



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:58 AM UTC

PDB ID : 9GM2 / pdb_00009gm2
Title : Human SMUG1 in complex with DNA
Authors : Ludaescher, J.M.; Scaletti Hutchinson, E.; Stenmark, P.
Deposited on : 2024-08-28
Resolution : 2.10 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

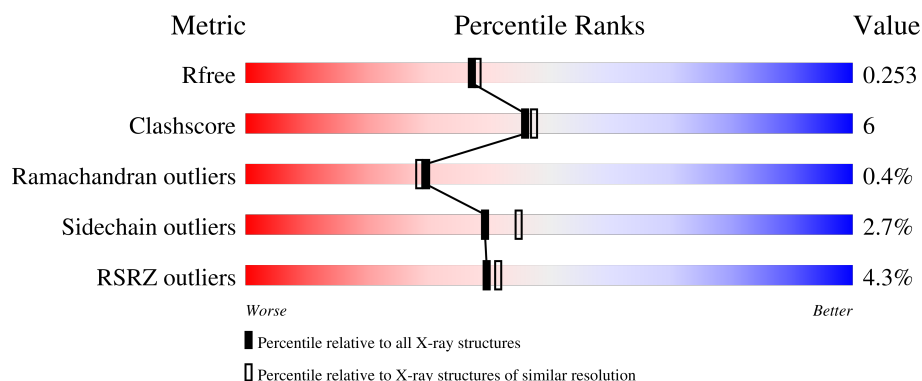
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	247	<div> <div>2%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	B	247	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	C	247	<div> <div>7%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	D	247	<div> <div>6%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
2	E	12	<div> <div>8%</div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	12	
3	F	12	
3	H	12	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17403 atoms, of which 8389 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 Single-strand selective monofunctional uracil DNA glycosylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	247	Total	C	H	N	O	S	38	4	0
			3910	1248	1962	346	343	11			
1	B	247	Total	C	H	N	O	S	38	5	0
			3923	1251	1968	349	344	11			
1	C	247	Total	C	H	N	O	S	37	1	0
			3896	1244	1955	346	340	11			
1	D	247	Total	C	H	N	O	S	37	5	0
			3930	1254	1972	348	344	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP Q53HV7
B	24	SER	-	expression tag	UNP Q53HV7
C	24	SER	-	expression tag	UNP Q53HV7
D	24	SER	-	expression tag	UNP Q53HV7

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	12	Total	C	H	N	O	P	5	0	0
			372	112	131	46	71	12			
2	G	12	Total	C	H	N	O	P	5	0	0
			372	112	131	46	71	12			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	12	Total	C	H	N	O	P	7	0	0
			379	115	135	44	73	12			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	12	Total 379	C 115	H 135	N 44	O 73	P 12	7	0	0

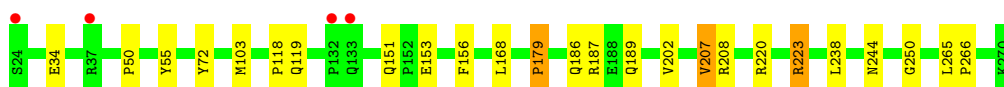
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total 69	O 69	0	0
4	B	67	Total 67	O 67	0	0
4	C	57	Total 57	O 57	0	0
4	D	42	Total 42	O 42	0	0
4	E	3	Total 3	O 3	0	0
4	F	1	Total 1	O 1	0	0
4	G	2	Total 2	O 2	0	0
4	H	1	Total 1	O 1	0	0

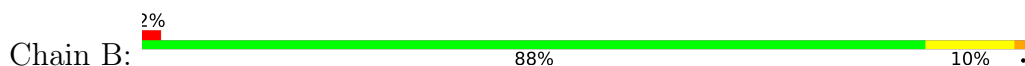
3 Residue-property plots [i](#)

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.

