



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 12:50 PM BST

PDB ID : 4IBZ
Title : Human p53 core domain with hot spot mutation R273C and second-site suppressor mutation T284R
Authors : Eldar, A.; Rozenberg, H.; Diskin-Posner, Y.; Shakked, Z.
Deposited on : 2012-12-09
Resolution : 1.92 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

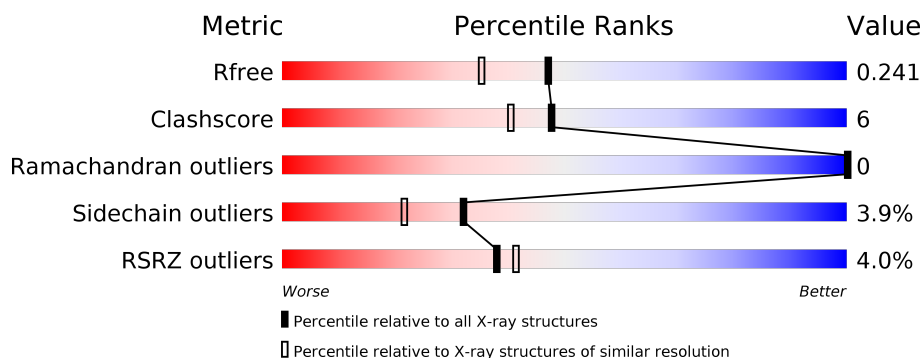
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 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	200	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	200	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>• •</div> </div> </div>
1	C	200	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>•</div> </div> </div>
1	D	200	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• • •</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6929 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	12	0
			1579	972	286	299	22			
1	B	192	Total	C	N	O	S	0	7	0
			1531	949	277	286	19			
1	C	192	Total	C	N	O	S	0	9	0
			1528	946	279	283	20			
1	D	192	Total	C	N	O	S	0	11	0
			1567	966	289	293	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	CYS	ARG	ENGINEERED MUTATION	UNP P04637
A	284	ARG	THR	ENGINEERED MUTATION	UNP P04637
B	273	CYS	ARG	ENGINEERED MUTATION	UNP P04637
B	284	ARG	THR	ENGINEERED MUTATION	UNP P04637
C	273	CYS	ARG	ENGINEERED MUTATION	UNP P04637
C	284	ARG	THR	ENGINEERED MUTATION	UNP P04637
D	273	CYS	ARG	ENGINEERED MUTATION	UNP P04637
D	284	ARG	THR	ENGINEERED MUTATION	UNP P04637

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



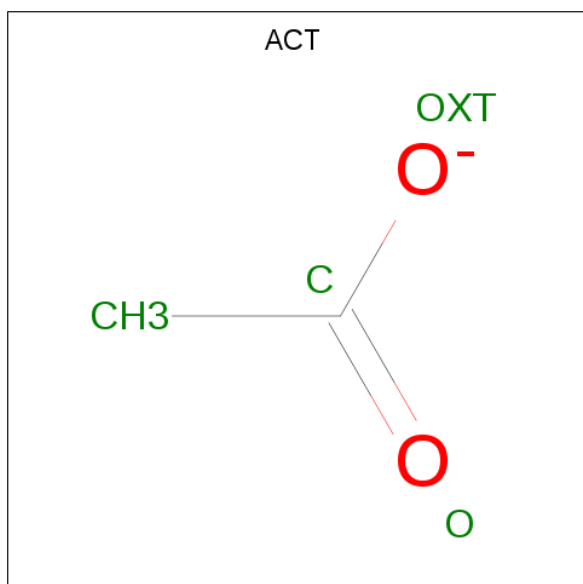
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	1
			8	4	4		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	165	Total	O	0	7
			172	172		

Continued on next page...

