



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:38 PM UTC

PDB ID : 4IOX / pdb_00004iox
Title : The structure of the herpes simplex virus DNA-packaging motor pUL15 C-terminal nuclease domain provides insights into cleavage of concatemeric viral genome precursors
Authors : Selvarajan Sigamani, S.; Zhao, H.; Kamau, Y.; Tang, L.
Deposited on : 2013-01-08
Resolution : 2.46 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

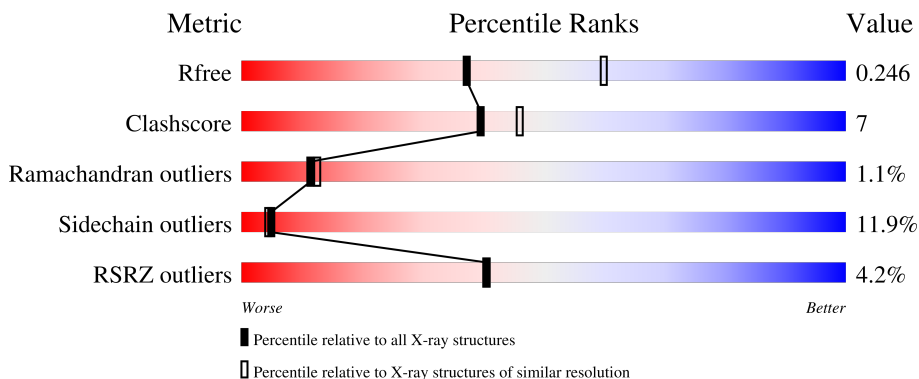
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	286	 3% 62% 14% 5% 21%
1	B	286	 2% 58% 12% 5% 24%
1	C	286	 4% 60% 13% 5% 23%
2	D	6	 100%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 5172 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 Tripartite terminase subunit UL15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	Total 1727	C 1109	N 295	O 316	S 7	0	0	0
1	B	216	Total 1653	C 1064	N 279	O 303	S 7	0	0	0
1	C	220	Total 1682	C 1085	N 283	O 307	S 7	0	0	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	MET	-	expression tag	UNP P04295
A	451	GLY	-	expression tag	UNP P04295
A	452	SER	-	expression tag	UNP P04295
A	453	SER	-	expression tag	UNP P04295
A	454	HIS	-	expression tag	UNP P04295
A	455	HIS	-	expression tag	UNP P04295
A	456	HIS	-	expression tag	UNP P04295
A	457	HIS	-	expression tag	UNP P04295
A	458	HIS	-	expression tag	UNP P04295
A	459	HIS	-	expression tag	UNP P04295
A	460	SER	-	expression tag	UNP P04295
A	461	SER	-	expression tag	UNP P04295
A	462	GLY	-	expression tag	UNP P04295
A	463	LEU	-	expression tag	UNP P04295
A	464	VAL	-	expression tag	UNP P04295
A	465	PRO	-	expression tag	UNP P04295
A	466	ARG	-	expression tag	UNP P04295
A	467	GLY	-	expression tag	UNP P04295
A	468	SER	-	expression tag	UNP P04295
A	469	HIS	-	expression tag	UNP P04295
A	470	MET	-	expression tag	UNP P04295
B	450	MET	-	expression tag	UNP P04295
B	451	GLY	-	expression tag	UNP P04295

