WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:08 am GMT

PDB ID	:	4IOX
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

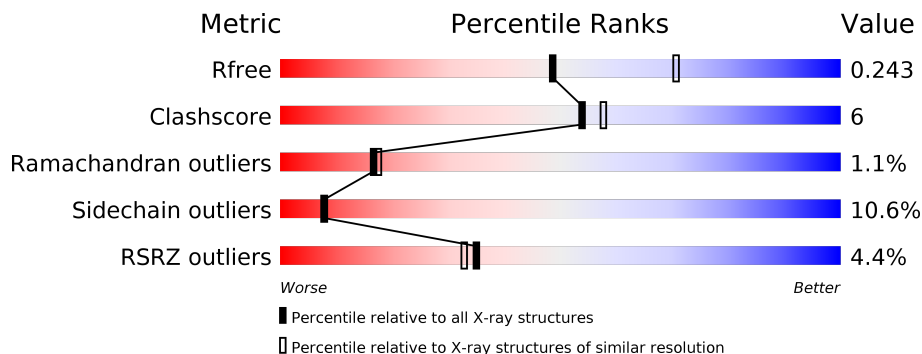|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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	Percentile Ranks	Value
Rfree		0.243
Clashscore		6
Ramachandran outliers		1.1%
Sidechain outliers		10.6%
RSRZ outliers		4.4%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	62% 15% • 21%
1	B	286	60% 11% • 24%
1	C	286	62% 12% • 23%
2	D	6	100%

2   Entry composition ⓘ

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
1	A	225	Total	C	N	O	S	0	0	0
			1727	1109	295	316	7			
1	B	216	Total	C	N	O	S	0	0	0
			1653	1064	279	303	7			
1	C	220	Total	C	N	O	S	0	0	0
			1682	1085	283	307	7			

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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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
2	D	6	Total 30	C 18	N 6	O 6	0	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).
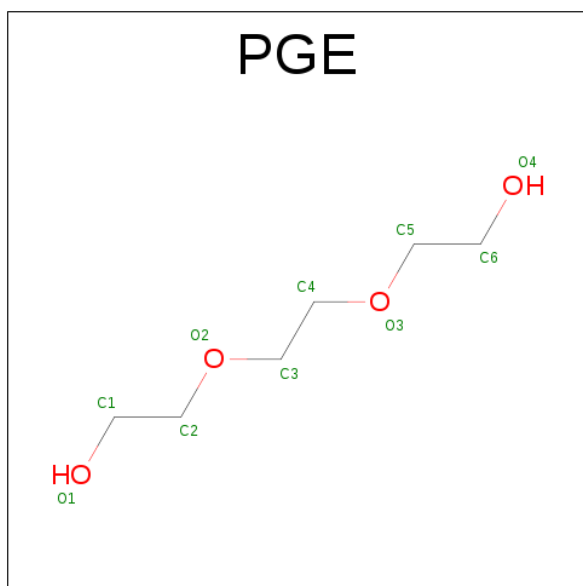
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 10	C 6	O 4	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
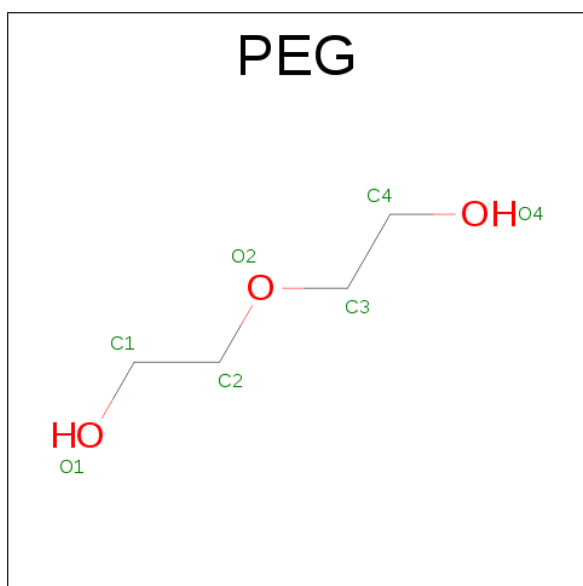
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 7	C 4	O 3	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
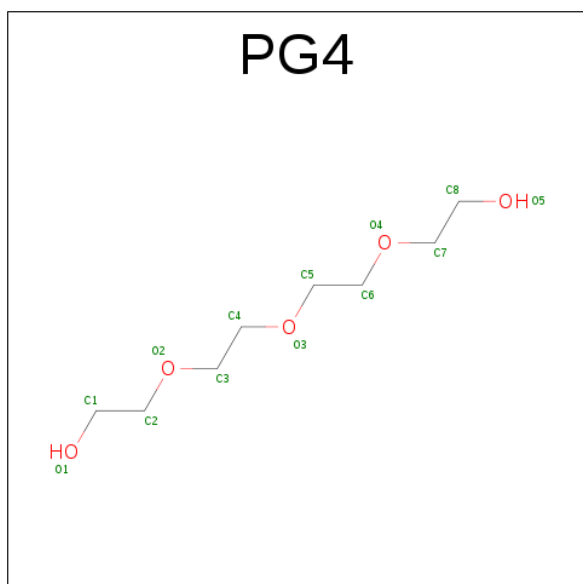
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 13	C 8	O 5	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
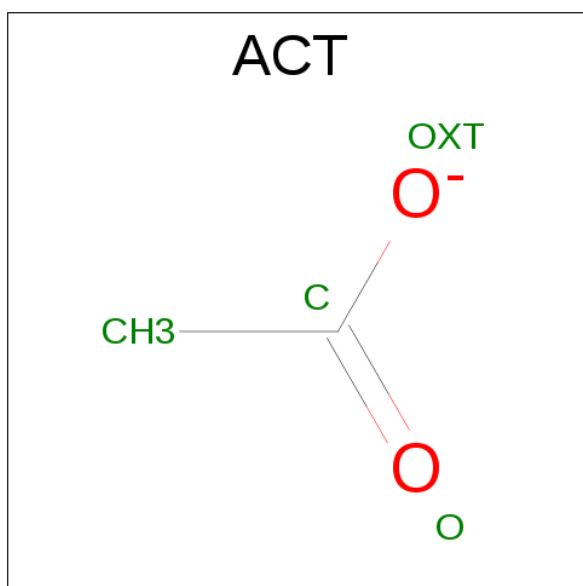
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total C O 4 2 2			0	0

