



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2024 – 10:24 AM EDT

PDB ID : 9DP4
Title : APE1 N174Q Product Complex with Abasic DNA
Authors : DeHart, K.D.; Hoitsma, N.M.; Freudenthal, B.D.
Deposited on : 2024-09-20
Resolution : 2.25 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

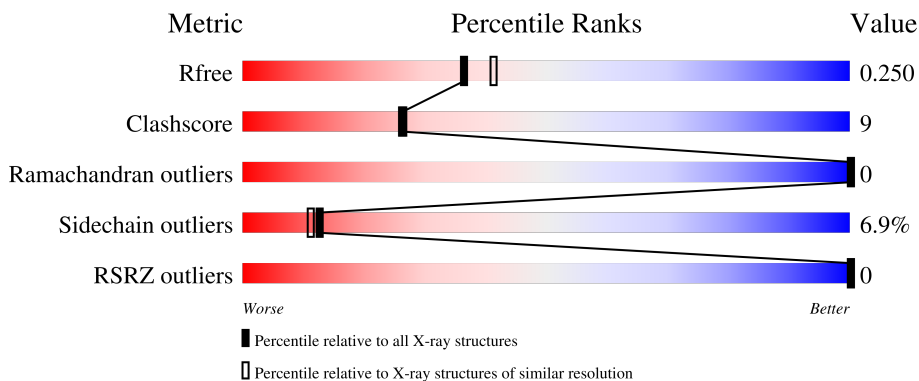
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	276	
1	B	276	
2	D	11	
2	G	11	
3	E	10	

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Mol	Chain	Length	Quality of chain
3	H	10	 70% 30%
4	F	21	 57% 43%
4	I	21	 62% 38%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6371 atoms, of which 20 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 DNA repair nuclease/redox regulator APEX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	Total	C	N	O	S	0	1	0
			2197	1402	381	406	8			
1	B	276	Total	C	N	O	S	0	0	0
			2191	1399	379	405	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	ALA	CYS	engineered mutation	UNP P27695
A	174	GLN	ASN	engineered mutation	UNP P27695
B	138	ALA	CYS	engineered mutation	UNP P27695
B	174	GLN	ASN	engineered mutation	UNP P27695

- Molecule 2 is a DNA chain called DNA (5'-D(P*(3DR)P*CP*GP*AP*CP*GP*GP*AP*T P*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	11	Total	C	N	O	P	0	0	0
			216	101	39	65	11			
2	G	11	Total	C	N	O	P	0	0	0
			216	101	39	65	11			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*TP*GP*AP*TP*GP*CP*GP*C)-3').

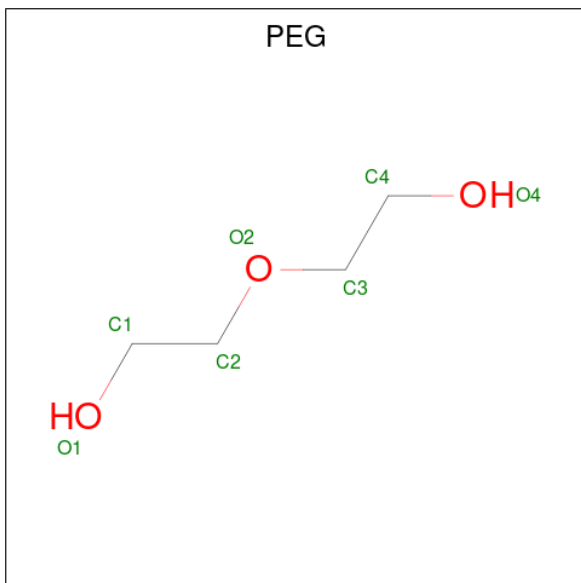
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			
3	H	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			

- Molecule 4 is a DNA chain called DNA (5'-D(*GP*GP*AP*TP*CP*CP*GP*TP*CP*GP*

GP*GP*CP*GP*CP*AP*TP*CP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	21	Total	C	N	O	P	0	0	0
			428	203	82	123	20			
4	I	21	Total	C	N	O	P	0	0	0
			432	203	82	126	21			

