



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:57 AM UTC

PDB ID : 2J6I / pdb_00002j6i
Title : Candida boidinii formate dehydrogenase (FDH) C-terminal mutant
Authors : Schirwitz, K.; Schmidt, A.; Lamzin, V.S.
Deposited on : 2006-09-29
Resolution : 1.55 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

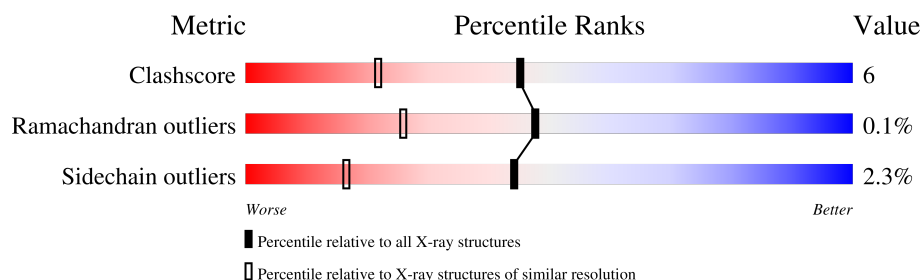
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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))
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	364	88% 8% . .
1	B	364	84% 12% . .
1	C	364	87% 9% . .
1	D	364	84% 12% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13261 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 FORMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	2	0
			2759	1758	473	522	6			
1	B	353	Total	C	N	O	S	0	2	0
			2765	1763	473	523	6			
1	C	352	Total	C	N	O	S	0	2	0
			2755	1757	472	520	6			
1	D	352	Total	C	N	O	S	0	3	0
			2768	1765	473	524	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	VAL	LYS	engineered mutation	UNP O93968
B	328	VAL	LYS	engineered mutation	UNP O93968
C	328	VAL	LYS	engineered mutation	UNP O93968
D	328	VAL	LYS	engineered mutation	UNP O93968

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	578	Total	O	0	0
			578	578		
3	B	534	Total	O	0	0
			534	534		
3	C	560	Total	O	0	0
			560	560		
3	D	503	Total	O	0	0
			503	503		

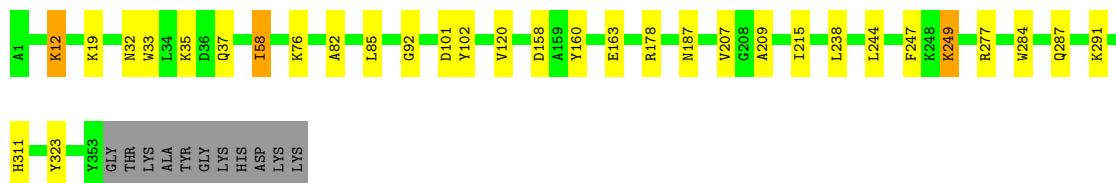
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

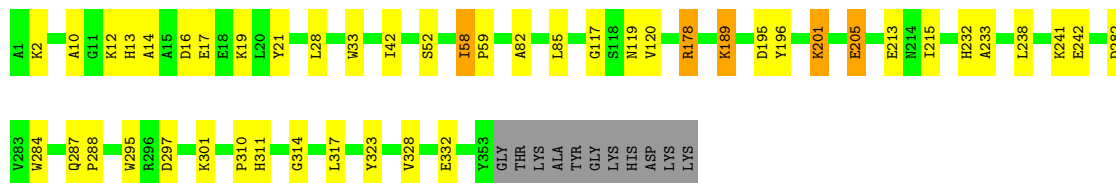
• Molecule 1: FORMATE DEHYDROGENASE

Chain A:  88% 8% ..



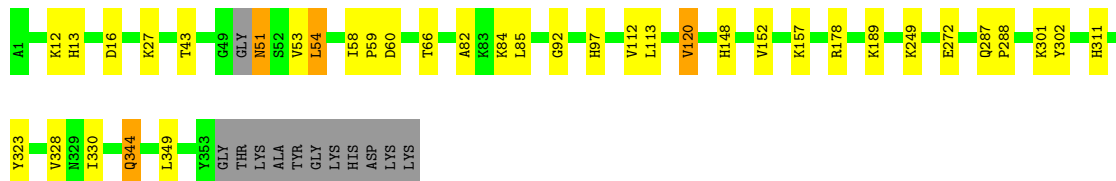
• Molecule 1: FORMATE DEHYDROGENASE

Chain B:  84% 12% ..



• Molecule 1: FORMATE DEHYDROGENASE

Chain C:  87% 9% ..



• Molecule 1: FORMATE DEHYDROGENASE

Chain D:  84% 12% ..



