



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:59 am GMT

PDB ID : 4YPR
Title : Crystal Structure of D144N MutY bound to its anti-substrate
Authors : Wang, L.; Lee, S.; Verdine, G.L.
Deposited on : 2015-03-13
Resolution : 2.59 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

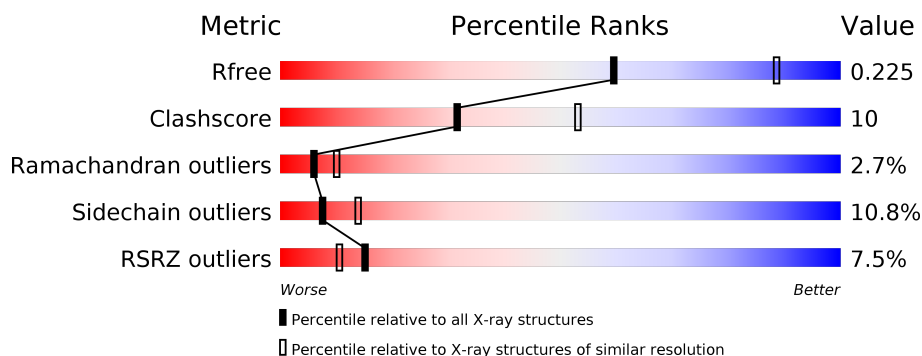
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 $\leq 5\%$. 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	369	<div> <div>5%</div> <div> <div>69%</div> <div>23%</div> <div>• • •</div> </div> </div>
1	B	369	<div> <div>10%</div> <div> <div>68%</div> <div>23%</div> <div>• • 5%</div> </div> </div>
2	C	11	<div> <div>55%</div> <div>27%</div> <div>9%</div> <div>9%</div> </div>
2	E	11	<div> <div>55%</div> <div>9%</div> <div>27%</div> <div>9%</div> </div>
3	D	11	<div> <div>55%</div> <div>45%</div> </div>
3	F	11	<div> <div>82%</div> <div>18%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	A	400	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6575 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 A/G-specific adenine glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2860	1831	494	524	11			
1	B	350	Total	C	N	O	S	0	0	0
			2818	1804	488	515	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P83847
A	-1	SER	-	expression tag	UNP P83847
A	0	HIS	-	expression tag	UNP P83847
A	164	CYS	PRO	engineered mutation	UNP P83847
B	-2	GLY	-	expression tag	UNP P83847
B	-1	SER	-	expression tag	UNP P83847
B	0	HIS	-	expression tag	UNP P83847
B	164	CYS	PRO	engineered mutation	UNP P83847

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			198	96	33	60	9			
2	E	10	Total	C	N	O	P	0	0	0
			198	96	33	60	9			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3').

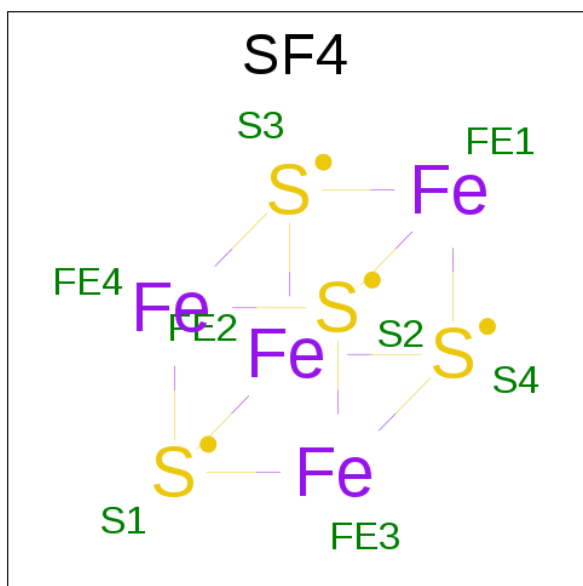
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	11	Total	C	N	O	P	0	0	0
			228	108	48	62	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	11	Total	C	N	O	P	0	0	0
			228	108	48	62	10			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