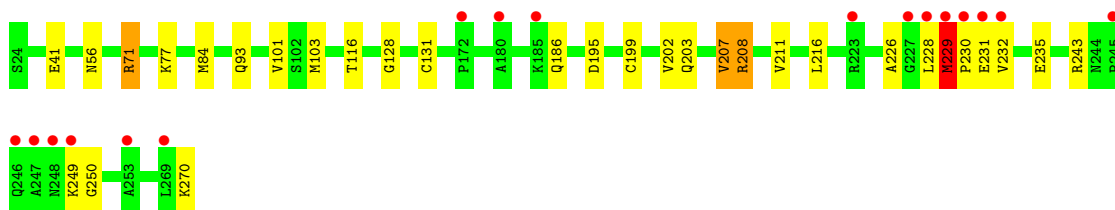
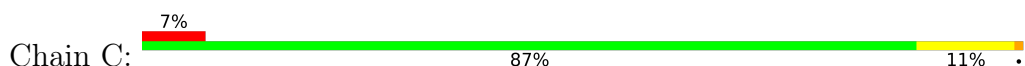
- Molecule 1: Single-strand selective monofunctional uracil DNA glycosylase



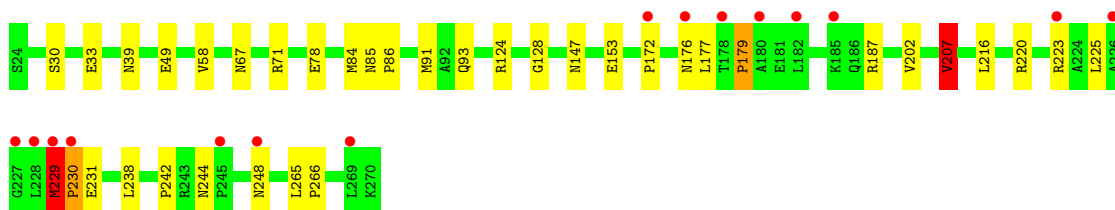
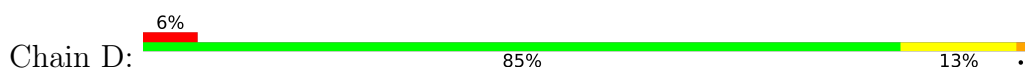
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- Molecule 1: Single-strand selective monofunctional uracil DNA glycosylase



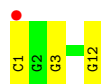
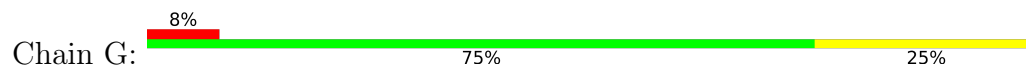
- Molecule 1: Single-strand selective monofunctional uracil DNA glycosylase



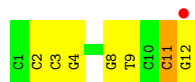
- Molecule 2: DNA (5'-D(P*CP*GP*GP*AP*CP*T*ORP*AP*CP*GP*GP*G)-3')



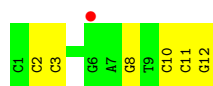
- Molecule 2: DNA (5'-D(P*CP*GP*GP*AP*CP*T*ORP*AP*CP*GP*GP*G)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.07Å 84.37Å 88.26Å 90.00° 113.40° 90.00°	Depositor
Resolution (Å)	72.05 – 2.10 72.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	79.7 (72.05-2.10) 79.7 (72.05-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.207 , 0.253 0.206 , 0.253	Depositor DCC
R_{free} test set	2374 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17403	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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: ORP

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	0/2011	1.02	3/2733 (0.1%)
1	B	0.54	0/2020	1.03	2/2746 (0.1%)
1	C	0.52	0/1993	1.04	3/2710 (0.1%)
1	D	0.55	0/2028	1.00	2/2755 (0.1%)
2	E	0.47	0/256	0.91	1/391 (0.3%)
2	G	0.48	0/256	1.16	1/391 (0.3%)
3	F	0.41	0/272	1.04	1/417 (0.2%)
3	H	0.44	0/272	1.11	4/417 (1.0%)
All	All	0.53	0/9108	1.03	17/12560 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	7

