.63	0.78
1:A:62:TRP:CE2	1:A:145:ARG:NH1	2.52	0.77
1:A:294:ALA:HB3	1:A:338:GLU:HG3	1.65	0.77
1:B:304:LEU:HD22	1:B:308:TRP:CH2	2.19	0.76
1:B:62:TRP:CE2	1:B:145:ARG:NH1	2.55	0.75
1:C:62:TRP:CE2	1:C:145:ARG:NH1	2.55	0.75
1:C:304:LEU:HD22	1:C:308:TRP:CH2	2.23	0.73
1:A:304:LEU:HD22	1:A:308:TRP:CH2	2.24	0.73
2:D:60:LYS:HD3	2:D:73:VAL:HG11	1.71	0.72
1:B:122:ARG:HH11	1:B:122:ARG:CG	2.02	0.71
1:B:220:GLN:O	1:B:224:THR:HG23	1.90	0.71
1:C:350:THR:CG2	1:C:360:GLN:HB3	2.21	0.70
1:A:220:GLN:O	1:A:224:THR:HG23	1.92	0.69
1:C:220:GLN:O	1:C:224:THR:HG23	1.92	0.69
2:D:25:VAL:HG12	2:D:26:THR:H	1.58	0.68
1:B:350:THR:CG2	1:B:360:GLN:HB3	2.22	0.68
1:A:98:LEU:O	1:A:101:ASP:HB2	1.95	0.67
1:C:340:ARG:NH1	2:D:11:ASP:HA	2.10	0.67
1:B:336:ARG:HH21	1:C:322:LYS:HE3	1.61	0.65
1:A:84:ARG:NH2	1:B:71:PRO:O	2.31	0.63
1:A:350:THR:CG2	1:A:360:GLN:HB3	2.27	0.63
1:B:336:ARG:NH1	1:C:322:LYS:C	2.56	0.62
1:C:271:TYR:CE2	1:C:273:GLY:HA2	2.35	0.61
1:B:62:TRP:CD2	1:B:145:ARG:NH1	2.68	0.61
1:B:336:ARG:CZ	1:C:322:LYS:O	2.48	0.61
1:B:134:ILE:HG13	1:B:137:ARG:HH22	1.65	0.60
1:B:336:ARG:HA	1:B:339:GLU:HB2	1.83	0.60
1:C:340:ARG:HH21	2:D:14:LYS:HD2	1.66	0.60
1:B:336:ARG:HH21	1:C:322:LYS:HG3	1.59	0.60
1:B:329:ARG:O	1:C:329:ARG:NH2	2.34	0.60
1:A:134:ILE:HG13	1:A:137:ARG:HH22	1.67	0.59
1:A:62:TRP:CD2	1:A:145:ARG:NH1	2.70	0.58
1:C:62:TRP:CD2	1:C:145:ARG:NH1	2.72	0.57
1:C:134:ILE:HG13	1:C:137:ARG:HH22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:LEU:HD21	2:D:39:LEU:HD22	1.86	0.57
1:C:336:ARG:HA	1:C:339:GLU:HB2	1.87	0.56
1:C:257:ASP:O	1:C:261:LYS:HG3	2.06	0.55
2:D:12:ILE:HG23	2:D:47:ASN:HD22	1.71	0.55
2:D:12:ILE:CG2	2:D:47:ASN:HD22	2.19	0.55
2:D:25:VAL:HG12	2:D:26:THR:N	2.20	0.54
1:B:350:THR:HG22	1:B:360:GLN:HB3	1.89	0.54
1:B:262:LYS:NZ	2:D:38:SEP:O2P	2.35	0.54
1:A:331:PRO:HB2	1:A:332:PRO:HD3	1.89	0.54
1:B:257:ASP:O	1:B:261:LYS:HG3	2.08	0.54
1:B:128:SER:O	1:B:137:ARG:NH2	2.42	0.53
1:C:331:PRO:HB2	1:C:332:PRO:HD3	1.91	0.53
1:A:257:ASP:O	1:A:261:LYS:HG3	2.08	0.53
1:A:128:SER:O	1:A:137:ARG:NH2	2.41	0.52
1:C:350:THR:HG22	1:C:360:GLN:HB3	1.91	0.52
1:C:270:MET:HE2	1:C:355:TRP:CH2	2.45	0.51
1:A:332:PRO:O	1:A:336:ARG:HB2	2.11	0.51
1:B:122:ARG:HG2	1:B:122:ARG:NH1	2.10	0.51
1:A:336:ARG:HA	1:A:339:GLU:HB2	1.93	0.51
1:C:36:LYS:O	1:C:39:ILE:HG13	2.12	0.50
1:C:121:VAL:HB	1:C:132:TRP:HB3	1.95	0.49
