



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:34 PM UTC

PDB ID : 4F1L / pdb_00004f1l
Title : Human Artd8 (Parp14, Bal2) - catalytic domain in complex with inhibitor A16(Z)
Authors : Karlberg, T.; Andersson, C.D.; Lindgren, A.; Spjut, S.; Thorsell, A.G.; Ekblad, T.; Weigelt, J.; Elofsson, M.; Linusson, A.; Schuler, H.
Deposited on : 2012-05-07
Resolution : 1.90 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

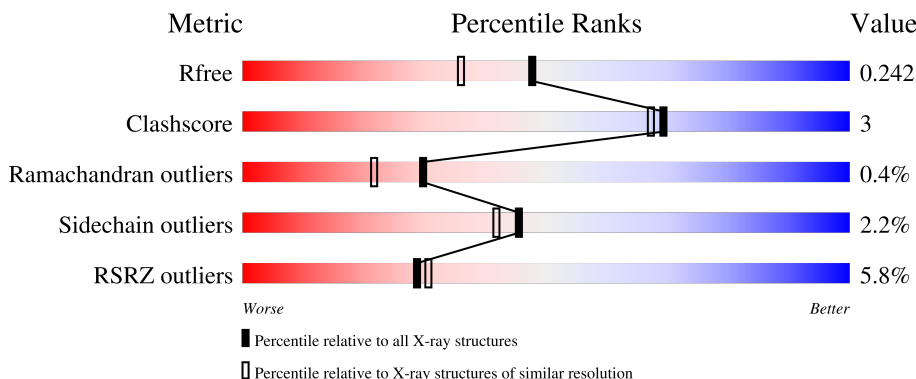
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	193	5% 92% 5% .
1	B	193	6% 85% 7% . 6%
1	C	193	5% 89% 6% . .
1	D	193	7% 88% 7% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6320 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.

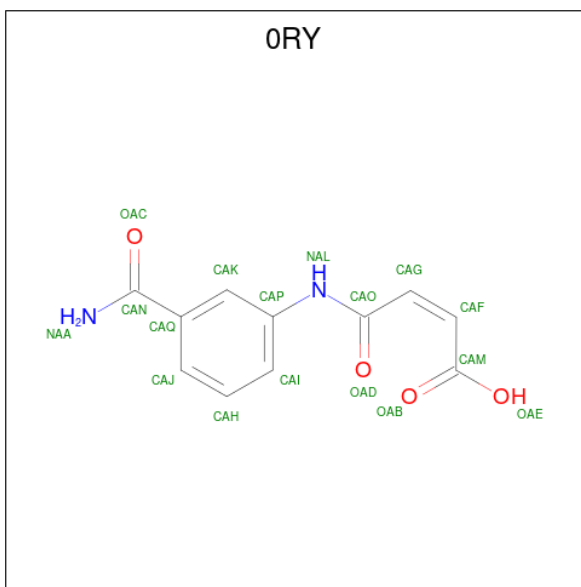
- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	1	0
			1513	957	266	286	4			
1	B	181	Total	C	N	O	S	0	1	0
			1479	935	262	278	4			
1	C	187	Total	C	N	O	S	0	0	0
			1512	956	267	285	4			
1	D	185	Total	C	N	O	S	0	0	0
			1495	946	263	282	4			

There are 8 discrepancies between the modelled and reference sequences:

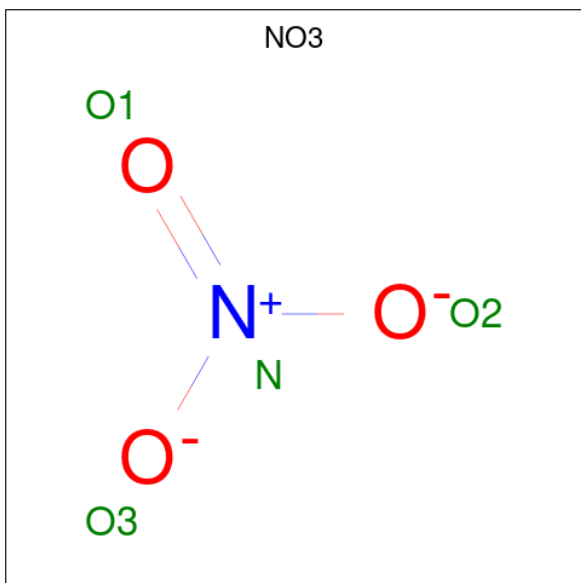
Chain	Residue	Modelled	Actual	Comment	Reference
A	1528	SER	-	expression tag	UNP Q460N5
A	1529	MET	-	expression tag	UNP Q460N5
B	1528	SER	-	expression tag	UNP Q460N5
B	1529	MET	-	expression tag	UNP Q460N5
C	1528	SER	-	expression tag	UNP Q460N5
C	1529	MET	-	expression tag	UNP Q460N5
D	1528	SER	-	expression tag	UNP Q460N5
D	1529	MET	-	expression tag	UNP Q460N5