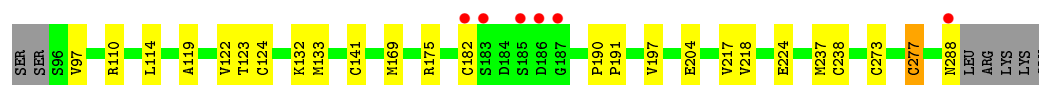
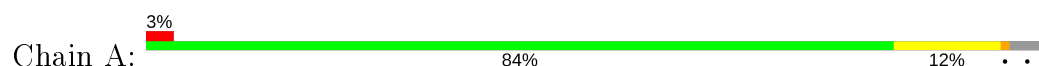
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	162	Total 166	O 166	0	5
5	C	139	Total 144	O 144	0	7
5	D	147	Total 150	O 150	0	5

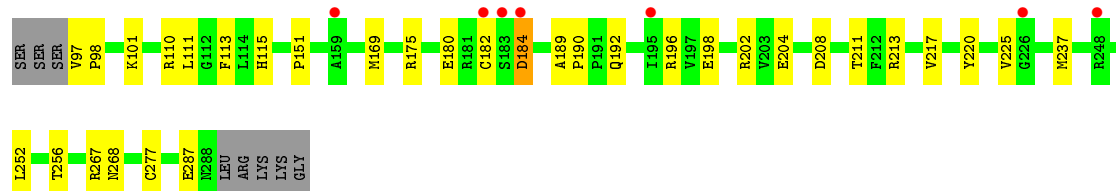
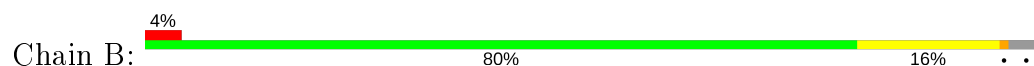
3 Residue-property plots [i](#)

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.

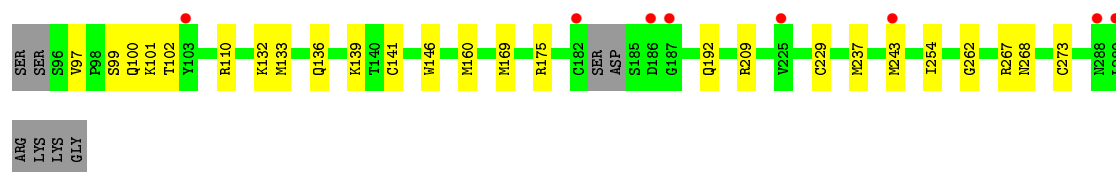
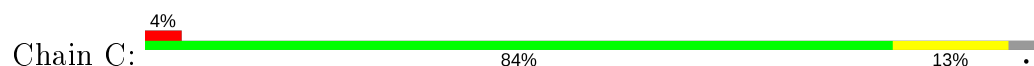
- Molecule 1: Cellular tumor antigen p53



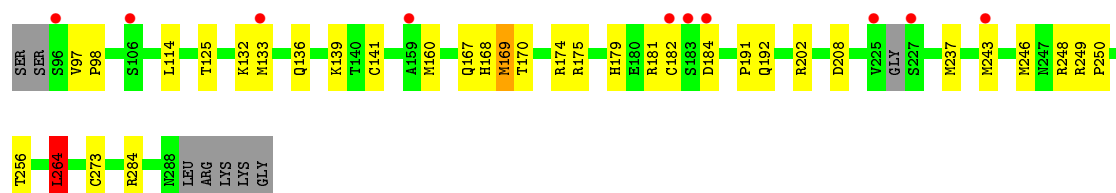
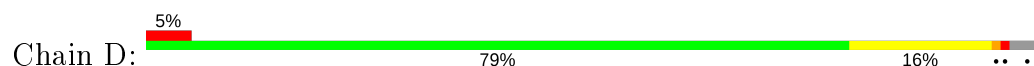
- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.74Å 70.41Å 84.58Å 90.00° 89.92° 90.00°	Depositor
Resolution (Å)	26.69 – 1.92 26.69 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.4 (26.69-1.92) 91.5 (26.69-1.92)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, R_{free}	0.179 , 0.233 0.187 , 0.241	Depositor DCC
R_{free} test set	2485 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.996	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l 0.009 for -k,-h,-l 0.119 for h,-k,-l	Xtriage
Reported twinning fraction	0.070 for h,-k,-l	Depositor
Outliers	1 of 59996 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6929	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.76% 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: ZN, EDO, 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	0.39	0/1617	0.55	0/2196
1	B	0.38	0/1571	0.55	0/2135
1	C	0.39	0/1571	0.55	0/2132
1	D	0.34	0/1607	0.55	1/2181 (0.0%)
All	All	0.38	0/6366	0.55	1/8644 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	264	LEU	CA-CB-CG	5.15	127.16	115.30