1:C:259:MET:SD	1:C:301:LEU:HD11	2.52	0.49
1:B:331:PRO:HB2	1:B:332:PRO:HD3	1.94	0.49
1:B:274:ARG:HG2	1:B:274:ARG:HH11	1.77	0.49
2:D:17:LEU:HD21	2:D:36:ALA:HB2	1.94	0.49
1:A:121:VAL:HB	1:A:132:TRP:HB3	1.95	0.48
1:B:332:PRO:HB2	1:C:325:ASP:OD2	2.13	0.48
1:C:40:PHE:CE2	1:C:185:PRO:HB2	2.48	0.48
1:B:344:ARG:NH1	2:D:56:VAL:O	2.47	0.48
1:A:350:THR:HG22	1:A:360:GLN:HB3	1.93	0.48
1:C:71:PRO:HA	1:C:76:PHE:CD1	2.48	0.48
1:C:180:ARG:NH2	1:C:261:LYS:HB3	2.29	0.48
1:A:40:PHE:CE2	1:A:185:PRO:HB2	2.48	0.47
1:A:67:PHE:CZ	1:A:224:THR:HG21	2.49	0.47
1:A:35:GLN:C	1:A:37:ILE:H	2.22	0.47
2:D:75:GLU:HA	2:D:78:LEU:HB2	1.96	0.47
1:B:121:VAL:HB	1:B:132:TRP:HB3	1.96	0.47
1:C:128:SER:O	1:C:137:ARG:NH2	2.46	0.47
1:B:33:PRO:HA	1:B:34:PRO:HD3	1.79	0.47
1:B:40:PHE:CE2	1:B:185:PRO:HB2	2.49	0.47
1:A:71:PRO:HA	1:A:76:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TYR:CE2	1:A:273:GLY:HA2	2.50	0.46
1:C:271:TYR:CZ	1:C:273:GLY:HA2	2.51	0.46
1:A:33:PRO:HA	1:A:34:PRO:HD3	1.71	0.46
1:B:36:LYS:O	1:B:39:ILE:HG13	2.17	0.45
1:C:108:LEU:HA	1:C:111:TYR:CD2	2.52	0.45
1:C:340:ARG:NH1	2:D:11:ASP:OD1	2.45	0.45
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.17	0.45
1:C:340:ARG:NH2	2:D:14:LYS:HD2	2.32	0.45
1:A:35:GLN:C	1:A:37:ILE:N	2.75	0.45
1:A:35:GLN:H	1:A:35:GLN:HG3	1.38	0.45
1:B:336:ARG:HH12	1:C:326:TYR:H	1.65	0.45
1:B:336:ARG:HH21	1:C:322:LYS:CE	2.29	0.44
1:C:350:THR:HG23	1:C:360:GLN:HB3	1.96	0.44
1:B:177:MET:SD	1:B:266:PRO:HA	2.57	0.44
1:B:336:ARG:NH1	1:C:322:LYS:HA	2.32	0.44
1:C:106:GLU:C	1:C:108:LEU:H	2.26	0.44
1:B:108:LEU:HA	1:B:111:TYR:CD2	2.53	0.44
1:C:340:ARG:HH21	2:D:14:LYS:CD	2.30	0.44
1:B:242:LYS:HE3	1:B:246:ILE:HD11	2.00	0.44
1:C:67:PHE:CZ	1:C:224:THR:HG21	2.52	0.43
1:B:35:GLN:HG2	1:B:36:LYS:N	2.32	0.43
1:B:350:THR:HG23	1:B:360:GLN:HB3	2.00	0.43
1:A:106:GLU:C	1:A:108:LEU:H	2.27	0.43
1:A:137:ARG:HB3	1:B:174:GLY:HA2	2.00	0.43
1:A:242:LYS:HE3	1:A:246:ILE:HD11	2.00	0.43
1:A:296:ASP:O	1:A:300:ILE:HG13	2.18	0.43
1:B:271:TYR:CE2	1:B:273:GLY:HA2	2.54	0.43
1:B:106:GLU:C	1:B:108:LEU:H	2.27	0.42
2:D:75:GLU:O	2:D:79:GLU:HG2	2.19	0.42
1:A:146:HIS:CD2	1:A:225:ILE:HG23	2.54	0.42
1:A:180:ARG:NH2	1:A:261:LYS:HB3	2.34	0.42
1:A:62:TRP:CZ2	1:A:145:ARG:NH1	2.87	0.42
1:B:274:ARG:HG2	1:B:274:ARG:NH1	2.34	0.42
1:A:177:MET:SD	1:A:266:PRO:HA	2.58	0.42
1:C:336:ARG:HD3	2:D:15:GLU:HG2	2.02	0.42
1:C:196:GLU:HA	1:C:196:GLU:OE1	2.19	0.41