- Molecule 2 is (2Z)-4-[(3-carbamoylphenyl)amino]-4-oxobut-2-enoic acid (CCD ID: 0RY) (formula: C₁₁H₁₀N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	11	2	4		
2	B	1	Total	C	N	O	0	0
			17	11	2	4		
2	C	1	Total	C	N	O	0	0
			17	11	2	4		
2	D	1	Total	C	N	O	0	0
			17	11	2	4		

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



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

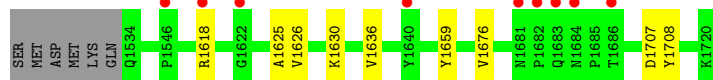
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total	O	0	0
			56	56		
4	B	71	Total	O	0	0
			71	71		
4	C	58	Total	O	0	0
			58	58		
4	D	60	Total	O	0	0
			60	60		

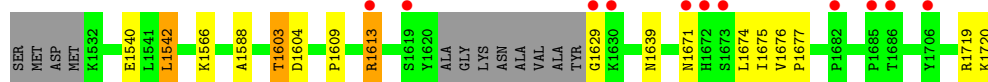
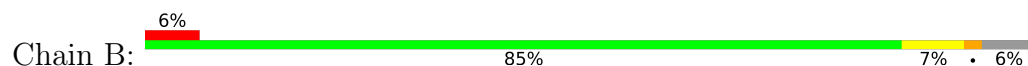
3 Residue-property plots [i](#)

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.

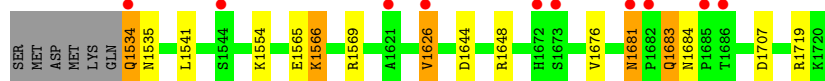
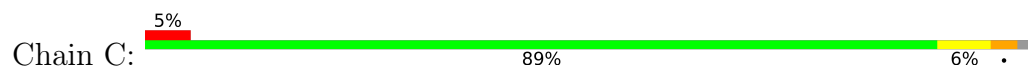
- Molecule 1: Poly [ADP-ribose] polymerase 14



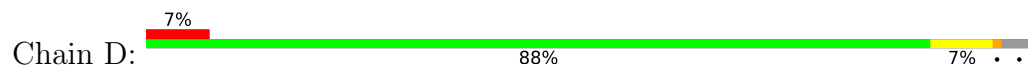
- Molecule 1: Poly [ADP-ribose] polymerase 14



- Molecule 1: Poly [ADP-ribose] polymerase 14



- Molecule 1: Poly [ADP-ribose] polymerase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	39.65Å 81.89Å 83.19Å 60.12° 78.32° 80.31°	Depositor
Resolution (Å)	34.89 – 1.90 34.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.89-1.90) 97.0 (34.89-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.57 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.197 , 0.239 0.201 , 0.242	Depositor DCC
R_{free} test set	3386 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6320	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.28% 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: NO3, ORY

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	1.03	1/1560 (0.1%)	0.95	2/2123 (0.1%)
1	B	1.08	1/1523 (0.1%)	0.97	1/2068 (0.0%)
1	C	1.01	0/1556	1.00	4/2117 (0.2%)
1	D	1.04	0/1538	0.97	2/2092 (0.1%)
All	All	1.04	2/6177 (0.0%)	0.97	9/8400 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1636	VAL	CA-CB	5.56	1.61	1.54
1	B	1588	ALA	CA-CB	5.26	1.62	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1676	VAL	CA-C-N	-6.47	113.72	120.38
1	A	1676	VAL	C-N-CA	-6.47	113.72	120.38
1	C	1707	ASP	N-CA-C	5.81	118.36	111.33
1	B	1639	ASN	N-CA-C	5.45	117.92	111.33
1	C	1676	VAL	N-CA-C	-5.26	103.07	109.01
1	D	1681	ASN	CA-C-N	5.21	125.52	119.47
1	D	1681	ASN	C-N-CA	5.21	125.52	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1681	ASN	CA-C-N	-5.11	114.34	119.56
1	C	1681	ASN	C-N-CA	-5.11	114.34	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1659	TYR	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	1513	0	1429	4	0
1	B	1479	0	1406	17	0
1	C	1512	0	1431	14	0
1	D	1495	0	1411	9	0
2	A	17	0	9	0	0
2	B	17	0	9	1	0
2	C	17	0	9	1	0
2	D	17	0	9	1	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
4	A	56	0	0	0	0
4	B	71	0	0	1	0
4	C	58	0	0	1	0
4	D	60	0	0	2	0
All	All	6320	0	5713	41	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 3.