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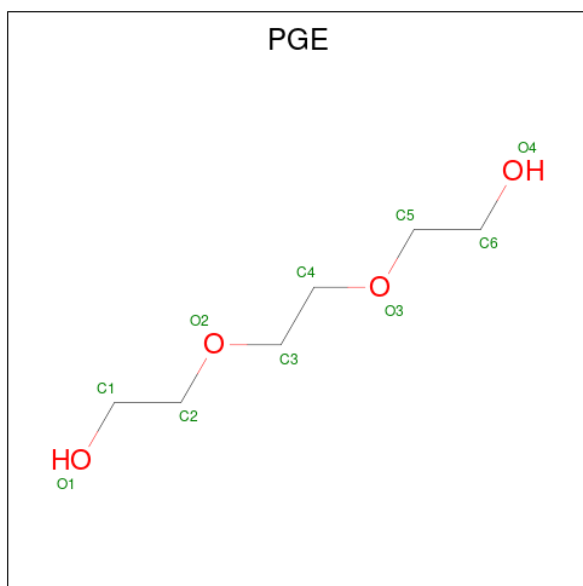
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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	SER	-	expression tag	UNP P04295
B	453	SER	-	expression tag	UNP P04295
B	454	HIS	-	expression tag	UNP P04295
B	455	HIS	-	expression tag	UNP P04295
B	456	HIS	-	expression tag	UNP P04295
B	457	HIS	-	expression tag	UNP P04295
B	458	HIS	-	expression tag	UNP P04295
B	459	HIS	-	expression tag	UNP P04295
B	460	SER	-	expression tag	UNP P04295
B	461	SER	-	expression tag	UNP P04295
B	462	GLY	-	expression tag	UNP P04295
B	463	LEU	-	expression tag	UNP P04295
B	464	VAL	-	expression tag	UNP P04295
B	465	PRO	-	expression tag	UNP P04295
B	466	ARG	-	expression tag	UNP P04295
B	467	GLY	-	expression tag	UNP P04295
B	468	SER	-	expression tag	UNP P04295
B	469	HIS	-	expression tag	UNP P04295
B	470	MET	-	expression tag	UNP P04295
C	450	MET	-	expression tag	UNP P04295
C	451	GLY	-	expression tag	UNP P04295
C	452	SER	-	expression tag	UNP P04295
C	453	SER	-	expression tag	UNP P04295
C	454	HIS	-	expression tag	UNP P04295
C	455	HIS	-	expression tag	UNP P04295
C	456	HIS	-	expression tag	UNP P04295
C	457	HIS	-	expression tag	UNP P04295
C	458	HIS	-	expression tag	UNP P04295
C	459	HIS	-	expression tag	UNP P04295
C	460	SER	-	expression tag	UNP P04295
C	461	SER	-	expression tag	UNP P04295
C	462	GLY	-	expression tag	UNP P04295
C	463	LEU	-	expression tag	UNP P04295
C	464	VAL	-	expression tag	UNP P04295
C	465	PRO	-	expression tag	UNP P04295
C	466	ARG	-	expression tag	UNP P04295
C	467	GLY	-	expression tag	UNP P04295
C	468	SER	-	expression tag	UNP P04295
C	469	HIS	-	expression tag	UNP P04295
C	470	MET	-	expression tag	UNP P04295

- Molecule 2 is a protein called peptide.

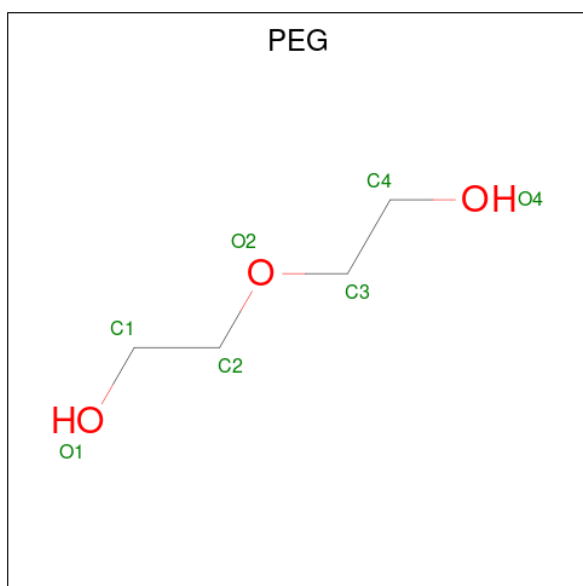
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	6	30	18	6	6	0	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



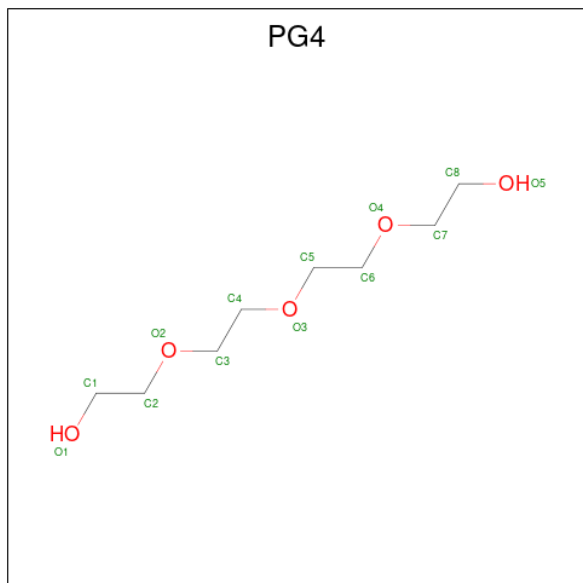
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	10	6	4	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