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

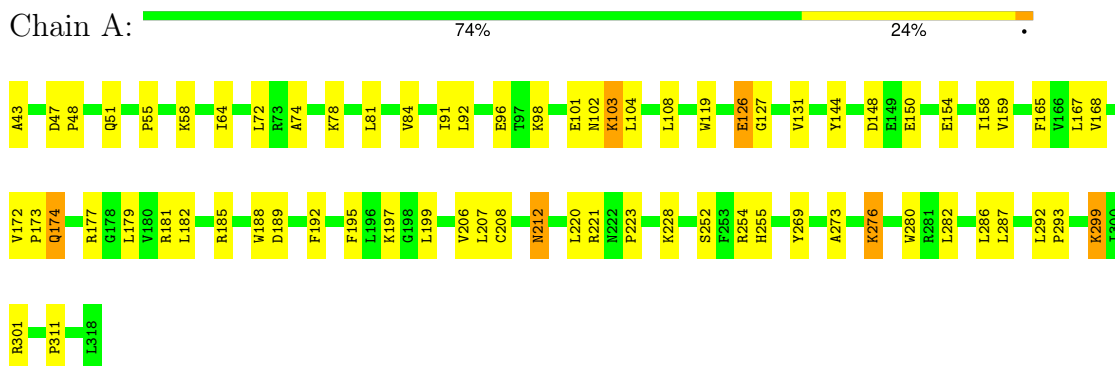
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	103	Total 103	O 103	0	0
7	B	86	Total 86	O 86	0	0
7	D	9	Total 9	O 9	0	0
7	E	7	Total 7	O 7	0	0
7	F	16	Total 16	O 16	0	0
7	G	6	Total 6	O 6	0	0
7	H	10	Total 10	O 10	0	0
7	I	12	Total 12	O 12	0	0

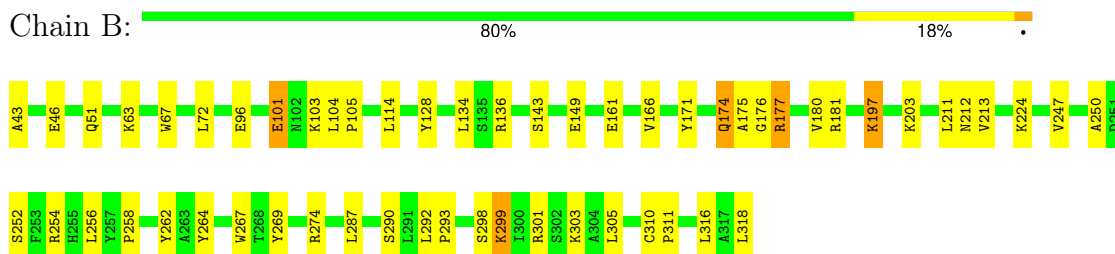
3 Residue-property plots [i](#)

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.

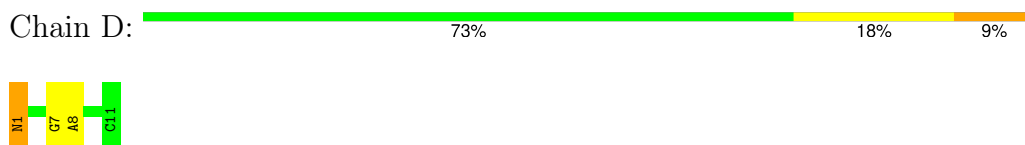
- Molecule 1: DNA repair nuclease/redox regulator APEX1



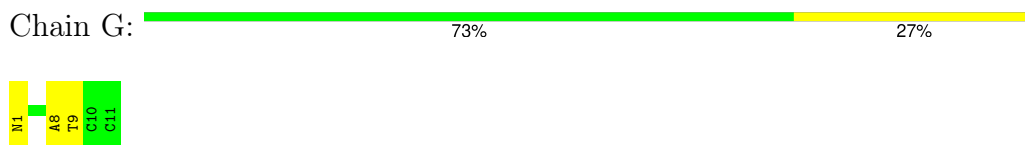
- Molecule 1: DNA repair nuclease/redox regulator APEX1



- Molecule 2: DNA (5'-D(P*(3DR)P*CP*GP*AP*CP*GP*GP*AP*TP*CP*C)-3')