All (41) 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:C:1534:GLN:HG2	1:C:1535:ASN:H	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1609:PRO:O	1:B:1613[A]:ARG:HG2	1.79	0.81
1:B:1542:LEU:N	1:B:1542:LEU:HD12	2.00	0.77
1:B:1719:ARG:NH2	4:B:1924:HOH:O	2.16	0.73
1:C:1534:GLN:CG	1:C:1535:ASN:H	2.04	0.70
1:D:1541:LEU:HD23	1:D:1541:LEU:N	2.07	0.69
2:B:1801:ORY:OAE	2:B:1801:ORY:NAL	2.24	0.66
1:A:1625:ALA:HB2	1:A:1630:LYS:CD	2.31	0.61
1:B:1675:ILE:HD12	1:B:1676:VAL:HG13	1.82	0.61
1:D:1540:GLU:HG2	1:D:1541:LEU:O	2.01	0.60
1:B:1542:LEU:HD12	1:B:1542:LEU:H	1.66	0.59
1:B:1542:LEU:N	1:B:1542:LEU:CD1	2.68	0.56
1:A:1625:ALA:HB2	1:A:1630:LYS:HD3	1.87	0.56
1:D:1547:GLU:OE2	1:D:1569:ARG:NH1	2.39	0.56
1:B:1540:GLU:H	1:C:1535:ASN:HD21	1.56	0.53
1:D:1616:PHE:O	1:D:1617:ASN:O	2.26	0.53
1:C:1534:GLN:CG	1:C:1535:ASN:N	2.72	0.52
1:C:1534:GLN:HG2	1:C:1535:ASN:N	2.17	0.51
1:B:1613[A]:ARG:CZ	1:C:1566:LYS:NZ	2.74	0.51
1:D:1626:VAL:HG21	2:D:1801:ORY:H3	1.93	0.51
1:D:1589:LYS:HE3	1:D:1687:ASP:OD1	2.10	0.51
1:D:1720:LYS:NZ	4:D:1932:HOH:O	2.44	0.51
1:B:1542:LEU:H	1:B:1542:LEU:CD1	2.24	0.50
1:D:1672:HIS:ND1	4:D:1945:HOH:O	2.35	0.50
1:A:1625:ALA:HB2	1:A:1630:LYS:HD2	1.93	0.50
1:B:1540:GLU:H	1:C:1535:ASN:ND2	2.10	0.50
1:C:1644:ASP:O	1:C:1648:ARG:HG3	2.13	0.49
1:B:1676:VAL:HB	1:B:1677:PRO:CD	2.44	0.48
1:C:1683:GLN:OE1	1:C:1684:ASN:HB2	2.14	0.47
1:B:1613[A]:ARG:NH1	1:C:1566:LYS:HZ1	2.13	0.47
1:B:1674:LEU:HD22	1:B:1676:VAL:O	2.14	0.46
1:B:1609:PRO:O	1:B:1613[A]:ARG:CG	2.58	0.46
1:B:1603:THR:HG23	1:B:1604:ASP:O	2.16	0.45
1:B:1675:ILE:HD12	1:B:1675:ILE:C	2.42	0.45
1:C:1626:VAL:HG21	2:C:1801:ORY:CAF	2.47	0.45
1:A:1707[A]:ASP:OD2	1:A:1708:TYR:N	2.49	0.44
1:C:1554:LYS:HE3	4:C:1928:HOH:O	2.18	0.43
1:B:1629:GLY:O	1:B:1675:ILE:O	2.36	0.43
1:C:1541:LEU:HD21	1:C:1569:ARG:NH1	2.34	0.42
1:C:1565:GLU:OE2	1:C:1719:ARG:NE	2.43	0.42
1:D:1608:VAL:HB	1:D:1609:PRO:HD3	2.03	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	186/193 (96%)	183 (98%)	2 (1%)	1 (0%)	24	16
1	B	178/193 (92%)	177 (99%)	1 (1%)	0	100	100
1	C	185/193 (96%)	180 (97%)	4 (2%)	1 (0%)	24	16
1	D	181/193 (94%)	175 (97%)	5 (3%)	1 (1%)	21	13
All	All	730/772 (95%)	715 (98%)	12 (2%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1617	ASN
1	A	1626	VAL
1	C	1626	VAL