- Molecule 7 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Tripartite terminase subunit UL15

• Molecule 1: Tripartite terminase subunit UL15

• Molecule 1: Tripartite terminase subunit UL15

• 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 33.75 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.80-2.46) 95.7 (33.75-2.46)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.01 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.203 , 0.247 0.198 , 0.243	Depositor DCC
R_{free} test set	1721 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5172	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage'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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PG4, PEG, PGE, ACT

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	0.48	0/1770	0.61	0/2412
1	B	0.49	0/1692	0.67	1/2303 (0.0%)
1	C	0.45	0/1722	0.61	0/2345
All	All	0.47	0/5184	0.63	1/7060 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	723	GLY	N-CA-C	9.96	138.00	113.10

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 ⓘ

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	21	0
1	C	1682	0	1661	19	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	62	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 6.

All (62) 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:A:491:PRO:HG3	3:A:801:PGE:H22	1.77	0.67
1:C:636:LEU:HD21	1:C:714:MET:HE3	1.76	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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:559:VAL:HG13	1:A:600:MET:HE2	1.94	0.49
1:A:621:HIS:CE1	5:A:803:PG4:H31	2.36	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: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:538:LEU:HD22	1:B:708:LEU:HD21	2.00	0.43
1:B:492:SER:HA	1:B:661:GLU:OE2	2.18	0.43
1:B:494:THR:HG23	1:B:661:GLU:HG3	2.00	0.43
1:A:614:GLY:CA	1:B:670:GLN:HG3	2.48	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:HG3	1:B:602:ARG:H	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:548:GLY:C	1:C:550:ALA:H	2.24	0.41
1:C:559:VAL:HG13	1:C:600:MET:HE3	2.01	0.41
1:C:504:LEU:HA	1:C:504:LEU:HD12	1.86	0.40
1:C:708:LEU:HA	1:C:708:LEU:HD23	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 (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	219/286 (77%)	210 (96%)	8 (4%)	1 (0%)	32	39
1	B	206/286 (72%)	195 (95%)	8 (4%)	3 (2%)	12	11
1	C	210/286 (73%)	197 (94%)	10 (5%)	3 (1%)	13	12
All	All	635/858 (74%)	602 (95%)	26 (4%)	7 (1%)	17	17

