



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:35 PM UTC

PDB ID : 8PQ7 / pdb_00008pq7
Title : The Potato Late Blight pathogen (*Phytophthora infestans*) effector protein Pi04134 in complex with potato protein phosphatase type 1c (PP1c).
Authors : Bentham, A.R.; Banfield, M.J.
Deposited on : 2023-07-10
Resolution : 2.10 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

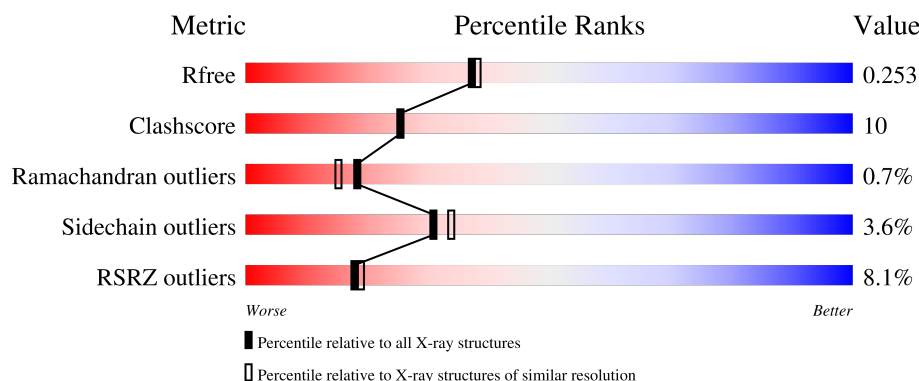
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	295	8% 78% 17% ...
1	C	295	6% 74% 20% ...
2	B	89	8% 67% 16% .. 15%
2	D	89	10% 75% 10% . 13%

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
4	EDO	A	303	-	-	X	-
4	EDO	C	303	-	-	X	-
4	EDO	C	304	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6116 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 Serine/threonine-protein phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2305	1477	385	426	17			
1	C	289	Total	C	N	O	S	0	0	0
			2312	1482	386	427	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP M1C5B8
A	2	PRO	-	expression tag	UNP M1C5B8
A	186	GLY	ASN	conflict	UNP M1C5B8
A	210	GLU	ASP	conflict	UNP M1C5B8
A	238	ASP	GLU	conflict	UNP M1C5B8
C	1	GLY	-	expression tag	UNP M1C5B8
C	2	PRO	-	expression tag	UNP M1C5B8
C	186	GLY	ASN	conflict	UNP M1C5B8
C	210	GLU	ASP	conflict	UNP M1C5B8
C	238	ASP	GLU	conflict	UNP M1C5B8

- Molecule 2 is a protein called RxLR effector protein PexRD24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	0
			632	411	109	110	2			
2	D	77	Total	C	N	O	S	0	0	0
			640	418	111	109	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	66	GLY	-	expression tag	UNP D0N0Z8
B	67	PRO	-	expression tag	UNP D0N0Z8

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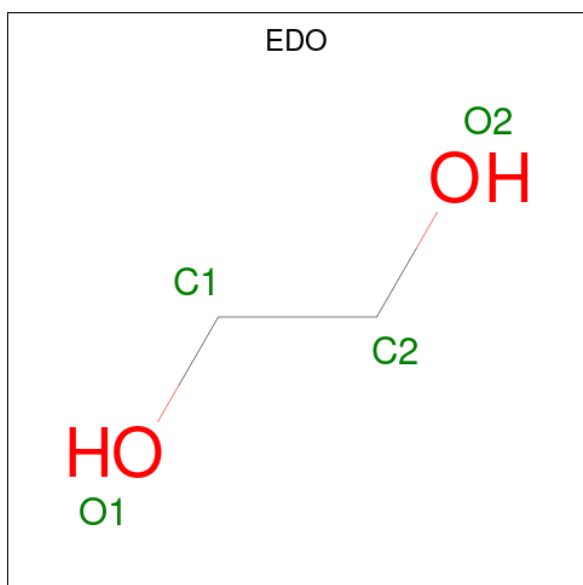
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Chain	Residue	Modelled	Actual	Comment	Reference
D	66	GLY	-	expression tag	UNP D0N0Z8
D	67	PRO	-	expression tag	UNP D0N0Z8