- Molecule 2: DNA (5'-D(P*(3DR)P*CP*GP*AP*CP*GP*GP*AP*TP*CP*C)-3')



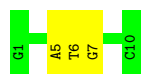
- Molecule 3: DNA (5'-D(*GP*CP*TP*GP*AP*TP*GP*CP*GP*C)-3')

Chain E:  70% 20% 10%



- Molecule 3: DNA (5'-D(*GP*CP*TP*GP*AP*TP*GP*CP*GP*C)-3')

Chain H:  70% 30%



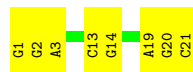
- Molecule 4: DNA (5'-D(*GP*GP*AP*TP*CP*CP*GP*TP*CP*GP*GP*GP*CP*GP*CP*AP*TP*CP*AP*GP*C)-3')

Chain F:  57% 43%



- Molecule 4: DNA (5'-D(*GP*GP*AP*TP*CP*CP*GP*TP*CP*GP*GP*GP*CP*GP*CP*AP*TP*CP*AP*GP*C)-3')

Chain I:  62% 38%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	153.42Å 153.42Å 45.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.52 – 2.25 48.52 – 2.25	Depositor EDS
% Data completeness (in resolution range)	65.5 (48.52-2.25) 72.9 (48.52-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.24Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.215 , 0.248 0.218 , 0.250	Depositor DCC
R_{free} test set	35096 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtrriage
Anisotropy	0.109	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 17.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6371	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: 3DR, PEG, MG

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	0.69	0/2255	0.94	0/3060
1	B	0.68	0/2249	0.96	0/3050
2	D	0.51	0/228	0.79	0/349
2	G	0.62	0/228	0.85	0/349
3	E	0.64	1/227 (0.4%)	0.82	0/349
3	H	0.51	0/227	0.77	0/349
4	F	0.59	0/480	0.84	0/740
4	I	0.58	0/484	0.82	0/745
All	All	0.65	1/6378 (0.0%)	0.91	0/8991

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	7	DG	O3'-P	5.38	1.67	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2197	0	2155	53	0
1	B	2191	0	2154	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	216	0	120	2	0
2	G	216	0	120	1	0
3	E	203	0	114	2	0
3	H	203	0	114	2	0
4	F	428	0	233	7	0
4	I	432	0	235	6	0
5	A	7	10	10	1	0
5	B	7	10	10	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	103	0	0	6	0
7	B	86	0	0	7	0
7	D	9	0	0	0	0
7	E	7	0	0	0	0
7	F	16	0	0	1	0
7	G	6	0	0	0	0
7	H	10	0	0	1	0
7	I	12	0	0	2	0
All	All	6351	20	5265	104	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 9.