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	1579	0	1502	12	0
1	B	1531	0	1454	24	0
1	C	1528	0	1469	16	0
1	D	1567	0	1498	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	16	0	24	0	0
3	B	20	0	30	8	0
3	C	16	0	24	4	0
3	D	28	0	42	9	0
4	B	4	0	3	0	0
4	D	4	0	3	0	0
5	A	172	0	0	2	1
5	B	166	0	0	3	1
5	C	144	0	0	3	0
5	D	150	0	0	2	0
All	All	6929	0	6049	75	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 (75) 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:192:GLN:HB2	3:B:304:EDO:H22	1.55	0.87
1:D:114:LEU:HB2	3:D:303:EDO:H22	1.58	0.83
1:D:191:PRO:HD2	3:D:302:EDO:H22	1.70	0.73
1:A:97:VAL:HG11	1:A:169[B]:MET:HG2	1.69	0.73
1:C:160:MET:HB3	3:C:302:EDO:H22	1.71	0.72
1:B:287:GLU:HA	1:D:202:ARG:HD3	1.76	0.68
1:C:262:GLY:HA3	3:C:304:EDO:H12	1.80	0.63
1:B:175[A]:ARG:HD3	1:B:237:MET:HB2	1.81	0.63
1:A:277[A]:CYS:SG	5:A:460:HOH:O	2.56	0.60
1:C:209[A]:ARG:NH2	5:C:521:HOH:O	2.26	0.60
1:B:111:LEU:HG	1:B:268:ASN:HB3	1.85	0.59
1:B:208:ASP:HB2	3:B:306:EDO:C1	2.33	0.58
1:C:209[B]:ARG:HB3	3:C:303:EDO:H12	1.87	0.56
1:A:97:VAL:HG11	1:A:169[A]:MET:HG2	1.87	0.56
3:D:305[B]:EDO:H12	5:D:442:HOH:O	2.07	0.55
1:B:190:PRO:HB2	3:B:304:EDO:H21	1.88	0.54
1:B:190:PRO:CB	3:B:304:EDO:H21	2.38	0.54
1:D:256[A]:THR:HG23	1:D:264:LEU:HD23	1.89	0.54
1:A:175:ARG:HD3	1:A:237[A]:MET:HB2	1.88	0.54
1:B:211:THR:HG23	1:B:213:ARG:H	1.74	0.52
1:C:100:GLN:HG2	1:C:254:ILE:HD11	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:HIS:NE2	3:D:302:EDO:H21	2.26	0.51
1:C:132:LYS:HE2	1:C:273:CYS:HB2	1.93	0.51
1:C:133:MET:SD	1:C:141[A]:CYS:SG	3.09	0.51
1:D:97:VAL:HG11	1:D:169:MET:HE2	1.93	0.51
1:C:254:ILE:HB	3:C:302:EDO:H21	1.93	0.50
1:D:133[B]:MET:SD	1:D:141[B]:CYS:SG	3.10	0.49
1:A:123:THR:OG1	5:A:462:HOH:O	2.20	0.49
1:A:204:GLU:HB3	1:A:217[A]:VAL:HG13	1.94	0.49
1:C:136:GLN:HB2	1:C:139[A]:LYS:HG3	1.95	0.49
3:B:305:EDO:H21	3:D:302:EDO:H12	1.92	0.49
1:D:160:MET:HE2	3:D:305[B]:EDO:H21	1.95	0.49
1:D:179:HIS:O	1:D:182:CYS:HB2	2.13	0.49
1:B:113:PHE:O	3:B:305:EDO:O2	2.20	0.49
1:C:97:VAL:HG11	1:C:169:MET:HG2	1.95	0.48
1:B:277:CYS:N	5:B:477:HOH:O	2.38	0.48
1:C:101:LYS:O	1:C:267:ARG:HD2	2.14	0.48
1:D:284:ARG:NH2	5:D:497:HOH:O	2.45	0.48
1:B:202:ARG:NH2	5:B:483:HOH:O	2.47	0.47
1:B:256[B]:THR:HG22	1:B:267:ARG:HG3	1.97	0.46
1:D:175[B]:ARG:HD3	1:D:191:PRO:O	2.14	0.46
1:B:208:ASP:CG	1:B:211:THR:HG22	2.35	0.46
1:B:184:ASP:O	1:B:196[A]:ARG:NH1	2.43	0.46
1:C:209[B]:ARG:HG3	5:C:481:HOH:O	2.15	0.46
1:A:124:CYS:SG	1:A:133[A]:MET:SD	3.13	0.45
1:D:136:GLN:HB2	1:D:139:LYS:HG3	1.99	0.45
1:D:97:VAL:HG11	1:D:169:MET:HG2	1.98	0.45
1:B:101:LYS:O	1:B:267:ARG:HD2	2.17	0.45
1:B:204:GLU:HB3	1:B:217:VAL:HG13	1.99	0.44
1:D:175[A]:ARG:HD3	1:D:237:MET:HB2	1.99	0.44
1:A:119:ALA:O	1:A:122[A]:VAL:HG22	2.18	0.44
1:B:208:ASP:HB2	3:B:306:EDO:H12	1.98	0.44
1:B:97:VAL:HA	1:B:98:PRO:HD3	1.88	0.44
1:C:175:ARG:HD3	1:C:237:MET:HB2	2.00	0.43
1:D:97:VAL:HA	1:D:98:PRO:HD3	1.81	0.43
1:B:208:ASP:HB2	3:B:306:EDO:H11	2.00	0.43
1:D:249[B]:ARG:HA	1:D:250:PRO:HD3	1.89	0.43
1:D:248:ARG:HA	3:D:304:EDO:H11	2.00	0.43
1:A:133[B]:MET:SD	1:A:141[B]:CYS:SG	3.16	0.43
1:A:190:PRO:HA	1:A:191:PRO:HD3	1.89	0.43
1:B:151:PRO:HD2	1:B:220:TYR:CE2	2.54	0.42
1:A:132:LYS:HE2	1:A:273:CYS:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ALA:HA	1:B:190:PRO:HD3	1.84	0.42
1:B:211:THR:HG21	5:B:562:HOH:O	2.20	0.42
1:C:209[A]:ARG:HG3	5:C:496:HOH:O	2.21	0.41
1:D:208:ASP:OD2	3:D:305[A]:EDO:H21	2.19	0.41
1:C:99:SER:HB2	1:C:267:ARG:CZ	2.50	0.41
1:D:125:THR:HA	3:D:303:EDO:H11	2.02	0.41
1:C:146:TRP:CE2	1:C:229:CYS:HB3	2.56	0.41
1:D:132:LYS:HE2	1:D:273:CYS:HB2	2.02	0.41
1:D:246:MET:O	1:D:249[B]:ARG:HD3	2.21	0.41
1:B:180:GLU:O	1:B:182:CYS:N	2.46	0.41
1:D:182:CYS:C	1:D:184:ASP:H	2.25	0.41
1:D:168:HIS:HB3	1:D:249[B]:ARG:HH21	1.86	0.40
1:A:197:VAL:HG11	1:A:218[A]:VAL:HG11	2.03	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)
5:A:530:HOH:O	5:B:546:HOH:O[2_444]	2.08	0.12