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	164/170 (96%)	163 (99%)	1 (1%)	78	81
1	B	162/170 (95%)	155 (96%)	7 (4%)	26	18
1	C	164/170 (96%)	160 (98%)	4 (2%)	43	38
1	D	162/170 (95%)	159 (98%)	3 (2%)	50	47
All	All	652/680 (96%)	637 (98%)	15 (2%)	45	40

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1618	ARG
1	B	1542	LEU
1	B	1566	LYS
1	B	1603	THR
1	B	1613[A]	ARG
1	B	1613[B]	ARG
1	B	1671	ASN
1	B	1720	LYS
1	C	1534	GLN
1	C	1566	LYS
1	C	1681	ASN
1	C	1683	GLN
1	D	1541	LEU
1	D	1544	SER
1	D	1618	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1561	HIS
1	B	1571	GLN
1	B	1614	ASN
1	B	1637	ASN
1	C	1535	ASN
1	C	1614	ASN
1	C	1709	GLN
1	D	1571	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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
2	ORY	C	1801	-	17,17,17	1.54	4 (23%)	22,22,22	2.07	8 (36%)
3	NO3	A	1802	-	1,3,3	2.78	1 (100%)	0,3,3	-	-
2	ORY	D	1801	-	17,17,17	1.96	6 (35%)	22,22,22	1.70	5 (22%)
3	NO3	C	1802	-	1,3,3	2.54	1 (100%)	0,3,3	-	-
2	ORY	B	1801	-	17,17,17	1.89	4 (23%)	22,22,22	1.34	3 (13%)
2	ORY	A	1801	-	17,17,17	2.00	5 (29%)	22,22,22	1.50	4 (18%)

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	ORY	A	1801	-	-	3/13/13/13	0/1/1/1
2	ORY	D	1801	-	-	2/13/13/13	0/1/1/1
2	ORY	C	1801	-	-	2/13/13/13	0/1/1/1
2	ORY	B	1801	-	-	2/13/13/13	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1801	ORY	CAQ-CAN	4.74	1.57	1.50
2	B	1801	ORY	CAP-NAL	-4.23	1.33	1.41
2	D	1801	ORY	CAG-CAO	-3.75	1.40	1.48
2	A	1801	ORY	CAP-NAL	-3.65	1.34	1.41
2	B	1801	ORY	CAG-CAO	-3.62	1.40	1.48
2	D	1801	ORY	CAP-NAL	-3.46	1.34	1.41
2	D	1801	ORY	CAG-CAF	3.28	1.42	1.33
2	C	1801	ORY	CAG-CAO	-2.90	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1801	0RY	CAG-CAO	-2.89	1.42	1.48
2	A	1801	0RY	CAG-CAF	2.87	1.41	1.33
2	B	1801	0RY	CAG-CAF	2.81	1.41	1.33
3	A	1802	NO3	O1-N	2.78	1.38	1.24
2	D	1801	0RY	CAK-CAP	-2.66	1.35	1.39
2	B	1801	0RY	CAF-CAM	-2.62	1.41	1.48
2	C	1801	0RY	CAG-CAF	2.59	1.40	1.33
3	C	1802	NO3	O1-N	2.54	1.36	1.24
2	A	1801	0RY	CAF-CAM	-2.51	1.42	1.48
2	C	1801	0RY	CAF-CAM	-2.42	1.42	1.48
2	D	1801	0RY	CAF-CAM	-2.41	1.42	1.48
2	C	1801	0RY	CAO-NAL	-2.29	1.31	1.35
2	D	1801	0RY	CAO-NAL	-2.12	1.32	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1801	0RY	CAG-CAO-NAL	4.54	122.31	113.93
2	A	1801	0RY	CAG-CAO-NAL	3.75	120.86	113.93
2	D	1801	0RY	CAG-CAO-NAL	3.60	120.58	113.93
2	A	1801	0RY	OAD-CAO-CAG	-3.30	115.33	122.95
2	C	1801	0RY	CAK-CAP-NAL	3.24	130.66	120.13
2	B	1801	0RY	OAD-CAO-CAG	-2.94	116.17	122.95
2	C	1801	0RY	OAD-CAO-CAG	-2.92	116.21	122.95
2	C	1801	0RY	CAI-CAP-CAK	-2.88	116.17	119.66
2	D	1801	0RY	CAJ-CAQ-CAK	2.78	122.46	119.25
2	A	1801	0RY	CAK-CAP-NAL	2.64	128.70	120.13
2	B	1801	0RY	CAP-NAL-CAO	2.63	133.02	128.07
2	C	1801	0RY	CAH-CAJ-CAQ	-2.50	117.90	120.36
2	D	1801	0RY	CAH-CAJ-CAQ	-2.50	117.91	120.36
2	D	1801	0RY	CAH-CAI-CAP	2.38	122.47	119.73
2	A	1801	0RY	CAI-CAP-NAL	-2.37	112.46	120.41
2	C	1801	0RY	CAH-CAI-CAP	2.33	122.42	119.73
2	B	1801	0RY	OAD-CAO-NAL	2.30	126.14	123.11
2	C	1801	0RY	CAJ-CAQ-CAN	-2.29	114.81	121.06
2	D	1801	0RY	CAK-CAQ-CAN	-2.19	114.17	119.94
2	C	1801	0RY	CAI-CAP-NAL	-2.17	113.14	120.41