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	75	Total O 75 75	0	0

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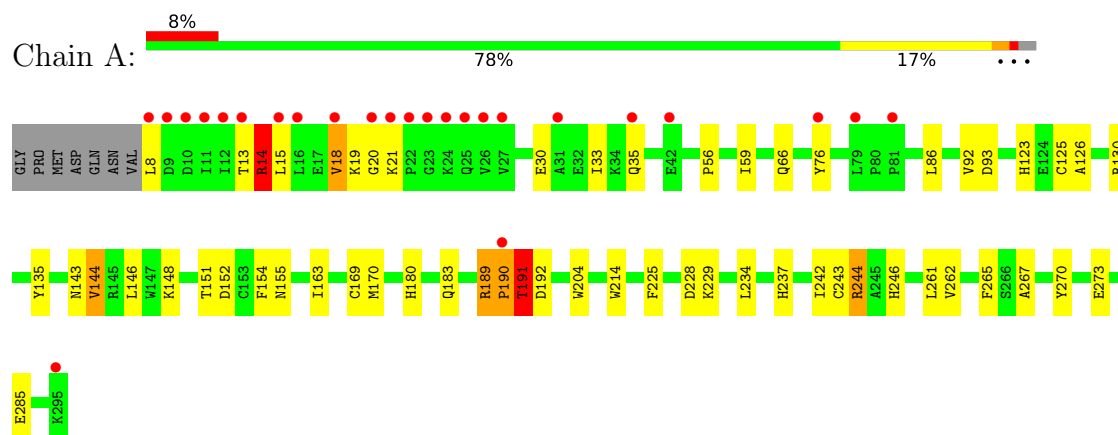
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	26	Total 26	O 26	0	0
5	C	79	Total 79	O 79	0	0
5	D	31	Total 31	O 31	0	0

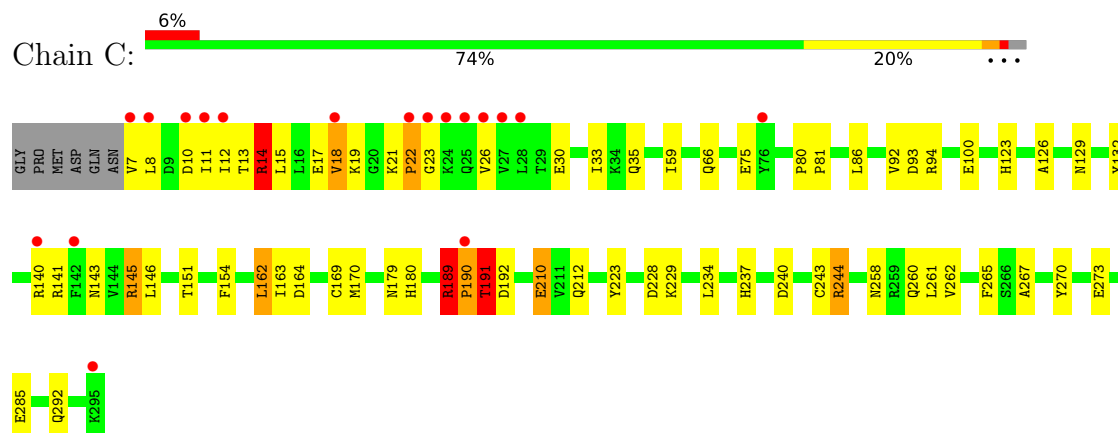
3 Residue-property plots [i](#)

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.

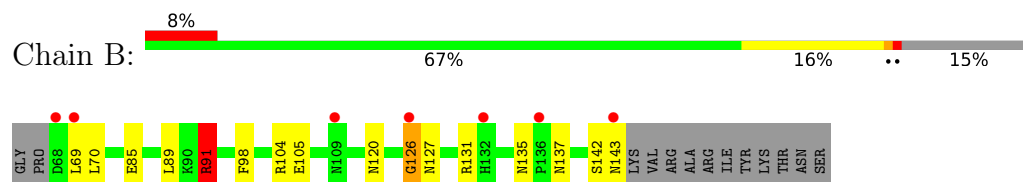
- Molecule 1: Serine/threonine-protein phosphatase



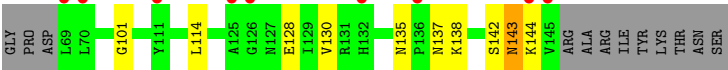
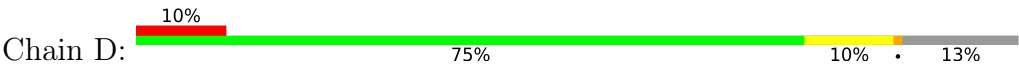
- Molecule 1: Serine/threonine-protein phosphatase