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.92	0.41
1:B:101:ASP:OD2	1:B:203:HIS:CE1	2.73	0.41
2:D:48:LEU:HD13	2:D:74:ILE:HD11	2.01	0.41
1:B:67:PHE:CZ	1:B:224:THR:HG21	2.56	0.41
1:A:108:LEU:HA	1:A:111:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:N	1:B:109:PRO:CD	2.84	0.41
1:B:128:SER:HA	1:B:129:PRO:HD3	1.83	0.41
1:C:340:ARG:NH1	2:D:11:ASP:CA	2.79	0.41
1:A:299:ASP:OD1	1:A:335:ARG:NH2	2.54	0.41
1:B:336:ARG:NH1	1:C:326:TYR:H	2.19	0.41
1:B:38:GLU:O	1:B:41:LYS:N	2.54	0.41
1:C:187:LEU:HB3	1:C:258:MET:SD	2.61	0.41
1:A:86:ARG:HD3	1:A:86:ARG:HA	1.88	0.41
1:C:242:LYS:HE3	1:C:246:ILE:HD11	2.03	0.40
1:B:294:ALA:CB	1:B:338:GLU:HG3	2.43	0.40
1:C:62:TRP:CZ2	1:C:145:ARG:NH1	2.89	0.40
1:C:102:MET:HE3	1:C:151:ASN:HA	2.02	0.40
1:A:235:ALA:O	1:A:239:ILE:HG13	2.21	0.40
1:A:268:HIS:HA	1:A:279:PHE:CD1	2.56	0.40
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.96	0.40
1:B:336:ARG:NE	1:C:322:LYS:HG3	2.26	0.40
1:C:38:GLU:O	1:C:41:LYS:N	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLY:CA	1:B:315:GLY:CA[4_555]	2.02	0.18
1:C:71:PRO:O	1:C:84:ARG:NH2[6_555]	2.16	0.04

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	344/363 (95%)	324 (94%)	19 (6%)	1 (0%)	36 70
1	B	344/363 (95%)	326 (95%)	17 (5%)	1 (0%)	36 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	344/363 (95%)	325 (94%)	18 (5%)	1 (0%)	36	70
2	D	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
All	All	1111/1171 (95%)	1050 (94%)	58 (5%)	3 (0%)	36	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	LYS
1	B	262	LYS
1	C	262	LYS

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	300/315 (95%)	293 (98%)	7 (2%)	44	74
1	B	300/315 (95%)	296 (99%)	4 (1%)	61	81
1	C	300/315 (95%)	294 (98%)	6 (2%)	48	76
2	D	68/68 (100%)	67 (98%)	1 (2%)	57	80
All	All	968/1013 (96%)	950 (98%)	18 (2%)	50	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	35	GLN
1	A	122	ARG
1	A	216	ILE
1	A	224	THR
1	A	339	GLU
1	A	340	ARG
1	B	122	ARG
1	B	224	THR

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Mol	Chain	Res	Type
1	B	274	ARG
1	B	339	GLU
1	C	35	GLN
1	C	86	ARG
1	C	122	ARG
1	C	224	THR
1	C	301	LEU
1	C	339	GLU
2	D	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	63	GLN
1	B	112	GLN
1	B	203	HIS
1	C	203	HIS
2	D	47	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	SEP	D	38	2	8,9,10	1.62	1 (12%)	7,12,14	1.22	1 (14%)