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	203/200 (102%)	199 (98%)	4 (2%)	0	100	100
1	B	197/200 (98%)	193 (98%)	4 (2%)	0	100	100
1	C	197/200 (98%)	193 (98%)	4 (2%)	0	100	100
1	D	199/200 (100%)	195 (98%)	4 (2%)	0	100	100
All	All	796/800 (100%)	780 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	180/179 (101%)	172 (96%)	8 (4%)	28	18
1	B	169/179 (94%)	163 (96%)	6 (4%)	35	24
1	C	171/179 (96%)	165 (96%)	6 (4%)	36	25
1	D	177/179 (99%)	168 (95%)	9 (5%)	24	13
All	All	697/716 (97%)	668 (96%)	29 (4%)	32	19

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ARG
1	A	114	LEU
1	A	182	CYS
1	A	224	GLU
1	A	238	CYS
1	A	277[A]	CYS
1	A	277[B]	CYS
1	A	288	ASN
1	B	110	ARG
1	B	169	MET
1	B	184	ASP
1	B	198	GLU
1	B	225	VAL
1	B	252	LEU
1	C	102	THR
1	C	110	ARG
1	C	192	GLN
1	C	243[A]	MET
1	C	243[B]	MET
1	C	268	ASN
1	D	167	GLN
1	D	169	MET
1	D	170	THR
1	D	174	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	181	ARG
1	D	192[A]	GLN
1	D	192[B]	GLN
1	D	243	MET
1	D	264	LEU