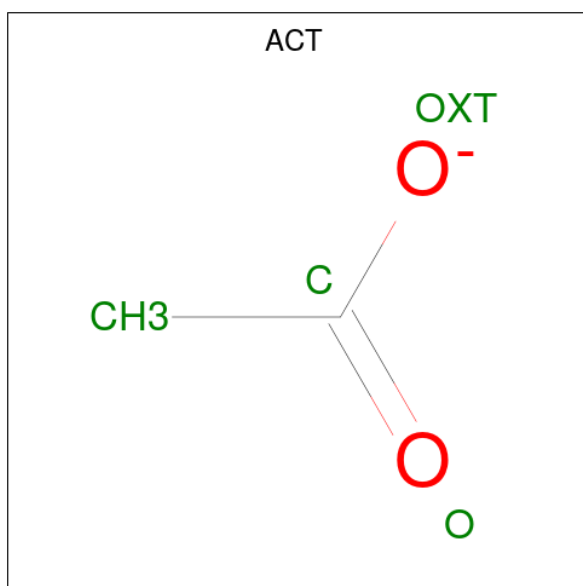
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

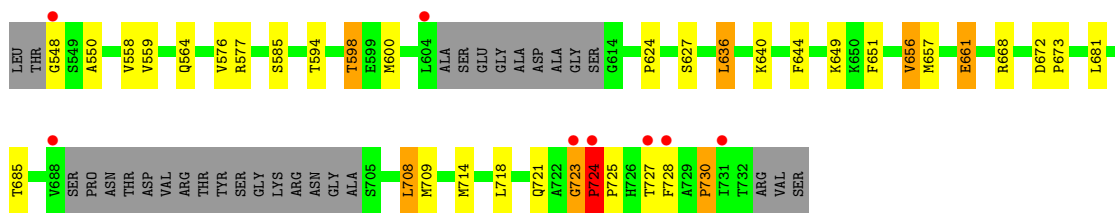
- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	16	Total	O	0	0
			16	16		
7	B	21	Total	O	0	0
			21	21		
7	C	9	Total	O	0	0
			9	9		



- Molecule 2: peptide

Chain D: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.94Å 96.94Å 194.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.46 19.80 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.80-2.46) 95.4 (19.80-2.46)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.203 , 0.247 0.210 , 0.246	Depositor DCC
R_{free} test set	1722 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtrriage
Anisotropy	0.332	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5172	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: PGE, ACT, PEG, PG4

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	0/1770	0.94	5/2412 (0.2%)
1	B	0.66	1/1692 (0.1%)	1.03	7/2303 (0.3%)
1	C	0.62	1/1722 (0.1%)	0.96	6/2345 (0.3%)
All	All	0.64	2/5184 (0.0%)	0.97	18/7060 (0.3%)