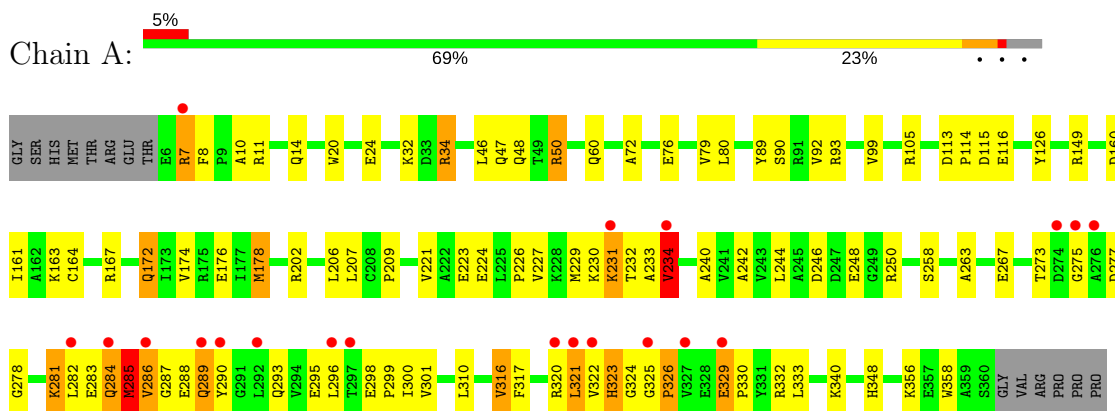
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	11	Total	O	0	0
			11	11		
5	C	2	Total	O	0	0
			2	2		
5	D	3	Total	O	0	0
			3	3		
5	E	2	Total	O	0	0
			2	2		
5	F	4	Total	O	0	0
			4	4		

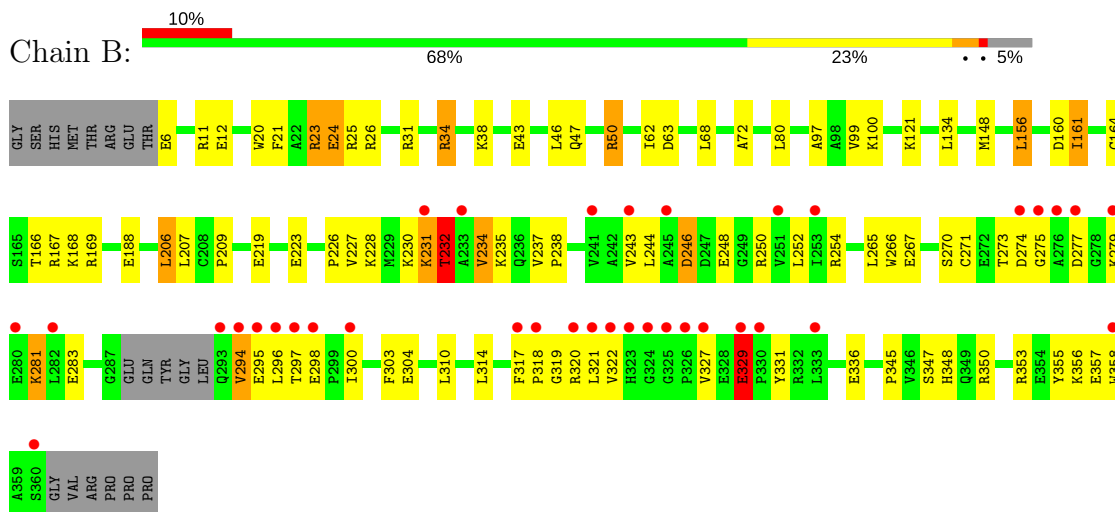
3 Residue-property plots

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: A/G-specific adenine glycosylase



- Molecule 1: A/G-specific adenine glycosylase



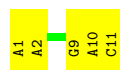
- Molecule 2: DNA (5'-D(*T*GP*TP*CP*CP*AP*CP*GP*TP*CP*T)-3')



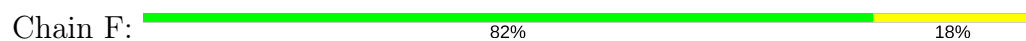
- Molecule 2: DNA (5'-D(*T*GP*TP*CP*CP*AP*CP*GP*TP*CP*T)-3')