- Molecule 2: RxLR effector protein PexRD24



- Molecule 2: RxLR effector protein PexRD24



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.49Å 57.04Å 59.02Å 84.35° 86.49° 89.85°	Depositor
Resolution (Å)	58.62 – 2.10 58.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (58.62-2.10) 97.4 (58.62-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.202 , 0.251 0.212 , 0.253	Depositor DCC
R_{free} test set	1979 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6116	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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: EDO, MN

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	0.65	0/2355	1.11	5/3185 (0.2%)
1	C	0.67	0/2362	1.13	7/3195 (0.2%)
2	B	0.66	0/645	1.15	2/861 (0.2%)
2	D	0.61	0/653	1.08	1/871 (0.1%)
All	All	0.66	0/6015	1.12	15/8112 (0.2%)

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	2
1	C	0	2
2	B	0	4
All	All	0	8

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	PRO	N-CA-C	-8.33	95.30	112.47
1	A	190	PRO	N-CA-C	-8.23	95.51	112.47
2	B	91	ARG	CG-CD-NE	-7.24	96.07	112.00
1	C	189	ARG	CA-CB-CG	-6.74	100.62	114.10
2	B	105	GLU	CB-CG-CD	6.61	123.84	112.60
1	C	22	PRO	N-CA-C	6.37	121.34	111.21
1	A	191	THR	CB-CA-C	-6.01	96.84	110.07
2	D	128	GLU	CB-CG-CD	5.93	122.69	112.60
1	C	191	THR	CB-CA-C	-5.73	97.45	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	228	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	189	ARG	N-CA-CB	5.17	119.58	110.37
1	C	190	PRO	CB-CA-C	5.17	120.10	111.56
1	A	190	PRO	CB-CA-C	5.14	120.05	111.56
1	A	225	PHE	CA-CB-CG	5.12	118.92	113.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	8	LEU	Peptide
2	B	104	ARG	Sidechain
2	B	126	GLY	Peptide
2	B	131	ARG	Sidechain
2	B	91	ARG	Sidechain
1	C	14	ARG	Sidechain
1	C	23	GLY	Peptide

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	2305	0	2281	46	0
1	C	2312	0	2290	54	0
2	B	632	0	654	11	0
2	D	640	0	672	9	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
4	A	4	0	6	8	0
4	C	8	0	12	15	0
5	A	75	0	0	3	0
5	B	26	0	0	0	0
5	C	79	0	0	3	0
5	D	31	0	0	0	0
All	All	6116	0	5915	114	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 10.