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	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	724	PRO	CA-C	6.90	1.58	1.52
1	C	724	PRO	CA-C	6.22	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	723	GLY	N-CA-C	12.58	138.00	112.34
1	C	723	GLY	CA-C-N	10.83	131.53	120.38
1	C	723	GLY	C-N-CA	10.83	131.53	120.38
1	B	723	GLY	CA-C-N	10.67	131.37	120.38
1	B	723	GLY	C-N-CA	10.67	131.37	120.38
1	B	724	PRO	N-CA-C	9.39	122.15	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	PRO	CA-C-N	-8.57	109.12	119.84
1	A	724	PRO	C-N-CA	-8.57	109.12	119.84
1	A	724	PRO	N-CA-C	7.54	119.90	110.70
1	B	542	PHE	N-CA-C	6.62	123.32	114.12
1	A	722	ALA	N-CA-C	6.42	117.91	108.86
1	C	531	ASP	N-CA-CB	-5.83	101.86	110.49
1	C	724	PRO	N-CA-C	5.46	117.36	110.70
1	B	729	ALA	CA-C-N	5.33	126.51	119.84
1	B	729	ALA	C-N-CA	5.33	126.51	119.84
1	A	477	VAL	N-CA-C	5.20	115.82	110.36
1	C	724	PRO	CA-C-N	5.13	126.26	119.84
1	C	724	PRO	C-N-CA	5.13	126.26	119.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	721	GLN	Peptide
1	B	721	GLN	Peptide
1	B	723	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1727	0	1710	27	0
1	B	1653	0	1627	24	0
1	C	1682	0	1661	22	0
2	D	30	0	9	0	0
3	A	10	0	14	1	0
4	A	7	0	10	0	0
5	A	13	0	18	3	0
6	A	4	0	3	0	0
7	A	16	0	0	1	0
7	B	21	0	0	0	0
7	C	9	0	0	0	0
All	All	5172	0	5052	68	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 7.