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 ⓘ

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%)	165 (90%)	19 (10%)	8	9
1	B	176/233 (76%)	155 (88%)	21 (12%)	6	5
1	C	179/233 (77%)	162 (90%)	17 (10%)	10	11
All	All	539/699 (77%)	482 (89%)	57 (11%)	8	8

All (57) 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
1	A	506	VAL
1	A	508	VAL
1	A	517	ARG
1	A	525	VAL
1	A	561	SER
1	A	587	ASP
1	A	616	GLU
1	A	618	LEU
1	A	636	LEU
1	A	638	LYS
1	A	656	VAL
1	A	657	MET
1	A	661	GLU
1	A	708	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	561	SER
1	B	562	LEU

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Mol	Chain	Res	Type
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	639	GLN
1	B	650	LYS
1	B	656	VAL
1	B	657	MET
1	B	668	ARG
1	B	708	LEU
1	B	718	LEU
1	B	721	GLN
1	C	488	LEU
1	C	504	LEU
1	C	506	VAL
1	C	508	VAL
1	C	564	GLN
1	C	576	VAL
1	C	577	ARG
1	C	585	SER
1	C	587	ASP
1	C	636	LEU
1	C	639	GLN
1	C	656	VAL
1	C	657	MET
1	C	661	GLU
1	C	708	LEU
1	C	718	LEU
1	C	721	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	621	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
3	PGE	A	801	-	9,9,9	0.63	0	8,8,8	1.46	0
4	PEG	A	802	-	6,6,6	0.58	0	5,5,5	1.46	0
5	PG4	A	803	-	12,12,12	0.70	0	11,11,11	1.41	0
6	ACT	A	804	-	1,3,3	1.44	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	A	801	-	-	0/7/7/7	0/0/0/0
4	PEG	A	802	-	-	0/4/4/4	0/0/0/0
5	PG4	A	803	-	-	0/10/10/10	0/0/0/0
6	ACT	A	804	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.21	4 (1%)	69	65	35, 49, 82, 114	0
1	B	216/286 (75%)	-0.09	10 (4%)	33	31	35, 51, 87, 106	0
1	C	220/286 (76%)	0.21	15 (6%)	18	15	34, 54, 92, 121	0
2	D	0/6	-	-			-	-
All	All	661/864 (76%)	-0.03	29 (4%)	35	33	34, 51, 87, 121	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	543	LEU	9.2
1	C	687	THR	4.1
1	B	543	LEU	3.7
1	B	728	PHE	3.6
1	C	548	GLY	3.4
1	B	548	GLY	3.3
1	C	688	VAL	3.3
1	A	517	ARG	3.2
1	B	542	PHE	3.1
1	C	728	PHE	3.1
1	C	542	PHE	2.9
1	B	705	SER	2.8
1	A	620	TYR	2.8
1	B	613	SER	2.7
1	C	711	ALA	2.7
1	B	683	ASN	2.7
1	C	638	LYS	2.6
1	A	728	PHE	2.5
1	C	723	GLY	2.5
1	B	614	GLY	2.5
1	C	549	SER	2.5
1	C	626	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	626	GLY	2.4
1	C	712	VAL	2.4
1	C	685	THR	2.2
1	C	526	VAL	2.2
1	A	722	ALA	2.1
1	B	685	THR	2.0
1	C	524	ALA	2.0

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	PGE	A	801	10/10	0.83	0.19	1.41	50,61,69,73	0
6	ACT	A	804	4/4	0.77	0.19	1.05	78,85,87,90	0
5	PG4	A	803	13/13	0.85	0.20	0.40	66,80,86,88	0
4	PEG	A	802	7/7	0.74	0.13	-	72,76,83,85	0

6.5 Other polymers ⓘ

There are no such residues in this entry.