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

Mol	Chain	Res	Type
1	B	239	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	$\# Z > 2$
3	EDO	C	303	-	3,3,3	0.55	0	2,2,2	0.09	0
3	EDO	D	305[B]	-	3,3,3	0.41	0	2,2,2	0.28	0
3	EDO	A	304	-	3,3,3	0.47	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	D	305[A]	-	3,3,3	0.41	0	2,2,2	0.40	0
3	EDO	D	302	-	3,3,3	0.45	0	2,2,2	0.15	0
3	EDO	A	303	-	3,3,3	0.45	0	2,2,2	0.20	0
3	EDO	B	305	-	3,3,3	0.46	0	2,2,2	0.26	0
3	EDO	B	304	-	3,3,3	0.41	0	2,2,2	0.59	0
3	EDO	D	304	-	3,3,3	0.48	0	2,2,2	0.32	0
3	EDO	D	306	-	3,3,3	0.51	0	2,2,2	0.32	0
3	EDO	C	302	-	3,3,3	0.47	0	2,2,2	0.18	0
3	EDO	B	302	-	3,3,3	0.50	0	2,2,2	0.13	0
3	EDO	B	306	-	3,3,3	0.42	0	2,2,2	0.27	0
4	ACT	D	308	-	1,3,3	1.51	0	0,3,3	0.00	-
3	EDO	C	304	-	3,3,3	0.46	0	2,2,2	0.37	0
3	EDO	B	303	-	3,3,3	0.49	0	2,2,2	0.29	0
3	EDO	D	307	-	3,3,3	0.45	0	2,2,2	0.37	0
3	EDO	D	303	-	3,3,3	0.52	0	2,2,2	0.08	0
3	EDO	A	302	-	3,3,3	0.54	0	2,2,2	0.20	0
3	EDO	C	305[A]	-	3,3,3	0.50	0	2,2,2	0.29	0
4	ACT	B	307	-	1,3,3	1.64	0	0,3,3	0.00	-
3	EDO	A	305	-	3,3,3	0.48	0	2,2,2	0.33	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
3	EDO	C	303	-	-	1/1/1/1	-
3	EDO	D	305[B]	-	-	0/1/1/1	-
3	EDO	B	305	-	-	0/1/1/1	-
3	EDO	B	304	-	-	1/1/1/1	-
3	EDO	D	304	-	-	0/1/1/1	-
3	EDO	A	304	-	-	0/1/1/1	-
3	EDO	D	305[A]	-	-	0/1/1/1	-
3	EDO	C	304	-	-	0/1/1/1	-
3	EDO	B	303	-	-	1/1/1/1	-
3	EDO	D	307	-	-	0/1/1/1	-
3	EDO	D	306	-	-	0/1/1/1	-
3	EDO	D	303	-	-	1/1/1/1	-
3	EDO	A	305	-	-	1/1/1/1	-
3	EDO	C	302	-	-	0/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	305[A]	-	-	0/1/1/1	-
3	EDO	A	303	-	-	0/1/1/1	-
3	EDO	B	306	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	306	EDO	O1-C1-C2-O2
3	B	303	EDO	O1-C1-C2-O2
3	D	303	EDO	O1-C1-C2-O2
3	C	303	EDO	O1-C1-C2-O2
3	B	304	EDO	O1-C1-C2-O2
3	A	302	EDO	O1-C1-C2-O2
3	A	305	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	303	EDO	1	0
3	D	305[B]	EDO	2	0
3	D	305[A]	EDO	1	0
3	D	302	EDO	3	0
3	B	305	EDO	2	0
3	B	304	EDO	3	0
3	D	304	EDO	1	0
3	C	302	EDO	2	0
3	B	306	EDO	3	0
3	C	304	EDO	1	0
3	D	303	EDO	2	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	193/200 (96%)	0.03	6 (3%)	49	52	13, 26, 54, 83	0