All (68) 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:681:LEU:HD23	1:A:709:MET:HG3	1.53	0.91
1:A:525:VAL:HG13	1:A:537:ALA:HB3	1.59	0.84
1:A:621:HIS:HE1	5:A:803:PG4:H31	1.45	0.80
1:A:619:PHE:H	5:A:803:PG4:H32	1.48	0.79
1:C:681:LEU:HD23	1:C:709:MET:HG3	1.68	0.76
1:C:728:PHE:O	1:C:730:PRO:HD3	1.88	0.73
1:C:543:LEU:HD13	1:C:550:ALA:HB1	1.73	0.70
1:C:636:LEU:HD11	1:C:714:MET:HE3	1.74	0.68
1:A:491:PRO:HG3	3:A:801:PGE:H22	1.77	0.67
1:A:516:THR:HG22	1:A:518:ALA:H	1.62	0.64
1:B:503:ASP:OD1	1:B:577:ARG:NH2	2.30	0.63
1:A:651:PHE:HA	1:A:656:VAL:HG13	1.82	0.62
1:B:681:LEU:HD23	1:B:709:MET:HG3	1.81	0.61
1:B:721:GLN:HA	1:B:722:ALA:HB2	1.82	0.61
1:C:494:THR:HG23	1:C:661:GLU:HG3	1.84	0.59
1:B:651:PHE:HA	1:B:656:VAL:HG13	1.84	0.58
1:B:506:VAL:HG13	1:B:578:VAL:HG22	1.85	0.58
1:A:559:VAL:HG13	1:A:600:MET:CE	2.34	0.57
1:B:724:PRO:HB2	1:B:725:PRO:HD2	1.87	0.55
1:C:640:LYS:HA	1:C:714:MET:HE1	1.87	0.55
1:A:570:PRO:HB3	1:B:668:ARG:O	2.07	0.55
1:C:651:PHE:HA	1:C:656:VAL:HG13	1.90	0.54
1:B:491:PRO:HG2	1:B:657:MET:HE3	1.89	0.54
1:B:728:PHE:O	1:B:730:PRO:HD3	2.08	0.54
1:C:508:VAL:HB	1:C:523:VAL:HG22	1.90	0.53
1:B:706:ASP:HB2	1:B:709:MET:HE2	1.90	0.53
1:B:562:LEU:HD11	1:B:576:VAL:HG21	1.91	0.53
1:C:559:VAL:HG13	1:C:600:MET:CE	2.39	0.52
1:A:614:GLY:N	1:B:670:GLN:HE21	2.07	0.52
1:A:559:VAL:HG13	1:A:600:MET:HE2	1.91	0.52
1:A:494:THR:HG23	1:A:661:GLU:HG3	1.91	0.52
1:A:525:VAL:CG1	1:A:537:ALA:HB3	2.37	0.51
1:A:504:LEU:HG	1:A:525:VAL:HG23	1.92	0.51
1:C:559:VAL:HG13	1:C:600:MET:HE2	1.93	0.50
1:A:576:VAL:HG22	1:A:617:LEU:HD12	1.93	0.50
1:A:728:PHE:O	1:A:730:PRO:HD3	2.12	0.49
1:A:621:HIS:CE1	5:A:803:PG4:H31	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:PHE:HE1	1:C:714:MET:HE2	1.78	0.48
1:A:543:LEU:N	7:A:907:HOH:O	2.43	0.48
1:A:614:GLY:HA2	1:B:670:GLN:HG3	1.96	0.47
1:A:505:TYR:CE2	1:A:577:ARG:HD2	2.50	0.46
1:C:548:GLY:C	1:C:550:ALA:H	2.24	0.45
1:B:570:PRO:HB3	1:C:668:ARG:O	2.15	0.45
1:A:513:THR:O	1:A:519:SER:HB2	2.17	0.45
1:A:516:THR:HB	1:A:519:SER:HB3	1.99	0.44
1:C:723:GLY:HA2	1:C:724:PRO:HD3	1.45	0.44
1:B:492:SER:HA	1:B:661:GLU:OE2	2.18	0.43
1:B:538:LEU:HD22	1:B:708:LEU:HD21	2.00	0.43
1:A:614:GLY:CA	1:B:670:GLN:HG3	2.48	0.43
1:B:494:THR:HG23	1:B:661:GLU:HG3	2.00	0.43
1:B:724:PRO:HB2	1:B:725:PRO:CD	2.47	0.43
1:B:588:SER:O	1:B:592:ILE:HG13	2.18	0.43
1:C:594:THR:O	1:C:598:THR:HG23	2.19	0.42
1:C:672:ASP:HA	1:C:673:PRO:HD3	1.87	0.42
1:A:621:HIS:HA	1:A:631:TYR:O	2.19	0.42
1:A:504:LEU:HD12	1:A:504:LEU:HA	1.87	0.42
1:B:542:PHE:O	1:B:543:LEU:HB2	2.19	0.42
1:C:494:THR:CG2	1:C:661:GLU:HG3	2.49	0.42
1:B:494:THR:CG2	1:B:661:GLU:HG3	2.50	0.41
1:A:586:GLN:O	1:A:590:VAL:HG23	2.21	0.41
1:B:602:ARG:H	1:B:602:ARG:HG3	1.64	0.41
1:B:602:ARG:HA	1:B:603:LEU:C	2.46	0.41
1:C:476:PRO:HD2	1:C:685:THR:HG22	2.03	0.41
1:A:620:TYR:CZ	1:A:718:LEU:HG	2.55	0.41
1:C:500:MET:HE2	1:C:500:MET:HB2	1.81	0.40
1:C:504:LEU:HD12	1:C:504:LEU:HA	1.86	0.40
1:C:708:LEU:HD23	1:C:708:LEU:HA	1.89	0.40
1:C:624:PRO:O	1:C:627:SER:HB3	2.22	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	219/286 (77%)	210 (96%)	8 (4%)	1 (0%)	24	32
1	B	206/286 (72%)	195 (95%)	8 (4%)	3 (2%)	8	7
1	C	210/286 (73%)	197 (94%)	10 (5%)	3 (1%)	9	8
All	All	635/858 (74%)	602 (95%)	26 (4%)	7 (1%)	11	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	730	PRO
1	C	730	PRO
1	B	724	PRO
1	B	725	PRO
1	C	724	PRO
1	A	724	PRO
1	C	725	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/233 (79%)	164 (89%)	20 (11%)	6	5
1	B	176/233 (76%)	151 (86%)	25 (14%)	3	2
1	C	179/233 (77%)	160 (89%)	19 (11%)	6	6
All	All	539/699 (77%)	475 (88%)	64 (12%)	5	4

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	480	LYS
1	A	488	LEU
1	A	504	LEU