- Molecule 3: DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3')



- Molecule 3: DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	105.27 Å 105.27 Å 235.37 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.01 – 2.59 85.01 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (85.01-2.59) 100.0 (85.01-2.59)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.58 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.169 , 0.228 0.171 , 0.225	Depositor DCC
R_{free} test set	2311 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6575	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: 8OG, SF4

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	0.54	0/2932	0.69	0/3982
1	B	0.51	0/2888	0.66	0/3921
2	C	1.33	1/220 (0.5%)	1.32	1/337 (0.3%)
2	E	1.51	4/220 (1.8%)	1.44	4/337 (1.2%)
3	D	1.05	0/230	1.06	0/351
3	F	1.24	0/230	1.15	1/351 (0.3%)
All	All	0.68	5/6720 (0.1%)	0.79	6/9279 (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	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	17	DA	C3'-O3'	-6.36	1.35	1.44
2	E	13	DG	C5'-C4'	5.78	1.57	1.51
2	E	17	DA	O5'-C5'	-5.65	1.28	1.42
2	C	13	DG	C5'-C4'	5.59	1.57	1.51
2	E	18	DC	O5'-C5'	-5.49	1.28	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	18	DC	O5'-P-OP2	-6.81	99.57	105.70
2	E	17	DA	O5'-P-OP2	-5.57	100.68	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	17	DA	P-O3'-C3'	-5.51	113.09	119.70
2	E	17	DA	O4'-C4'-C3'	-5.32	102.37	104.50
3	F	7	DT	C1'-O4'-C4'	-5.26	104.84	110.10
2	E	18	DC	O4'-C4'-C3'	-5.21	102.42	104.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	MET	Peptide
1	A	322	VAL	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	2860	0	2821	57	0
1	B	2818	0	2783	60	0
2	C	198	0	115	5	0
2	E	198	0	115	9	0
3	D	228	0	124	5	0
3	F	228	0	124	3	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	7	0	0	0	0
5	B	11	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
5	E	2	0	0	0	0
5	F	4	0	0	0	0
All	All	6575	0	6082	129	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (129) 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:B:294:VAL:HG11	1:B:321:LEU:HA	1.48	0.96
1:A:246:ASP:HB3	1:A:248:GLU:H	1.27	0.95
1:B:50:ARG:HH11	1:B:50:ARG:HG3	1.35	0.91
3:F:1:DA:HO5'	3:F:1:DA:H8	1.21	0.87
1:B:254:ARG:HH21	1:B:270:SER:H	1.25	0.80
1:B:297:THR:HG22	1:B:298:GLU:H	1.46	0.80
1:A:329:GLU:HB3	1:A:330:PRO:HD2	1.68	0.76
1:B:254:ARG:NH2	1:B:270:SER:H	1.84	0.74
1:B:281:LYS:HZ2	1:B:281:LYS:HB2	1.57	0.69
1:A:50:ARG:NH1	3:D:9:DG:N3	2.40	0.69
1:B:46:LEU:HB3	2:E:18:DC:H2'	1.76	0.68
2:E:18:DC:H5''	2:E:18:DC:H6	1.58	0.68