All (114) 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:189:ARG:O	1:A:191:THR:N	1.95	0.99
1:C:189:ARG:O	1:C:191:THR:N	1.95	0.99
1:A:189:ARG:O	1:A:190:PRO:C	2.09	0.93
1:C:189:ARG:O	1:C:190:PRO:C	2.09	0.93
1:C:273:GLU:OE2	5:C:401:HOH:O	1.86	0.93
1:A:214:TRP:H	2:B:120:ASN:HD21	1.22	0.87
1:C:151:THR:HG23	4:C:304:EDO:H21	1.55	0.87
4:C:303:EDO:H11	2:D:101:GLY:HA2	1.63	0.81
1:A:123:HIS:HE1	5:A:468:HOH:O	1.65	0.79
1:A:273:GLU:OE2	5:A:401:HOH:O	2.04	0.76
1:C:14:ARG:HH11	1:C:18:VAL:HG21	1.52	0.75
1:A:14:ARG:HH11	1:A:18:VAL:HG21	1.54	0.71
1:A:33:ILE:CG2	1:A:146:LEU:HD11	2.21	0.71
2:B:85:GLU:O	2:B:89:LEU:HD13	1.91	0.70
1:C:93:ASP:OD2	1:C:123:HIS:HD2	1.73	0.70
1:C:154:PHE:HD2	4:C:304:EDO:H12	1.57	0.69
1:C:223:TYR:HE2	4:C:303:EDO:H22	1.58	0.69
1:A:33:ILE:HG22	1:A:146:LEU:HD11	1.73	0.69
1:A:151:THR:HA	4:A:303:EDO:H11	1.75	0.69
1:A:93:ASP:OD2	1:A:123:HIS:HD2	1.77	0.66
1:C:33:ILE:CG2	1:C:146:LEU:HD11	2.25	0.66
1:A:66:GLN:HE22	1:A:270:TYR:HA	1.60	0.66
4:C:303:EDO:C1	2:D:101:GLY:HA2	2.26	0.65
1:C:33:ILE:HG22	1:C:146:LEU:HD11	1.77	0.65
1:C:66:GLN:HE22	1:C:270:TYR:HA	1.60	0.65
1:A:154:PHE:HB2	4:A:303:EDO:H11	1.82	0.62
1:C:26:VAL:HG23	1:C:141:ARG:HH11	1.64	0.61
2:B:126:GLY:O	2:B:127:ASN:HB2	2.01	0.61
1:A:234:LEU:HD21	1:A:242:ILE:HG13	1.83	0.60
1:A:204:TRP:O	1:A:246:HIS:HE1	1.85	0.59
1:A:183:GLN:HA	1:C:212:GLN:HG3	1.85	0.58
1:C:126:ALA:N	4:C:304:EDO:H22	2.18	0.58
1:A:191:THR:HB	1:A:192:ASP:O	2.04	0.58
2:B:135:ASN:HD21	2:B:137:ASN:HB2	1.68	0.58
2:D:135:ASN:HD21	2:D:137:ASN:HB2	1.69	0.56
1:C:191:THR:HB	1:C:192:ASP:O	2.06	0.56
1:A:244:ARG:C	1:A:244:ARG:HD3	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:TYR:HE2	4:C:303:EDO:C2	2.18	0.55
1:A:148:LYS:HE2	1:A:152:ASP:OD1	2.07	0.55
1:C:17:GLU:O	1:C:21:LYS:HG3	2.05	0.55
1:A:125:CYS:C	4:A:303:EDO:H21	2.33	0.54
1:C:244:ARG:HD3	1:C:244:ARG:C	2.33	0.53
1:A:126:ALA:N	4:A:303:EDO:H21	2.24	0.53
1:C:145:ARG:HB3	1:C:145:ARG:NH2	2.24	0.53
1:C:179:ASN:O	1:C:237:HIS:HE1	1.91	0.52
1:A:154:PHE:HB2	4:A:303:EDO:C1	2.40	0.52
1:A:19:LYS:C	1:A:21:LYS:H	2.18	0.51
1:A:237:HIS:HE1	5:A:454:HOH:O	1.93	0.51
1:C:123:HIS:HE1	5:C:464:HOH:O	1.93	0.51
2:B:142:SER:O	2:B:143:ASN:C	2.54	0.50
1:C:19:LYS:O	1:C:22:PRO:HD2	2.10	0.50
1:C:154:PHE:HB2	4:C:304:EDO:O2	2.13	0.49
2:D:135:ASN:ND2	2:D:137:ASN:HB2	2.27	0.49
2:D:130:VAL:HG12	2:D:130:VAL:O	2.12	0.49
1:A:261:LEU:HD23	1:A:262:VAL:N	2.28	0.49
4:C:304:EDO:H22	5:C:437:HOH:O	2.12	0.49
1:C:265:PHE:CE1	1:C:267:ALA:HB3	2.48	0.48
2:B:135:ASN:ND2	2:B:137:ASN:HB2	2.27	0.48
1:C:8:LEU:HB3	1:C:10:ASP:OD1	2.13	0.48
1:C:100:GLU:OE2	1:C:141:ARG:NH1	2.36	0.47
1:A:15:LEU:C	1:A:19:LYS:HZ3	2.22	0.47