D202	A203	E213	N214	I215	E216	I224	H232	A233	G234	L238	K246	W284	Q287	P288	W295	K301	H311	L317	Y323	Y353	GLY	THR	LYS	LYS	ALA	TYR	GLY	LYS	HIS	ASP	LYS	LYS
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.36Å 68.14Å 109.15Å 78.07° 89.41° 81.27°	Depositor
Resolution (Å)	19.26 – 1.55	Depositor
% Data completeness (in resolution range)	96.1 (19.26-1.55)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13261	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

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: PG4

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	0.63	0/2822	0.82	0/3832
1	B	0.65	1/2826 (0.0%)	0.79	1/3838 (0.0%)
1	C	0.68	3/2817 (0.1%)	0.82	1/3823 (0.0%)
1	D	0.64	1/2837 (0.0%)	0.80	0/3852
All	All	0.65	5/11302 (0.0%)	0.81	2/15345 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	GLU	C-O	-7.12	1.14	1.24
1	C	54	LEU	C-O	-6.94	1.16	1.24
1	D	5	LEU	C-O	-6.44	1.16	1.24
1	C	53	VAL	C-O	-5.35	1.18	1.24
1	C	272	GLU	C-O	-5.04	1.18	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	120	VAL	N-CA-C	5.61	115.81	110.42
1	B	52	SER	N-CA-C	5.01	116.75	110.24