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Mol	Chain	Res	Type
1	A	506	VAL
1	A	508	VAL
1	A	517	ARG
1	A	525	VAL
1	A	558	VAL
1	A	561	SER
1	A	576	VAL
1	A	616	GLU
1	A	618	LEU
1	A	636	LEU
1	A	656	VAL
1	A	657	MET
1	A	661	GLU
1	A	708	LEU
1	A	718	LEU
1	A	721	GLN
1	A	727	THR
1	B	488	LEU
1	B	504	LEU
1	B	506	VAL
1	B	508	VAL
1	B	528	ARG
1	B	558	VAL
1	B	561	SER
1	B	562	LEU
1	B	576	VAL
1	B	602	ARG
1	B	618	LEU
1	B	623	GLU
1	B	629	VAL
1	B	636	LEU
1	B	637	ASN
1	B	639	GLN
1	B	650	LYS
1	B	656	VAL
1	B	657	MET
1	B	661	GLU
1	B	668	ARG
1	B	708	LEU
1	B	718	LEU
1	B	721	GLN
1	B	727	THR

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Mol	Chain	Res	Type
1	C	488	LEU
1	C	504	LEU
1	C	506	VAL
1	C	508	VAL
1	C	558	VAL
1	C	564	GLN
1	C	576	VAL
1	C	577	ARG
1	C	585	SER
1	C	598	THR
1	C	636	LEU
1	C	649	LYS
1	C	656	VAL
1	C	657	MET
1	C	661	GLU
1	C	708	LEU
1	C	718	LEU
1	C	721	GLN
1	C	727	THR

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	564	GLN
1	A	621	HIS
1	B	564	GLN
1	B	621	HIS
1	C	564	GLN
1	C	637	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](#)

4 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
6	ACT	A	804	-	3,3,3	0.87	0	3,3,3	1.14	0
4	PEG	A	802	-	6,6,6	0.59	0	5,5,5	1.49	1 (20%)
3	PGE	A	801	-	9,9,9	0.63	0	8,8,8	1.48	0
5	PG4	A	803	-	12,12,12	0.71	0	11,11,11	1.43	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	802	-	-	3/4/4/4	-
3	PGE	A	801	-	-	5/7/7/7	-
5	PG4	A	803	-	-	3/10/10/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	PEG	O2-C2-C1	2.01	118.99	110.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	PGE	C1-C2-O2-C3
3	A	801	PGE	O1-C1-C2-O2
3	A	801	PGE	C6-C5-O3-C4
4	A	802	PEG	O1-C1-C2-O2
4	A	802	PEG	O2-C3-C4-O4
4	A	802	PEG	C4-C3-O2-C2
5	A	803	PG4	O2-C3-C4-O3
5	A	803	PG4	C4-C3-O2-C2
5	A	803	PG4	O4-C7-C8-O5
3	A	801	PGE	C3-C4-O3-C5
3	A	801	PGE	O2-C3-C4-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	PGE	1	0
5	A	803	PG4	3	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	225/286 (78%)	-0.24	10 (4%) 39 38	35, 49, 82, 114	0
1	B	216/286 (75%)	-0.20	7 (3%) 50 51	35, 51, 87, 106	0
1	C	220/286 (76%)	-0.03	11 (5%) 34 32	34, 54, 92, 121	0
2	D	0/6	-	-	-	-
All	All	661/864 (76%)	-0.16	28 (4%) 40 40	34, 51, 87, 121	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	728	PHE	4.0
1	A	727	THR	4.0
1	B	731	ILE	4.0
1	C	728	PHE	3.6
1	C	476	PRO	3.6
1	B	727	THR	3.5
1	B	723	GLY	3.5
1	C	723	GLY	3.5
1	A	620	TYR	3.3
1	A	722	ALA	3.1
1	C	543	LEU	3.1
1	A	728	PHE	3.1
1	C	731	ILE	3.1
1	B	724	PRO	3.0
1	C	727	THR	2.9
1	C	724	PRO	2.9
1	A	724	PRO	2.8
1	C	688	VAL	2.8
1	B	511	ALA	2.8
1	A	476	PRO	2.7
1	B	604	LEU	2.7
1	A	723	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	602	ARG	2.4
1	C	541	PHE	2.3
1	C	604	LEU	2.2
1	C	548	GLY	2.2
1	A	614	GLY	2.1
1	A	725	PRO	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(Å ²)	Q<0.9
6	ACT	A	804	4/4	0.21	0.31	78,85,87,90	0
4	PEG	A	802	7/7	0.49	0.31	72,76,83,85	0
5	PG4	A	803	13/13	0.68	0.16	66,80,86,88	0
3	PGE	A	801	10/10	0.83	0.18	50,61,69,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.