1:B:234:VAL:HG13	1:B:310:LEU:HA	1.76	0.67
1:B:254:ARG:NH2	1:B:270:SER:O	2.29	0.66
3:D:1:DA:H2''	3:D:2:DA:H5'	1.76	0.66
1:B:68:LEU:HG	1:B:99:VAL:HG13	1.78	0.65
1:B:160:ASP:HA	1:B:227:VAL:HG22	1.76	0.65
1:B:206:LEU:HD13	1:B:207:LEU:HG	1.79	0.64
1:A:293:GLN:NE2	3:F:1:DA:N1	2.45	0.64
1:B:246:ASP:HB3	1:B:248:GLU:H	1.63	0.64
3:D:10:DA:H2''	3:D:11:DC:H5''	1.79	0.64
1:A:113:ASP:HB3	1:A:116:GLU:HG3	1.78	0.64
2:E:18:DC:H5''	2:E:18:DC:C6	2.32	0.63
1:A:329:GLU:HB3	1:A:330:PRO:CD	2.27	0.63
1:A:285:MET:N	1:A:286:VAL:O	2.31	0.63
1:B:148:MET:HB3	1:B:161:ILE:HD11	1.79	0.62
1:A:300:ILE:HG13	1:A:301:VAL:HG12	1.82	0.61
1:A:293:GLN:HB3	2:E:22:DT:H2''	1.81	0.61
1:A:290:TYR:HB3	1:A:326:PRO:O	2.02	0.59
1:A:164:CYS:SG	3:D:2:DA:N6	2.75	0.59
1:A:229:MET:HB3	1:A:231:LYS:HG3	1.85	0.58
1:B:21:PHE:O	1:B:25:ARG:HB2	2.04	0.57
1:B:50:ARG:HG3	1:B:50:ARG:NH1	2.13	0.57
1:B:267:GLU:HB2	1:B:348:HIS:CE1	2.40	0.57
2:E:13:DG:C8	2:E:13:DG:H5''	2.41	0.56
1:A:160:ASP:HB3	1:A:163:LYS:HG3	1.86	0.56
1:B:160:ASP:OD1	1:B:228:LYS:HA	2.06	0.56
1:A:273:THR:O	1:A:275:GLY:N	2.37	0.56
1:B:297:THR:CG2	1:B:298:GLU:H	2.18	0.56
2:E:17:DA:C8	2:E:17:DA:H5''	2.41	0.56
2:E:17:DA:H8	2:E:17:DA:H5''	1.70	0.56
1:A:246:ASP:HB3	1:A:248:GLU:N	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:THR:HG22	1:B:298:GLU:N	2.18	0.55
1:B:329:GLU:HB3	1:B:331:TYR:HD2	1.71	0.55
1:A:149:ARG:HG3	1:A:226:PRO:HD3	1.87	0.55
1:A:244:LEU:HB3	1:A:321:LEU:HD13	1.89	0.55
2:E:18:DC:C6	2:E:18:DC:C5'	2.90	0.54
1:A:34:ARG:HE	1:A:34:ARG:HA	1.71	0.54
1:A:287:GLY:HA2	2:E:22:DT:H3'	1.89	0.54
1:A:278:GLY:H	1:A:281:LYS:HZ3	1.55	0.54
3:F:1:DA:H8	3:F:1:DA:O5'	1.87	0.53
1:A:46:LEU:HB3	2:C:18:DC:H2'	1.90	0.53
1:A:301:VAL:HG13	1:A:316:VAL:HG13	1.91	0.52
1:A:93:ARG:NH2	1:A:263:ALA:HB3	2.24	0.52
1:B:20:TRP:CD1	1:B:24:GLU:HG3	2.44	0.52
1:A:289:GLN:HG2	1:A:290:TYR:CE1	2.44	0.52
1:B:320:ARG:HG3	1:B:321:LEU:N	2.24	0.52
1:A:281:LYS:HZ2	1:A:281:LYS:H	1.58	0.52
1:B:161:ILE:HA	1:B:166:THR:HG21	1.91	0.52
3:D:1:DA:C2'	3:D:2:DA:H5'	2.39	0.51
1:B:244:LEU:HD12	1:B:252:LEU:HD23	1.92	0.51
1:A:47:GLN:HG2	2:C:19:DG:H4'	1.93	0.51
1:A:174:VAL:O	1:A:178:MET:HB3	2.11	0.51
1:B:296:LEU:HD23	1:B:319:GLY:HA3	1.93	0.50
1:A:89:TYR:O	1:A:92:VAL:HG12	2.12	0.49
1:B:273:THR:O	1:B:275:GLY:N	2.45	0.49
1:A:10:ALA:O	1:A:14:GLN:HG3	2.12	0.49
1:A:232:THR:OG1	1:A:233:ALA:N	2.44	0.49
1:A:79:VAL:HG12	1:A:92:VAL:HG22	1.94	0.48
1:B:167:ARG:HG3	1:B:168:LYS:N	2.28	0.48
1:B:20:TRP:CG	1:B:209:PRO:HG3	2.49	0.48
1:A:289:GLN:HG2	1:A:290:TYR:CZ	2.49	0.47
1:B:231:LYS:HB3	1:B:232:THR:H	1.41	0.47
1:B:246:ASP:HB2	1:B:250:ARG:H	1.80	0.47