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
2	SEP	D	38	2	-	3/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	38	SEP	P-O1P	3.55	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	38	SEP	OG-CB-CA	2.11	110.20	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	38	SEP	CB-OG-P-O2P
2	D	38	SEP	CB-OG-P-O3P
2	D	38	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	38	SEP	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	$\# Z > 2$
5	EDO	B	1367	-	3,3,3	0.57	0	2,2,2	0.31	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
5	EDO	B	1367	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1367	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	346/363 (95%)	-0.01	3 (0%) 81 61	29, 92, 175, 214	0
1	B	346/363 (95%)	0.38	30 (8%) 16 8	34, 87, 144, 166	0
1	C	346/363 (95%)	-0.04	3 (0%) 81 61	28, 84, 148, 176	0
2	D	81/82 (98%)	0.64	4 (4%) 35 18	129, 179, 199, 201	0
All	All	1119/1171 (95%)	0.15	40 (3%) 46 26	28, 92, 180, 214	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	259	MET	3.8
1	C	249	ASP	3.7
1	B	244	PHE	3.7
1	B	193	SER	3.6
1	B	120	GLY	3.4
1	B	249	ASP	3.2
1	B	256	ALA	3.2
1	A	186	TYR	3.1
1	B	40	PHE	2.9
1	B	43	LEU	2.9
1	B	248	PRO	2.8
1	B	35	GLN	2.8
2	D	41	THR	2.8
2	D	9	VAL	2.7
1	B	131	SER	2.7
1	B	313	LEU	2.7
1	B	314	THR	2.6
1	B	263	ILE	2.6
1	B	253	LEU	2.6
1	B	39	ILE	2.6
1	B	255	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	39	LEU	2.5
1	B	132	TRP	2.4
1	C	325	ASP	2.4
1	B	239	ILE	2.4
2	D	13	VAL	2.4
1	B	237	THR	2.3
1	B	191	TYR	2.3
1	B	186	TYR	2.3
1	A	255	PHE	2.3
1	B	194	PHE	2.3
1	B	251	THR	2.3
1	B	323	ALA	2.2
1	B	121	VAL	2.2
1	B	246	ILE	2.2
1	B	125	THR	2.1
1	B	190	ILE	2.1
1	B	259	MET	2.1
1	B	330	LEU	2.0
1	A	33	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	SEP	D	38	10/11	0.75	0.10	121,165,173,174	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	1367	4/4	0.48	0.41	133,135,144,151	0
4	ZN	B	1366	1/1	0.86	0.27	107,107,107,107	1
4	ZN	A	1366	1/1	0.92	0.21	71,71,71,71	1
4	ZN	C	1366	1/1	0.94	0.26	87,87,87,87	1
3	FE	C	1365	1/1	0.96	0.12	83,83,83,83	0
3	FE	B	1365	1/1	0.97	0.06	83,83,83,83	0
3	FE	B	1364	1/1	0.97	0.08	71,71,71,71	0
3	FE	C	1364	1/1	0.98	0.09	59,59,59,59	0
3	FE	A	1364	1/1	0.99	0.05	67,67,67,67	0
3	FE	A	1365	1/1	0.99	0.03	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.