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	232	VAL	N-CA-CB	7.47	120.57	111.60
2	G	3	DG	O3'-P-O5'	-7.13	93.31	104.00
1	B	34	GLU	N-CA-CB	6.68	119.94	110.12
1	B	34	GLU	CB-CA-C	-6.54	99.93	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	DG	O3'-P-O5'	-6.25	94.62	104.00
1	C	195	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	103	MET	CG-SD-CE	-5.62	88.55	100.90
3	H	3	DC	O3'-P-O5'	-5.58	95.64	104.00
3	H	2	DC	C2'-C3'-O3'	5.52	119.78	111.50
3	H	8	DG	O3'-P-O5'	-5.50	95.75	104.00
1	A	34	GLU	CB-CA-C	-5.33	101.79	110.85
1	A	189	GLN	CB-CA-C	-5.20	102.72	110.88
1	D	78	GLU	CB-CA-C	5.11	119.76	110.11
1	C	116	THR	CA-CB-OG1	-5.10	101.95	109.60
3	F	11	DC	O3'-P-O5'	-5.06	96.40	104.00
1	D	207	VAL	N-CA-CB	5.05	117.18	110.26
3	H	2	DC	C4'-C3'-O3'	-5.04	102.43	110.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ARG	Sidechain
1	B	223	ARG	Sidechain
1	B	37	ARG	Sidechain
1	C	208	ARG	Sidechain
1	C	71	ARG	Sidechain
1	D	229[A]	MET	Peptide
1	D	229[B]	MET	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	1948	1962	1939	13	0
1	B	1955	1968	1943	22	1
1	C	1941	1955	1946	20	0
1	D	1958	1972	1942	29	0
2	E	241	131	131	9	1
2	G	241	131	131	5	0
3	F	244	135	135	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	244	135	135	2	0
4	A	69	0	0	2	0
4	B	67	0	0	5	0
4	C	57	0	0	4	0
4	D	42	0	0	2	0
4	E	3	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
All	All	9014	8389	8302	99	1