1:B:265:LEU:HB3	1:B:345:PRO:HD3	1.95	0.47
1:B:23:ARG:O	1:B:25:ARG:N	2.48	0.47
1:A:172:GLN:O	1:A:176:GLU:HG3	2.15	0.46
1:B:336:GLU:OE2	1:B:356:LYS:NZ	2.27	0.46
1:A:221:VAL:O	1:A:224:GLU:HG2	2.16	0.46
1:B:271:CYS:SG	1:B:281:LYS:HB3	2.57	0.45
1:B:300:ILE:HG23	1:B:318:PRO:HG3	1.99	0.45
1:A:50:ARG:HH11	1:A:50:ARG:HG3	1.81	0.45
1:B:134:LEU:HD21	1:B:188:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:GLU:O	1:B:47:GLN:HG3	2.17	0.45
1:A:20:TRP:HB2	1:A:209:PRO:HB3	1.99	0.44
1:A:206:LEU:O	1:A:206:LEU:HD22	2.17	0.44
1:A:72:ALA:HB2	1:A:99:VAL:HG12	1.98	0.44
1:B:320:ARG:HG3	1:B:321:LEU:H	1.82	0.44
1:A:299:PRO:HD3	1:A:317:PHE:CE1	2.52	0.44
1:B:34:ARG:HE	1:B:34:ARG:HA	1.83	0.44
1:B:294:VAL:HG11	1:B:321:LEU:CA	2.34	0.43
1:B:266:TRP:O	1:B:345:PRO:HD2	2.18	0.43
1:A:324:GLY:O	1:A:326:PRO:N	2.51	0.43
1:B:25:ARG:HG2	1:B:31:ARG:NH1	2.34	0.43
1:B:21:PHE:CE1	1:B:25:ARG:HG3	2.53	0.43
1:A:283:GLU:HG2	1:A:296:LEU:HD12	2.00	0.43
1:B:237:VAL:HA	1:B:238:PRO:HD3	1.89	0.42
1:A:242:ALA:HB2	1:A:282:LEU:HG	2.01	0.42
1:B:206:LEU:HD22	1:B:206:LEU:O	2.19	0.42
1:A:20:TRP:CD1	1:A:24:GLU:HG3	2.54	0.42
1:A:267:GLU:HB2	1:A:348:HIS:CE1	2.55	0.42
1:A:356:LYS:HD2	1:A:356:LYS:HA	1.77	0.42
1:A:46:LEU:O	2:C:18:DC:H3'	2.19	0.42
1:A:296:LEU:HA	1:A:296:LEU:HD23	1.79	0.42
1:A:207:LEU:HA	1:A:207:LEU:HD23	1.79	0.42
1:A:113:ASP:HA	1:A:114:PRO:HD3	1.92	0.42
1:A:246:ASP:HB2	1:A:250:ARG:H	1.85	0.42
1:B:317:PHE:HA	1:B:318:PRO:HD2	1.93	0.42
1:B:72:ALA:HB2	1:B:99:VAL:HG12	2.01	0.42
1:A:284:GLN:O	1:A:288:GLU:HB2	2.19	0.42
1:A:20:TRP:NE1	1:A:24:GLU:HG3	2.35	0.41
1:B:161:ILE:HD12	1:B:226:PRO:HB2	2.02	0.41
1:A:234:VAL:O	1:A:310:LEU:HA	2.19	0.41
1:B:283:GLU:HG2	1:B:295:GLU:HA	2.02	0.41
1:B:97:ALA:O	1:B:100:LYS:HB2	2.20	0.41
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.88	0.41
1:B:303:PHE:CE1	1:B:314:LEU:HD13	2.55	0.41
1:B:355:TYR:O	1:B:358:TRP:HB3	2.21	0.41
1:B:148:MET:CB	1:B:161:ILE:HD11	2.48	0.41
1:B:244:LEU:HD23	1:B:319:GLY:HA3	2.03	0.41
2:C:17:DA:H8	2:C:17:DA:H5''	1.86	0.41
1:A:244:LEU:HD21	1:A:296:LEU:HD21	2.03	0.41
1:B:243:VAL:HG11	1:B:355:TYR:CG	2.56	0.41
1:A:282:LEU:O	1:A:285:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LEU:HB3	1:B:297:THR:H	1.46	0.41
1:B:350:ARG:HG3	1:B:353:ARG:NH2	2.36	0.41
1:A:126:TYR:HB3	2:C:19:DG:H3'	2.04	0.40
1:A:240:ALA:HB1	1:A:282:LEU:HD22	2.03	0.40
1:B:62:ILE:HA	1:B:62:ILE:HD13	1.77	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	353/369 (96%)	318 (90%)	24 (7%)	11 (3%)	5	8
1	B	346/369 (94%)	314 (91%)	24 (7%)	8 (2%)	7	13
All	All	699/738 (95%)	632 (90%)	48 (7%)	19 (3%)	6	10