All (104) 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:101:GLU:HA	1:A:104:LEU:HG	1.48	0.93
1:A:64:ILE:HD13	1:A:167:LEU:CD1	2.12	0.80
1:A:64:ILE:HD13	1:A:167:LEU:HD11	1.72	0.72
1:B:197:LYS:HG3	1:B:247:VAL:HA	1.77	0.66
1:A:64:ILE:HD13	1:A:167:LEU:HD12	1.78	0.66
1:A:255:HIS:CE1	1:A:292:LEU:HD13	2.31	0.65
1:B:72:LEU:CD2	1:B:105:PRO:HG2	2.27	0.65
1:A:159:VAL:HG13	1:A:168:VAL:HG22	1.79	0.65
1:A:177:ARG:HH22	4:F:11:DG:N2	1.96	0.64
1:A:84:VAL:HG11	1:A:92:LEU:HD22	1.80	0.63
1:A:185:ARG:HH12	1:A:212:ASN:HB3	1.65	0.62
1:B:301:ARG:HB2	1:B:311:PRO:HG2	1.81	0.62
4:I:1:DG:H2'	4:I:2:DG:C8	2.35	0.61
2:G:8:DA:H2''	2:G:9:DT:H5''	1.83	0.60
4:F:16:DA:H2''	4:F:17:DT:H72	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:CG2	1:A:158:ILE:HG13	2.35	0.57
1:A:189:ASP:HA	7:A:507:HOH:O	2.06	0.56
1:B:303:LYS:O	1:B:305:LEU:CD1	2.54	0.56
1:B:267:TRP:HZ3	1:B:310:CYS:HB3	1.72	0.55
4:I:3:DA:H1'	7:I:105:HOH:O	2.07	0.55
1:A:192:PHE:HB2	7:A:507:HOH:O	2.07	0.55
1:B:181:ARG:HB2	7:B:527:HOH:O	2.07	0.54
1:B:161:GLU:HG3	1:B:166:VAL:HG22	1.90	0.54
1:A:221:ARG:O	1:A:223:PRO:HD3	2.09	0.53
4:I:13:DC:H5''	7:I:102:HOH:O	2.08	0.53
1:B:252:SER:HB2	1:B:298:SER:HB2	1.91	0.53
4:I:13:DC:H2''	4:I:14:DG:H5'	1.91	0.52
1:A:173:PRO:HD2	1:A:188:TRP:CE2	2.44	0.52
1:A:47:ASP:HB3	7:A:552:HOH:O	2.10	0.52
1:A:292:LEU:N	1:A:293:PRO:HD2	2.25	0.52
3:H:5:DA:H1'	7:H:101:HOH:O	2.09	0.52
1:A:177:ARG:HH22	4:F:11:DG:H22	1.58	0.51
1:A:165:PHE:HB2	7:A:528:HOH:O	2.11	0.51
1:A:103:LYS:NZ	1:A:126:GLU:OE2	2.34	0.51
1:A:206:VAL:HG22	1:A:287:LEU:HG	1.93	0.51
1:B:303:LYS:O	1:B:305:LEU:HD12	2.11	0.51
1:A:64:ILE:CD1	1:A:167:LEU:HD12	2.41	0.50
1:A:47:ASP:OD2	1:A:299:LYS:HE2	2.12	0.50
1:A:255:HIS:HE1	1:A:292:LEU:HD13	1.72	0.50
1:A:131:VAL:HG23	1:A:158:ILE:HG13	1.93	0.50
1:B:166:VAL:HG23	1:B:203:LYS:HB3	1.94	0.50
1:A:98:LYS:HB3	1:A:127:GLY:HA2	1.93	0.49
1:B:262:TYR:HA	1:B:264:TYR:CZ	2.47	0.49
1:A:220:LEU:HD11	1:A:223:PRO:HA	1.94	0.49
1:B:72:LEU:HD22	1:B:105:PRO:CD	2.43	0.49
1:B:72:LEU:HD23	1:B:105:PRO:HG2	1.94	0.49
1:A:252:SER:HB2	1:A:287:LEU:HD13	1.95	0.49
1:A:273:ALA:HA	1:A:276:LYS:HE2	1.95	0.48
1:A:144:TYR:HE1	7:A:578:HOH:O	1.95	0.48
1:B:43:ALA:N	7:B:511:HOH:O	2.45	0.48
1:B:211:LEU:O	1:B:213:VAL:HG12	2.13	0.48
2:D:7:DG:H2''	2:D:8:DA:C8	2.50	0.47
1:B:96:GLU:HG3	1:B:171:TYR:CE2	2.50	0.47
1:A:173:PRO:HD2	1:A:188:TRP:NE1	2.31	0.46
1:B:267:TRP:CZ3	1:B:310:CYS:HB3	2.49	0.46
1:A:269:TYR:HB3	4:F:12:DG:H1'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LYS:HB3	1:B:299:LYS:HE3	1.41	0.46