1:C:59:ILE:HD11	1:C:163:ILE:CD1	2.45	0.47
1:A:229:LYS:HA	1:A:229:LYS:HE2	1.96	0.47
1:A:59:ILE:HD11	1:A:163:ILE:CD1	2.45	0.47
1:A:214:TRP:H	2:B:120:ASN:ND2	2.00	0.46
1:C:169:CYS:HA	1:C:243:CYS:O	2.16	0.46
1:A:204:TRP:O	1:A:246:HIS:CE1	2.67	0.46
1:A:30:GLU:OE1	1:A:143:ASN:ND2	2.43	0.46
1:C:94:ARG:NH1	1:C:132:TYR:CD1	2.83	0.46
1:C:26:VAL:CG2	1:C:141:ARG:HH11	2.28	0.46
1:C:129:ASN:HD21	4:C:304:EDO:C1	2.29	0.45
1:C:93:ASP:OD2	1:C:123:HIS:CD2	2.60	0.45
1:C:234:LEU:HD22	1:C:260:GLN:HB3	1.98	0.45
1:C:261:LEU:HD23	1:C:262:VAL:N	2.31	0.45
1:A:265:PHE:CE1	1:A:267:ALA:HB3	2.52	0.45
1:C:180:HIS:CD2	2:D:130:VAL:HG11	2.52	0.45
1:A:35:GLN:NE2	1:A:35:GLN:HA	2.31	0.45
1:A:126:ALA:O	1:A:130:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:HIS:CE1	1:C:210:GLU:HA	2.52	0.45
1:A:169:CYS:HA	1:A:243:CYS:O	2.17	0.45
1:C:223:TYR:CE2	4:C:303:EDO:C2	3.01	0.44
1:A:56:PRO:HD3	1:A:285:GLU:HG2	1.98	0.44
1:A:151:THR:HG23	4:A:303:EDO:H22	1.99	0.44
1:C:240:ASP:OD2	2:D:138:LYS:HA	2.17	0.44
1:C:145:ARG:HH21	1:C:145:ARG:CB	2.31	0.43
1:C:15:LEU:O	1:C:19:LYS:NZ	2.49	0.43
1:C:59:ILE:HA	1:C:86:LEU:O	2.17	0.43
1:C:154:PHE:CD2	4:C:304:EDO:H12	2.45	0.43
1:A:126:ALA:N	4:A:303:EDO:C2	2.81	0.43
2:B:69:LEU:HG	2:B:70:LEU:H	1.84	0.43
4:C:303:EDO:H11	2:D:101:GLY:CA	2.43	0.43
2:B:91:ARG:HA	2:B:91:ARG:HD3	1.86	0.43
1:C:7:VAL:CG2	1:C:12:ILE:HD11	2.48	0.43
1:C:92:VAL:O	1:C:93:ASP:HB2	2.17	0.43
1:C:129:ASN:HD21	4:C:304:EDO:H11	1.83	0.43
1:A:19:LYS:O	1:A:21:LYS:N	2.52	0.42
1:A:93:ASP:OD2	1:A:123:HIS:CD2	2.63	0.42
1:C:126:ALA:H	4:C:304:EDO:H22	1.84	0.42
1:A:59:ILE:HA	1:A:86:LEU:O	2.19	0.42
1:C:170:MET:O	1:C:244:ARG:HA	2.20	0.42
1:C:229:LYS:HA	1:C:229:LYS:HE2	2.00	0.42
1:A:135:TYR:CE1	1:A:144:VAL:CG2	3.03	0.42
2:B:98:PHE:HA	1:C:258:ASN:OD1	2.19	0.42
1:A:170:MET:O	1:A:244:ARG:HA	2.20	0.41
1:C:292:GLN:CD	1:C:292:GLN:N	2.78	0.41
2:B:85:GLU:O	2:B:89:LEU:CD1	2.66	0.41
1:C:162:LEU:HD23	1:C:162:LEU:HA	1.93	0.41
1:A:35:GLN:HA	1:A:35:GLN:HE21	1.86	0.41
1:C:80:PRO:HA	1:C:81:PRO:HA	1.88	0.41
2:D:142:SER:O	2:D:143:ASN:C	2.64	0.41
1:C:21:LYS:N	1:C:22:PRO:CD	2.83	0.40
1:A:155:ASN:OD1	4:A:303:EDO:O1	2.39	0.40
1:C:30:GLU:OE1	1:C:143:ASN:ND2	2.48	0.40
1:A:92:VAL:O	1:A:93:ASP:HB2	2.20	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	286/295 (97%)	268 (94%)	16 (6%)	2 (1%)	18	15
1	C	287/295 (97%)	267 (93%)	18 (6%)	2 (1%)	18	15
2	B	74/89 (83%)	70 (95%)	4 (5%)	0	100	100
2	D	75/89 (84%)	71 (95%)	3 (4%)	1 (1%)	9	6
All	All	722/768 (94%)	676 (94%)	41 (6%)	5 (1%)	18	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLY
2	D	144	LYS
1	A	189	ARG
1	C	189	ARG
1	C	164	ASP