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	231	LYS
1	A	234	VAL
1	A	325	GLY
1	A	326	PRO
1	A	329	GLU
1	B	231	LYS
1	B	232	THR
1	B	24	GLU
1	B	274	ASP
1	B	294	VAL
1	B	329	GLU
1	A	286	VAL

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Mol	Chain	Res	Type
1	A	298	GLU
1	A	358	TRP
1	A	8	PHE
1	A	323	HIS
1	B	230	LYS
1	B	327	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	303/315 (96%)	268 (88%)	35 (12%)	6	11
1	B	299/315 (95%)	269 (90%)	30 (10%)	9	17
All	All	602/630 (96%)	537 (89%)	65 (11%)	7	14

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	11	ARG
1	A	32	LYS
1	A	34	ARG
1	A	48	GLN
1	A	50	ARG
1	A	60	GLN
1	A	76	GLU
1	A	80	LEU
1	A	90	SER
1	A	105	ARG
1	A	115	ASP
1	A	161	ILE
1	A	167	ARG
1	A	172	GLN
1	A	178	MET
1	A	202	ARG

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Mol	Chain	Res	Type
1	A	223	GLU
1	A	227	VAL
1	A	230	LYS
1	A	234	VAL
1	A	258	SER
1	A	277	ASP
1	A	281	LYS
1	A	284	GLN
1	A	285	MET
1	A	289	GLN
1	A	295	GLU
1	A	316	VAL
1	A	320	ARG
1	A	321	LEU
1	A	323	HIS
1	A	332	ARG
1	A	333	LEU
1	A	340	LYS
1	B	6	GLU
1	B	11	ARG
1	B	12	GLU
1	B	23	ARG
1	B	26	ARG
1	B	34	ARG
1	B	38	LYS
1	B	50	ARG
1	B	63	ASP
1	B	80	LEU
1	B	121	LYS
1	B	156	LEU
1	B	161	ILE
1	B	164	CYS
1	B	169	ARG
1	B	206	LEU
1	B	219	GLU
1	B	223	GLU
1	B	232	THR
1	B	234	VAL
1	B	235	LYS
1	B	246	ASP
1	B	277	ASP
1	B	279	LYS

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Mol	Chain	Res	Type
1	B	281	LYS
1	B	304	GLU
1	B	322	VAL
1	B	329	GLU
1	B	347	SER
1	B	357	GLU

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	47	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
3	8OG	D	6	3	17,25,26	1.38	2 (11%)	22,37,40	2.71	5 (22%)
3	8OG	F	6	3	17,25,26	1.34	3 (17%)	22,37,40	2.26	6 (27%)