3:E:7:DG:H2''	3:E:8:DC:H5'	1.98	0.45
1:B:292:LEU:N	1:B:293:PRO:HD2	2.32	0.45
1:A:131:VAL:HG21	1:A:158:ILE:HG13	1.98	0.45
1:A:301:ARG:HB2	1:A:311:PRO:HG2	1.99	0.45
4:I:19:DA:H1'	4:I:20:DG:H5'	1.99	0.45
4:F:19:DA:H2''	4:F:20:DG:C8	2.52	0.45
1:A:172:VAL:HG13	1:A:188:TRP:HE1	1.81	0.45
1:B:174:GLN:HG3	1:B:176:GLY:H	1.82	0.45
1:B:290:SER:HB3	7:B:547:HOH:O	2.17	0.45
1:A:254:ARG:HA	1:A:254:ARG:HD3	1.67	0.44
1:B:177:ARG:HD2	1:B:177:ARG:HA	1.25	0.44
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.81	0.44
1:A:91:ILE:HD13	1:A:167:LEU:HD13	1.99	0.44
1:A:282:LEU:HD11	2:D:1:3DR:H2'	1.99	0.44
1:B:143:SER:HB2	7:B:545:HOH:O	2.18	0.44
1:B:114:LEU:HB3	1:B:134:LEU:HB3	1.99	0.44
3:H:6:DT:H2''	3:H:7:DG:H8	1.83	0.44
1:B:250:ALA:N	1:B:287:LEU:O	2.50	0.43
1:B:250:ALA:O	1:B:287:LEU:HD23	2.17	0.43
1:A:55:PRO:HG3	5:A:401:PEG:O2	2.18	0.43
1:A:174:GLN:NE2	3:E:10:DC:H3'	2.34	0.43
1:A:101:GLU:O	1:A:104:LEU:HB2	2.19	0.42
1:B:174:GLN:HG3	1:B:175:ALA:N	2.34	0.42
1:B:267:TRP:CD2	1:B:274:ARG:HG3	2.55	0.42
1:A:207:LEU:HD23	1:A:286:LEU:HD12	2.01	0.42
1:B:101:GLU:HA	1:B:104:LEU:HG	2.01	0.42
1:A:74:ALA:O	1:A:78:LYS:HE3	2.20	0.42
1:A:159:VAL:HG21	1:A:195:PHE:HZ	1.84	0.42
1:B:96:GLU:HG3	1:B:171:TYR:CZ	2.54	0.42
1:B:180:VAL:HG22	7:B:536:HOH:O	2.20	0.42
1:A:195:PHE:CZ	1:A:199:LEU:HD11	2.55	0.41
1:B:67:TRP:CE2	1:B:311:PRO:HD3	2.54	0.41
1:A:47:ASP:HA	1:A:48:PRO:HD3	1.81	0.41
1:A:108:LEU:HD13	1:A:119:TRP:CZ2	2.55	0.41
4:F:6:DC:H5'	7:F:106:HOH:O	2.20	0.41
4:I:20:DG:H2''	4:I:21:DC:C6	2.55	0.41
1:B:269:TYR:HA	7:B:508:HOH:O	2.18	0.41
1:B:316:LEU:HD23	1:B:318:LEU:HD11	2.01	0.41
1:A:173:PRO:O	1:A:185:ARG:HD3	2.20	0.41
1:A:72:LEU:HD21	1:A:108:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HB2	1:A:221:ARG:NH2	2.35	0.41
1:A:165:PHE:CE2	1:A:167:LEU:HB2	2.56	0.41
1:A:179:LEU:HD13	1:A:182:LEU:HD22	2.03	0.41
1:A:144:TYR:O	7:A:501:HOH:O	2.22	0.40
1:B:136:ARG:HD2	7:B:522:HOH:O	2.22	0.40
1:B:256:LEU:C	1:B:258:PRO:HD3	2.42	0.40
4:F:4:DT:H2''	4:F:5:DC:C6	2.56	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	275/276 (100%)	258 (94%)	17 (6%)	0	100	100
1	B	274/276 (99%)	258 (94%)	16 (6%)	0	100	100
All	All	549/552 (100%)	516 (94%)	33 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	233/235 (99%)	215 (92%)	18 (8%)	10	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	233/235 (99%)	219 (94%)	14 (6%)	16	15
All	All	466/470 (99%)	434 (93%)	32 (7%)	13	11