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 (99) 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)
2:E:6:DT:H2''	2:E:7:ORP:O1P	1.39	1.09
1:D:229[A]:MET:O	1:D:229[A]:MET:HG3	1.60	1.02
1:B:56[B]:ASN:H	1:B:56[B]:ASN:HD22	1.04	0.94
1:B:56[B]:ASN:HD22	1:B:56[B]:ASN:N	1.66	0.89
2:E:6:DT:C2'	2:E:7:ORP:O1P	2.27	0.81
1:D:229[A]:MET:O	1:D:229[A]:MET:CG	2.29	0.81
1:D:225:LEU:O	1:D:229[B]:MET:HG3	1.81	0.80
1:D:248[B]:ASN:HD22	1:D:248[B]:ASN:C	1.91	0.79
2:E:1:DC:P	2:E:1:DC:C6	2.82	0.73
1:B:56[B]:ASN:H	1:B:56[B]:ASN:ND2	1.86	0.70
1:A:153[B]:GLU:OE2	4:A:301:HOH:O	2.10	0.69
1:C:202:VAL:HG13	1:C:207:VAL:HG22	1.74	0.68
1:A:202:VAL:HG13	1:A:207:VAL:HG22	1.77	0.66
1:C:228:LEU:HG	1:C:228:LEU:O	1.96	0.65
1:D:67:ASN:HD21	1:D:71:ARG:HH11	1.43	0.65
1:D:248[B]:ASN:C	1:D:248[B]:ASN:ND2	2.52	0.65
1:C:229:MET:O	1:C:231:GLU:N	2.30	0.64
1:B:269:LEU:HA	4:B:343:HOH:O	1.97	0.64
1:C:56[B]:ASN:H	1:C:56[B]:ASN:HD22	1.45	0.63
1:C:101:VAL:HG21	1:C:131:CYS:HB3	1.79	0.62
1:C:228:LEU:C	1:C:230:PRO:CD	2.73	0.62
1:D:124:ARG:NH2	2:E:6:DT:OP1	2.24	0.61
1:A:151:GLN:HB3	1:A:153[B]:GLU:OE2	2.00	0.61
1:C:228:LEU:C	1:C:230:PRO:HD3	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:PRO:HD2	2:E:7:ORP:O1P	2.00	0.60
1:C:203:GLN:NE2	1:C:228:LEU:HD21	2.16	0.60
2:E:1:DC:P	2:E:1:DC:O4'	2.60	0.60
3:F:11:DC:H1'	3:F:12:DG:N7	2.17	0.60
1:A:118:PRO:HG2	1:B:33:GLU:HG3	1.84	0.59
2:G:1:DC:H2'	2:G:1:DC:O2	2.02	0.59
4:B:356:HOH:O	1:D:147:ASN:HB3	2.02	0.58
1:A:153[B]:GLU:H	1:A:153[B]:GLU:CD	2.12	0.57
1:B:56[B]:ASN:N	1:B:56[B]:ASN:ND2	2.41	0.57
1:B:265:LEU:N	1:B:266:PRO:HD2	2.21	0.56
2:E:1:DC:OP2	2:G:12:DG:H2''	2.06	0.55
1:C:199:CYS:O	1:C:203:GLN:HG2	2.07	0.55
3:F:12:DG:N3	3:F:12:DG:H2'	2.22	0.54
3:H:11:DC:H2''	3:H:12:DG:C8	2.42	0.54
1:B:56[B]:ASN:ND2	4:B:304:HOH:O	2.41	0.53
1:C:228:LEU:O	1:C:230:PRO:HD2	2.08	0.53
3:F:8:DG:H1'	3:F:9:DT:H5'	1.90	0.52
3:F:3:DC:H4'	3:F:4:DG:OP1	2.08	0.52
2:G:1:DC:O2	2:G:1:DC:C2'	2.57	0.52
1:B:246:GLN:O	1:B:249:LYS:HE3	2.11	0.51
1:C:208:ARG:HD2	4:C:306:HOH:O	2.12	0.50
1:D:230:PRO:HD2	1:D:231:GLU:H	1.77	0.49
1:C:226:ALA:HB3	4:C:330:HOH:O	2.12	0.49
1:C:56[B]:ASN:HD22	1:C:56[B]:ASN:N	2.08	0.49
1:B:202:VAL:HG13	1:B:207:VAL:HG22	1.93	0.49