1	B	192/200 (96%)	0.19	7 (3%)	42	46	14, 30, 59, 107	0
1	C	192/200 (96%)	0.25	8 (4%)	36	39	18, 32, 59, 87	0
1	D	192/200 (96%)	0.34	10 (5%)	27	30	15, 33, 62, 85	0
All	All	769/800 (96%)	0.20	31 (4%)	38	41	13, 30, 60, 107	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182	CYS	5.4
1	B	184	ASP	4.8
1	B	182	CYS	4.7
1	D	183	SER	4.4
1	C	289	LEU	4.3
1	A	288	ASN	3.5
1	D	182	CYS	3.3
1	A	183	SER	3.1
1	C	243[A]	MET	3.0
1	A	185	SER	2.9
1	B	226	GLY	2.8
1	A	182	CYS	2.8
1	C	103	TYR	2.7
1	C	187	GLY	2.5
1	D	96	SER	2.4
1	B	195	ILE	2.4
1	B	248	ARG	2.3
1	D	159	ALA	2.3
1	B	183	SER	2.3
1	D	227	SER	2.3
1	A	187	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	288	ASN	2.2
1	D	243	MET	2.2
1	D	184	ASP	2.2
1	C	186	ASP	2.1
1	C	225	VAL	2.1
1	D	225	VAL	2.1
1	D	106[A]	SER	2.1
1	A	186	ASP	2.1
1	D	133[A]	MET	2.0
1	B	159	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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
3	EDO	A	302	4/4	0.44	0.31	53,58,59,59	0
3	EDO	C	304	4/4	0.63	0.31	64,66,69,71	0
3	EDO	C	305[A]	4/4	0.64	0.31	49,53,55,58	0
3	EDO	D	304	4/4	0.68	0.33	58,60,61,62	0
3	EDO	B	302	4/4	0.73	0.31	60,61,65,68	0
3	EDO	D	303	4/4	0.73	0.27	44,47,48,51	0
3	EDO	D	305[B]	4/4	0.76	0.33	17,22,25,25	4
3	EDO	D	305[A]	4/4	0.76	0.33	17,19,23,25	4
3	EDO	A	305	4/4	0.77	0.23	65,66,67,67	0
3	EDO	C	303	4/4	0.80	0.21	38,40,40,41	0
3	EDO	B	303	4/4	0.80	0.33	51,55,56,57	0
4	ACT	D	308	4/4	0.80	0.19	65,68,69,69	0
3	EDO	B	305	4/4	0.81	0.20	40,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ACT	B	307	4/4	0.83	0.21	35,41,42,42	0
3	EDO	D	307	4/4	0.84	0.29	39,40,41,42	0
3	EDO	A	304	4/4	0.85	0.32	63,64,65,65	0
3	EDO	B	306	4/4	0.88	0.27	49,51,52,52	0
3	EDO	D	306	4/4	0.89	0.28	32,40,44,47	0
3	EDO	D	302	4/4	0.90	0.20	33,37,38,39	0
3	EDO	B	304	4/4	0.91	0.32	45,49,54,58	0
3	EDO	A	303	4/4	0.92	0.17	22,27,30,31	0
2	ZN	B	301	1/1	0.96	0.06	33,33,33,33	0
2	ZN	C	301	1/1	0.97	0.04	47,47,47,47	0
2	ZN	D	301	1/1	0.97	0.05	31,31,31,31	0
3	EDO	C	302	4/4	0.97	0.15	25,29,32,33	0
2	ZN	A	301	1/1	0.98	0.05	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.