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	58	LYS
1	A	96	GLU
1	A	102	ASN
1	A	103	LYS
1	A	126	GLU
1	A	148	ASP
1	A	150	GLU
1	A	154	GLU
1	A	174	GLN
1	A	181	ARG
1	A	197	LYS
1	A	208	CYS
1	A	212	ASN
1	A	228	LYS
1	A	276	LYS
1	A	280	TRP
1	A	299	LYS
1	B	46	GLU
1	B	51	GLN
1	B	63	LYS
1	B	101	GLU
1	B	103	LYS
1	B	128	TYR
1	B	149	GLU
1	B	174	GLN
1	B	177	ARG
1	B	197	LYS
1	B	212	ASN
1	B	224	LYS
1	B	254	ARG
1	B	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	51	GLN
1	B	277	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](#)

2 non-standard protein/DNA/RNA residues 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	3DR	D	1	2,6	12,12,12	2.91	5 (41%)	14,17,17	1.46	2 (14%)
2	3DR	G	1	2	12,12,12	2.91	4 (33%)	14,17,17	1.43	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3DR	D	1	2,6	-	5/6/16/16	0/1/1/1
2	3DR	G	1	2	-	5/6/16/16	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	3DR	C3'-C4'	-7.60	1.33	1.53
2	G	1	3DR	C3'-C4'	-7.23	1.34	1.53
2	G	1	3DR	O4'-C1'	-4.39	1.30	1.43
2	D	1	3DR	O4'-C1'	-4.24	1.30	1.43
2	D	1	3DR	C2'-C1'	3.05	1.59	1.51
2	G	1	3DR	C2'-C1'	2.93	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	3DR	O3'-C3'	2.70	1.49	1.43
2	D	1	3DR	P-OP3	-2.13	1.46	1.54
2	D	1	3DR	P-OP2	-2.06	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	3DR	C1'-C2'-C3'	-3.71	99.28	103.26
2	G	1	3DR	C1'-C2'-C3'	-2.82	100.24	103.26
2	D	1	3DR	O3'-C3'-C2'	-2.76	104.95	111.43
2	G	1	3DR	O4'-C4'-C3'	2.32	107.15	103.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	3DR	C5'-O5'-P-OP2
2	D	1	3DR	C5'-O5'-P-OP3
2	G	1	3DR	C5'-O5'-P-OP1
2	G	1	3DR	C5'-O5'-P-OP2
2	G	1	3DR	C5'-O5'-P-OP3
2	G	1	3DR	C3'-C4'-C5'-O5'
2	G	1	3DR	O4'-C4'-C5'-O5'
2	D	1	3DR	C3'-C4'-C5'-O5'
2	D	1	3DR	O4'-C4'-C5'-O5'
2	D	1	3DR	C5'-O5'-P-OP1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	3DR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	B	402	-	6,6,6	0.22	0	5,5,5	0.11	0
5	PEG	A	401	-	6,6,6	0.32	0	5,5,5	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	B	402	-	-	3/4/4/4	-
5	PEG	A	401	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	402	PEG	O2-C3-C4-O4
5	B	402	PEG	O1-C1-C2-O2
5	A	401	PEG	O2-C3-C4-O4
5	A	401	PEG	O1-C1-C2-O2
5	A	401	PEG	C4-C3-O2-C2
5	B	402	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	PEG	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	276/276 (100%)	-1.34	0 100 100	14, 27, 39, 50	1 (0%)
1	B	276/276 (100%)	-1.31	0 100 100	13, 30, 46, 54	0
2	D	10/11 (90%)	-1.53	0 100 100	33, 46, 60, 64	0
2	G	10/11 (90%)	-1.27	0 100 100	45, 62, 80, 81	0
3	E	10/10 (100%)	-1.48	0 100 100	48, 57, 66, 66	0
3	H	10/10 (100%)	-1.26	0 100 100	57, 70, 78, 86	0
4	F	21/21 (100%)	-1.51	0 100 100	35, 54, 62, 67	0
4	I	21/21 (100%)	-1.33	0 100 100	41, 63, 76, 81	0
All	All	634/636 (99%)	-1.34	0 100 100	13, 30, 62, 86	1 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	3DR	D	1	12/12	0.99	0.04	19,25,32,32	0
2	3DR	G	1	12/12	0.99	0.03	27,32,36,42	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
5	PEG	A	401	7/7	0.97	0.07	29,35,43,44	0
5	PEG	B	402	7/7	0.98	0.07	27,35,41,41	0
6	MG	D	101	1/1	0.98	0.04	35,35,35,35	0
6	MG	B	401	1/1	0.99	0.11	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.