1:D:84:MET:HE3	1:D:216:LEU:HB3	1.94	0.49
1:D:153:GLU:HG3	4:D:340:HOH:O	2.13	0.49
1:D:230:PRO:HD2	1:D:231:GLU:OE1	2.13	0.49
1:B:55:TYR:HB2	1:B:168:LEU:HB3	1.94	0.48
1:B:179:PRO:O	1:B:187:ARG:HD3	2.12	0.48
1:D:202:VAL:HG13	1:D:207:VAL:HG22	1.96	0.48
1:D:238:LEU:HD11	1:D:244:ASN:HD21	1.78	0.47
1:B:39[A]:ASN:OD1	1:B:56[A]:ASN:ND2	2.48	0.47
3:F:2:DC:H2''	3:F:3:DC:O5'	2.14	0.47
1:D:67:ASN:HD21	1:D:71:ARG:NH1	2.10	0.46
1:D:220:ARG:HA	1:D:220:ARG:HD2	1.66	0.46
1:B:231:GLU:HB3	4:B:359:HOH:O	2.16	0.46
3:H:10:DC:H2''	3:H:11:DC:OP2	2.15	0.46
1:B:107:TRP:CD1	1:B:146:ARG:HG3	2.51	0.46
1:D:172:PRO:HA	4:D:312:HOH:O	2.16	0.45
1:C:103:MET:HE3	4:C:310:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD11	1:A:244:ASN:HD21	1.81	0.45
1:B:37:ARG:HD2	4:B:333:HOH:O	2.16	0.45
1:D:39:ASN:HD21	1:D:58:VAL:CG1	2.30	0.45
1:A:179:PRO:O	1:A:187:ARG:HD3	2.16	0.45
1:D:86:PRO:HB3	1:D:91:MET:HB3	1.99	0.44
1:D:30:SER:O	1:D:33[B]:GLU:HG2	2.18	0.44
1:B:24:SER:OG	1:B:25:GLY:N	2.49	0.44
1:D:85:ASN:HB2	1:D:86:PRO:CD	2.48	0.44
1:D:230:PRO:HG2	1:D:231:GLU:OE2	2.17	0.44
1:C:71:ARG:HD2	4:C:349:HOH:O	2.17	0.43
2:E:1:DC:P	2:G:12:DG:H2''	2.59	0.43
1:D:265:LEU:N	1:D:266:PRO:CD	2.82	0.43
1:B:240:PRO:HB3	1:B:251:TRP:CE2	2.54	0.42
1:B:246:GLN:O	1:B:249:LYS:CE	2.67	0.42
2:E:1:DC:P	2:G:12:DG:C2'	3.07	0.42
1:D:93:GLN:O	1:D:128:GLY:HA2	2.19	0.42
1:A:220:ARG:NH1	1:A:223:ARG:HH12	2.17	0.42
3:F:3:DC:H2'	3:F:3:DC:OP2	2.20	0.42
1:D:179:PRO:O	1:D:187:ARG:HD3	2.19	0.42
1:A:119:GLN:HB3	1:B:29:GLU:CD	2.45	0.42
1:A:153[B]:GLU:HG3	4:A:357:HOH:O	2.19	0.42
1:A:55:TYR:HB2	1:A:168:LEU:HB3	2.00	0.42
1:C:56[B]:ASN:H	1:C:56[B]:ASN:ND2	2.14	0.42
1:B:39[B]:ASN:HD21	1:B:58:VAL:CG1	2.33	0.42
1:C:93:GLN:O	1:C:128:GLY:HA2	2.20	0.41
1:C:211:VAL:HA	1:C:235:GLU:O	2.20	0.41
1:A:265:LEU:N	1:A:266:PRO:CD	2.84	0.41
1:D:39:ASN:HD21	1:D:58:VAL:HG12	1.86	0.41
1:C:77:LYS:O	1:C:207:VAL:HA	2.21	0.41
1:D:176:ASN:HD22	1:D:177:LEU:N	2.18	0.41
1:D:230:PRO:CD	1:D:231:GLU:H	2.34	0.41
1:C:84:MET:HE3	1:C:216:LEU:C	2.45	0.40
1:B:39[B]:ASN:HD21	1:B:58:VAL:HG12	1.87	0.40
1:A:72:TYR:HB3	1:A:156:PHE:CD1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:SER:HG	2:E:1:DC:H5[2_455]	1.13	0.47