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	253/259 (98%)	246 (97%)	7 (3%)	38	43
1	C	254/259 (98%)	241 (95%)	13 (5%)	21	21
2	B	69/80 (86%)	68 (99%)	1 (1%)	59	67
2	D	70/80 (88%)	68 (97%)	2 (3%)	37	42
All	All	646/678 (95%)	623 (96%)	23 (4%)	31	34

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	14	ARG
1	A	18	VAL
1	A	76	TYR
1	A	144	VAL
1	A	191	THR
1	A	244	ARG
2	B	91	ARG
1	C	11	ILE
1	C	13	THR
1	C	14	ARG
1	C	18	VAL
1	C	35	GLN
1	C	75	GLU
1	C	140	ARG
1	C	145	ARG
1	C	162	LEU
1	C	191	THR
1	C	210	GLU
1	C	244	ARG
1	C	285	GLU
2	D	114	LEU
2	D	143	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	66	GLN
1	A	123	HIS
1	A	180	HIS
1	A	246	HIS
1	A	260	GLN
2	B	109	ASN
2	B	117	ASN
2	B	120	ASN
2	B	132	HIS
2	B	135	ASN
2	B	137	ASN
2	B	143	ASN
1	C	66	GLN

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Mol	Chain	Res	Type
1	C	123	HIS
1	C	180	HIS
1	C	260	GLN
2	D	132	HIS
2	D	135	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
4	EDO	A	303	-	3,3,3	0.33	0	2,2,2	0.68	0
4	EDO	C	303	-	3,3,3	0.53	0	2,2,2	0.60	0
4	EDO	C	304	-	3,3,3	0.17	0	2,2,2	0.46	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
4	EDO	A	303	-	-	1/1/1/1	-
4	EDO	C	303	-	-	1/1/1/1	-
4	EDO	C	304	-	-	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
4	A	303	EDO	O1-C1-C2-O2
4	C	304	EDO	O1-C1-C2-O2
4	C	303	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	EDO	8	0
4	C	303	EDO	6	0
4	C	304	EDO	9	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	288/295 (97%)	0.44	25 (8%) 16 16	16, 35, 74, 133	0
1	C	289/295 (97%)	0.42	18 (6%) 26 28	17, 35, 72, 145	0
2	B	76/89 (85%)	0.73	7 (9%) 14 15	22, 43, 76, 100	0
2	D	77/89 (86%)	0.76	9 (11%) 9 9	19, 40, 84, 113	0
All	All	730/768 (95%)	0.50	59 (8%) 18 19	16, 37, 76, 145	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	VAL	8.2
1	A	8	LEU	6.2
1	A	26	VAL	5.9
1	A	12	ILE	5.9
1	C	27	VAL	5.9
1	C	8	LEU	5.6
2	D	145	VAL	5.2
2	B	69	LEU	5.0
2	D	69	LEU	4.9
1	A	22	PRO	4.5
1	A	24	LYS	4.5
1	A	76	TYR	4.4
1	A	27	VAL	4.4
1	C	23	GLY	4.2
1	A	23	GLY	4.2
1	A	25	GLN	3.9
1	C	12	ILE	3.8
1	A	190	PRO	3.8
2	D	70	LEU	3.7
1	C	7	VAL	3.6
1	C	76	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	68	ASP	3.4
1	C	24	LYS	3.3
1	A	16	LEU	3.2
1	C	190	PRO	3.1
2	B	126	GLY	3.1
1	C	11	ILE	3.0
2	B	143	ASN	2.8
1	A	13	THR	2.8
1	A	31	ALA	2.7
2	D	111	TYR	2.7
1	A	81	PRO	2.7
2	B	109	ASN	2.7
1	C	22	PRO	2.7
2	D	144	LYS	2.7
1	C	25	GLN	2.6
1	A	21	LYS	2.5
1	C	140	ARG	2.5
1	A	79	LEU	2.5
1	C	295	LYS	2.5
2	D	125	ALA	2.4
1	A	35	GLN	2.4
2	D	126	GLY	2.4
2	B	136	PRO	2.4
1	A	295	LYS	2.3
1	C	142	PHE	2.3
1	A	11	ILE	2.3
1	A	15	LEU	2.3
1	C	18	VAL	2.2
2	D	132	HIS	2.2
2	D	136	PRO	2.2
1	A	18	VAL	2.2
1	A	20	GLY	2.2
1	C	28	LEU	2.2
2	B	132	HIS	2.1
1	A	42	GLU	2.1
1	A	9	ASP	2.1
1	A	10	ASP	2.1
1	C	10	ASP	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 [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
4	EDO	A	303	4/4	0.70	0.23	60,68,68,83	0
4	EDO	C	304	4/4	0.75	0.21	64,67,70,74	0
3	MN	A	301	1/1	0.84	0.17	103,103,103,103	0
3	MN	A	302	1/1	0.86	0.15	83,83,83,83	0
3	MN	C	302	1/1	0.89	0.17	93,93,93,93	0
3	MN	C	301	1/1	0.90	0.18	78,78,78,78	0
4	EDO	C	303	4/4	0.92	0.19	27,31,31,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.