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1801	0RY	CAF-CAG-CAO-OAD
2	C	1801	0RY	CAF-CAG-CAO-OAD
2	D	1801	0RY	CAF-CAG-CAO-OAD
2	A	1801	0RY	CAF-CAG-CAO-OAD
2	B	1801	0RY	CAF-CAG-CAO-NAL
2	C	1801	0RY	CAF-CAG-CAO-NAL
2	D	1801	0RY	CAF-CAG-CAO-NAL
2	A	1801	0RY	CAF-CAG-CAO-NAL
2	A	1801	0RY	OAC-CAN-CAQ-CAJ

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1801	0RY	1	0
2	D	1801	0RY	1	0
2	B	1801	0RY	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	187/193 (96%)	0.18	9 (4%) 35 38	12, 23, 38, 54	1 (0%)
1	B	181/193 (93%)	0.34	11 (6%) 27 29	11, 23, 40, 57	1 (0%)
1	C	187/193 (96%)	0.19	10 (5%) 32 34	14, 24, 39, 55	0
1	D	185/193 (95%)	0.30	13 (7%) 22 24	12, 23, 42, 54	0
All	All	740/772 (95%)	0.25	43 (5%) 29 30	11, 23, 42, 57	2 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1629	GLY	5.4
1	D	1622	GLY	4.7
1	B	1619	SER	4.5
1	B	1630	LYS	3.8
1	B	1672	HIS	3.4
1	B	1673	SER	3.4
1	C	1685	PRO	3.3
1	B	1685	PRO	3.2
1	D	1626	VAL	3.1
1	A	1681	ASN	2.9
1	D	1619	SER	2.8
1	C	1681	ASN	2.7
1	B	1682	PRO	2.7
1	C	1686	THR	2.7
1	B	1706	TYR	2.7
1	B	1686	THR	2.6
1	C	1621	ALA	2.6
1	C	1672	HIS	2.6
1	D	1625	ALA	2.6
1	D	1686	THR	2.6
1	A	1683	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	1544	SER	2.4
1	D	1683	GLN	2.4
1	A	1684	ASN	2.4
1	B	1613[A]	ARG	2.3
1	D	1618	ARG	2.3
1	D	1620	TYR	2.3
1	C	1534	GLN	2.2
1	B	1671	ASN	2.2
1	C	1544	SER	2.2
1	A	1546	PRO	2.2
1	A	1640	TYR	2.1
1	D	1547	GLU	2.1
1	C	1626	VAL	2.1
1	D	1621	ALA	2.1
1	C	1682	PRO	2.1
1	D	1684	ASN	2.1
1	C	1673	SER	2.1
1	A	1686	THR	2.1
1	A	1682	PRO	2.1
1	D	1627	ALA	2.0
1	A	1622	GLY	2.0
1	A	1618	ARG	2.0

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($\text{\AA}^2$)	Q<0.9
3	NO3	A	1802	4/4	0.90	0.13	27,27,27,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ORY	B	1801	17/17	0.92	0.12	17,28,48,49	0
2	ORY	D	1801	17/17	0.93	0.10	15,22,37,37	0
2	ORY	A	1801	17/17	0.95	0.07	14,18,33,36	0
2	ORY	C	1801	17/17	0.95	0.08	14,20,35,36	0
3	NO3	C	1802	4/4	0.95	0.10	26,26,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.