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	8OG	D	6	3	-	0/3/21/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	8OG	F	6	3	-	0/3/21/22	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	8OG	C8-N7	-2.39	1.31	1.34
3	F	6	8OG	C8-N7	-2.21	1.31	1.34
3	F	6	8OG	O5'-C5'	-2.04	1.41	1.44
3	F	6	8OG	C6-N1	3.72	1.39	1.33
3	D	6	8OG	C6-N1	4.19	1.40	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	6	8OG	C5-C6-N1	-9.11	110.50	123.48
3	F	6	8OG	C5-C6-N1	-7.04	113.45	123.48
3	F	6	8OG	N3-C2-N1	-3.35	122.57	127.46
3	D	6	8OG	N3-C2-N1	-2.88	123.26	127.46
3	F	6	8OG	C4-C5-N7	-2.33	107.28	109.47
3	F	6	8OG	C1'-N9-C4	-2.23	122.83	126.99
3	D	6	8OG	C4-C5-N7	-2.20	107.41	109.47
3	F	6	8OG	C8-N9-C1'	2.23	129.73	125.90
3	D	6	8OG	C2'-C1'-N9	2.57	118.40	115.79
3	F	6	8OG	C6-N1-C2	5.26	123.62	116.06
3	D	6	8OG	C6-N1-C2	6.54	125.47	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
4	SF4	A	400	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	400	1	0,12,12	0.00	-	0,24,24	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
4	SF4	A	400	1	-	0/0/48/48	0/6/5/5
4	SF4	B	400	1	-	0/0/48/48	0/6/5/5

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.

No monomer is involved in short contacts.

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	355/369 (96%)	0.52	20 (5%)	25 19	29, 49, 94, 138	0
1	B	350/369 (94%)	0.82	36 (10%)	7 4	31, 55, 111, 187	0
2	C	10/11 (90%)	0.15	0	100 100	38, 44, 58, 83	0
2	E	10/11 (90%)	0.11	0	100 100	38, 40, 51, 59	0
3	D	10/11 (90%)	0.24	0	100 100	38, 46, 92, 94	0
3	F	10/11 (90%)	0.03	0	100 100	38, 48, 62, 66	0
All	All	745/782 (95%)	0.64	56 (7%)	15 10	29, 51, 102, 187	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	PRO	20.1
1	B	324	GLY	6.7
1	B	325	GLY	6.3
1	B	321	LEU	6.0
1	B	322	VAL	5.1
1	B	327	VAL	4.9
1	B	282	LEU	4.9
1	B	333	LEU	4.9
1	B	329	GLU	4.7
1	B	296	LEU	4.5
1	B	323	HIS	4.4
1	A	290	TYR	4.3
1	A	274	ASP	4.2
1	A	286	VAL	4.1
1	B	320	ARG	3.9
1	B	245	ALA	3.8
1	A	325	GLY	3.7
1	A	296	LEU	3.7
1	A	275	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	292	LEU	3.5
1	B	294	VAL	3.3
1	A	329	GLU	3.2
1	B	243	VAL	3.2
1	A	289	GLN	3.2
1	B	280	GLU	3.1
1	B	293	GLN	3.1
1	B	275	GLY	3.1
1	B	360	SER	3.0
1	B	295	GLU	2.9
1	B	298	GLU	2.9
1	B	274	ASP	2.9
1	A	234	VAL	2.8
1	B	276	ALA	2.8
1	B	253	ILE	2.6
1	B	317	PHE	2.6
1	A	327	VAL	2.6
1	B	241	VAL	2.6
1	A	322	VAL	2.5
1	A	276	ALA	2.5
1	A	297	THR	2.5
1	B	279	LYS	2.5
1	B	277	ASP	2.5
1	A	284	GLN	2.4
1	A	282	LEU	2.4
1	B	231	LYS	2.4
1	B	330	PRO	2.3
1	B	300	ILE	2.2
1	B	251	VAL	2.1
1	B	233	ALA	2.1
1	A	7	ARG	2.1
1	B	297	THR	2.1
1	A	320	ARG	2.1
1	B	318	PRO	2.1
1	A	321	LEU	2.0
1	A	231	LYS	2.0
1	B	358	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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	8OG	D	6	23/24	0.99	0.18	-	29,42,50,54	0
3	8OG	F	6	23/24	0.99	0.19	-	34,41,51,54	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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
4	SF4	A	400	8/8	0.99	0.22	2.29	35,40,42,43	0
4	SF4	B	400	8/8	0.99	0.21	1.58	33,35,38,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.