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	249/247 (101%)	244 (98%)	4 (2%)	1 (0%)	30	28
1	B	250/247 (101%)	245 (98%)	5 (2%)	0	100	100
1	C	246/247 (100%)	237 (96%)	7 (3%)	2 (1%)	16	12
1	D	250/247 (101%)	240 (96%)	9 (4%)	1 (0%)	30	28
All	All	995/988 (101%)	966 (97%)	25 (2%)	4 (0%)	30	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	230	PRO
1	C	229	MET
1	C	250	GLY
1	A	250	GLY

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	210/207 (101%)	205 (98%)	5 (2%)	43	49
1	B	211/207 (102%)	206 (98%)	5 (2%)	43	49
1	C	208/207 (100%)	201 (97%)	7 (3%)	32	35
1	D	212/207 (102%)	206 (97%)	6 (3%)	38	43
All	All	841/828 (102%)	818 (97%)	23 (3%)	39	45

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	PRO
1	A	179	PRO
1	A	186	GLN
1	A	207	VAL
1	A	223	ARG
1	B	50	PRO
1	B	207	VAL
1	B	223	ARG
1	B	269	LEU
1	B	270	LYS
1	C	41	GLU
1	C	186	GLN
1	C	207	VAL
1	C	229	MET
1	C	243	ARG
1	C	249	LYS
1	C	270	LYS
1	D	49	GLU
1	D	179	PRO
1	D	207	VAL
1	D	223	ARG
1	D	229[A]	MET
1	D	229[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	74	GLN
1	A	147	ASN
1	A	157	HIS
1	A	219	GLN
1	A	233	GLN
1	A	244	ASN
1	B	44	GLN
1	B	189	GLN
1	B	219	GLN
1	B	244	ASN
1	C	46	GLN
1	C	157	HIS
1	C	158	HIS

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Mol	Chain	Res	Type
1	C	176	ASN
1	D	67	ASN
1	D	157	HIS
1	D	163	ASN
1	D	176	ASN
1	D	244	ASN

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	$\# Z > 2$
2	ORP	G	7	2	9,12,13	0.47	0	7,16,19	0.68	0
2	ORP	E	7	2	9,12,13	0.31	0	7,16,19	0.34	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
2	ORP	G	7	2	-	0/3/17/18	0/1/1/1
2	ORP	E	7	2	-	2/3/17/18	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	7	ORP	C3-C4-C5-O5
2	E	7	ORP	O4-C4-C5-O5

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	7	ORP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	247/247 (100%)	0.06	4 (1%) 70 73	11, 29, 57, 71	2 (0%)
1	B	247/247 (100%)	0.07	4 (1%) 70 73	11, 30, 53, 77	3 (1%)
1	C	247/247 (100%)	0.46	17 (6%) 23 24	12, 35, 72, 97	1 (0%)
1	D	247/247 (100%)	0.42	15 (6%) 27 29	16, 36, 64, 82	3 (1%)
2	E	11/12 (91%)	0.65	1 (9%) 15 15	38, 53, 82, 91	0
2	G	11/12 (91%)	0.75	1 (9%) 15 15	44, 50, 71, 97	0
3	F	12/12 (100%)	1.04	1 (8%) 17 18	54, 78, 101, 113	0
3	H	12/12 (100%)	1.07	1 (8%) 17 18	54, 80, 88, 108	0
All	All	1034/1036 (99%)	0.28	44 (4%) 40 41	11, 34, 67, 113	9 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	1	DC	4.9
1	D	229[A]	MET	4.2
1	C	247	ALA	4.1
1	C	229	MET	3.9
1	C	253	ALA	3.8
1	C	230	PRO	3.6
1	B	50	PRO	3.4
1	D	230	PRO	3.4
1	C	245	PRO	3.4
1	B	269	LEU	3.4
1	D	227	GLY	3.2
1	C	246	GLN	3.2
1	C	269	LEU	3.1
1	A	132	PRO	3.1
1	C	228	LEU	3.1
1	C	248	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	180	ALA	2.9
3	F	12	DG	2.9
1	D	269	LEU	2.8
1	C	231	GLU	2.8
1	D	248[A]	ASN	2.8
3	H	6	DG	2.8
1	B	24	SER	2.7
1	A	37	ARG	2.6
1	C	185	LYS	2.4
1	C	180	ALA	2.3
1	D	172	PRO	2.3
2	E	1	DC	2.3
1	C	232	VAL	2.3
1	C	172	PRO	2.3
1	D	182	LEU	2.3
1	B	48	SER	2.2
1	D	185	LYS	2.2
1	C	223	ARG	2.2
1	D	176	ASN	2.2
1	C	227	GLY	2.1
1	D	228	LEU	2.1
1	C	249	LYS	2.1
1	A	133	GLN	2.1
1	A	24	SER	2.1
1	D	226	ALA	2.1
1	D	178	THR	2.0
1	D	223	ARG	2.0
1	D	245	PRO	2.0

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	ORP	G	7	12/13	0.60	0.20	88,99,117,119	1
2	ORP	E	7	12/13	0.69	0.23	73,80,93,95	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.