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	2759	0	2762	23	0
1	B	2765	0	2762	48	0
1	C	2755	0	2763	33	0
1	D	2768	0	2769	33	0
2	A	13	0	18	0	0
2	C	13	0	18	1	0
2	D	13	0	18	0	0
3	A	578	0	0	6	0
3	B	534	0	0	11	0
3	C	560	0	0	8	0
3	D	503	0	0	8	0
All	All	13261	0	11110	131	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (131) 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:C:84:LYS:HG2	3:C:2048:HOH:O	1.67	0.92
1:C:344:GLN:H	1:C:344:GLN:HE21	1.15	0.90
1:B:10:ALA:HB3	1:B:14:ALA:HB2	1.53	0.90
1:D:216[C]:GLU:HG3	1:D:246:LYS:HD3	1.55	0.87
3:A:2072:HOH:O	1:C:12[B]:LYS:HE2	1.76	0.86
1:B:19:LYS:HD3	1:B:317:LEU:HB3	1.59	0.84
1:C:120:VAL:HG12	1:C:178:ARG:HD2	1.59	0.82
1:D:119:ASN:HD22	1:D:119:ASN:H	1.28	0.79
1:D:232:HIS:HD2	1:D:234:GLY:H	1.34	0.75
1:D:200:PRO:HG2	1:D:203:ALA:HB3	1.68	0.75
1:B:201:LYS:O	1:B:205:GLU:HG3	1.86	0.74
1:C:311:HIS:HD2	3:C:2487:HOH:O	1.69	0.74
1:A:249:LYS:H	1:A:249:LYS:CD	1.99	0.72
1:B:178:ARG:CG	1:B:178:ARG:HH11	2.03	0.71
1:A:249:LYS:H	1:A:249:LYS:HD2	1.55	0.71
1:C:120:VAL:CG1	1:C:178:ARG:HD2	2.19	0.71
1:A:12:LYS:HG3	3:A:2027:HOH:O	1.92	0.68
1:B:120:VAL:CG2	1:B:178:ARG:HE	2.06	0.67
1:B:201:LYS:CE	3:B:2335:HOH:O	2.42	0.67
1:B:297:ASP:OD1	1:C:148:HIS:HE1	1.79	0.67
1:D:232:HIS:CD2	1:D:234:GLY:H	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LYS:O	1:B:189:LYS:HD3	1.96	0.65
1:A:311:HIS:HD2	3:A:2284:HOH:O	1.80	0.65
1:B:19:LYS:CD	1:B:317:LEU:HB3	2.29	0.63
1:B:189:LYS:HD3	1:B:189:LYS:C	2.23	0.63
1:B:16:ASP:HB3	1:C:302:TYR:OH	2.00	0.61
1:B:19:LYS:HG2	3:B:2482:HOH:O	2.01	0.61
1:D:143:GLU:HG3	3:D:2249:HOH:O	2.00	0.61
1:B:120:VAL:HG23	1:B:178:ARG:HE	1.65	0.61
1:B:287:GLN:HA	1:B:288:PRO:C	2.27	0.60
1:B:301:LYS:HG2	3:B:2465:HOH:O	2.02	0.60
1:D:143:GLU:HG3	3:D:2091:HOH:O	2.02	0.60
1:C:178:ARG:NH1	3:C:2342:HOH:O	2.35	0.59
1:B:178:ARG:HH11	1:B:178:ARG:HG3	1.68	0.58
1:B:13:HIS:HB3	1:C:157:LYS:HD3	1.86	0.58
1:C:27:LYS:HG2	1:C:43:THR:HG21	1.85	0.58
1:C:60:ASP:HA	1:C:84:LYS:HD3	1.86	0.58
1:D:70[B]:HIS:CD2	3:D:2081:HOH:O	2.59	0.56
1:B:328:VAL:O	1:B:332:GLU:HG3	2.07	0.55
1:C:12[A]:LYS:HE3	1:C:13:HIS:CE1	2.42	0.54
1:D:12:LYS:HD3	1:D:13:HIS:CE1	2.43	0.54
1:B:301:LYS:CG	3:B:2465:HOH:O	2.56	0.54
1:B:201:LYS:HE3	3:B:2335:HOH:O	2.04	0.54
1:B:21:TYR:HB3	1:B:28:LEU:HA	1.90	0.53
1:B:17:GLU:HG3	1:C:157:LYS:O	2.08	0.53
1:A:12:LYS:HD3	3:C:2003:HOH:O	2.09	0.53
1:C:301:LYS:HE2	1:C:302:TYR:CZ	2.45	0.52
1:B:178:ARG:HG3	1:B:178:ARG:NH1	2.22	0.52
1:A:92:GLY:HA2	1:A:323:TYR:CD2	2.44	0.52
1:A:207:VAL:HG23	1:A:209:ALA:HB2	1.92	0.52
1:A:76:LYS:HG3	1:A:102:TYR:CZ	2.46	0.51
1:B:117:GLY:O	1:B:120:VAL:HG22	2.11	0.51
1:B:120:VAL:HG21	1:B:178:ARG:HH21	1.75	0.51
1:D:200:PRO:HG2	1:D:203:ALA:CB	2.37	0.51
1:C:51:ASN:N	1:C:51:ASN:ND2	2.58	0.51
1:B:297:ASP:OD1	1:C:148:HIS:CE1	2.63	0.50
1:D:24:THR:HG21	1:D:45:SER:OG	2.12	0.50
1:A:92:GLY:HA2	1:A:323:TYR:CE2	2.47	0.49
1:C:97:HIS:H	1:C:97:HIS:CD2	2.29	0.49
1:B:178:ARG:CG	1:B:178:ARG:NH1	2.68	0.49
1:C:66:THR:OG1	1:C:97:HIS:HE1	1.95	0.49
1:A:120:VAL:HG12	1:A:178:ARG:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ILE:CD1	1:B:238:LEU:HD21	2.42	0.49
1:A:33:TRP:CE2	1:A:37:GLN:NE2	2.81	0.48
1:D:19:LYS:HE3	3:D:2459:HOH:O	2.13	0.48
1:C:287:GLN:HA	1:C:288:PRO:C	2.38	0.48
1:B:178:ARG:NH1	3:B:2312:HOH:O	2.46	0.48
1:B:201:LYS:HE2	3:B:2335:HOH:O	2.08	0.48
1:D:47:LYS:HD3	1:D:72:ALA:HA	1.94	0.48
1:D:8:TYR:HB3	1:D:70[B]:HIS:CD2	2.48	0.48
1:A:158:ASP:OD2	1:A:277:ARG:HD2	2.14	0.48
1:A:244:LEU:HA	1:A:247:PHE:CD1	2.48	0.47
1:A:215:ILE:HD13	1:A:238:LEU:HD21	1.95	0.47
1:C:178:ARG:NE	3:C:2340:HOH:O	2.46	0.47
1:A:291:LYS:HG2	3:A:2491:HOH:O	2.14	0.47
1:B:311:HIS:HD2	3:B:2136:HOH:O	1.97	0.46
1:C:54:LEU:O	1:C:58:ILE:HG12	2.15	0.46
1:C:92:GLY:HA2	1:C:323:TYR:CD2	2.51	0.46
1:D:8:TYR:HB3	1:D:70[A]:HIS:CG	2.51	0.46
1:A:19:LYS:HE2	3:A:2045:HOH:O	2.15	0.46
1:C:178:ARG:NH1	3:C:2339:HOH:O	2.48	0.46
3:A:2510:HOH:O	1:D:152:VAL:HG21	2.16	0.46
1:D:215:ILE:HD13	1:D:238:LEU:HD21	1.98	0.46
1:A:12:LYS:HG3	1:A:12:LYS:H	1.47	0.45
1:B:33:TRP:HZ2	1:B:332:GLU:HG2	1.81	0.45
1:D:8:TYR:HB3	1:D:70[B]:HIS:CG	2.52	0.45
1:A:284:TRP:H	1:A:287:GLN:NE2	2.14	0.45
1:D:178:ARG:HD3	3:D:2293:HOH:O	2.17	0.45
1:D:53:VAL:O	1:D:57:HIS:HD2	1.99	0.45
1:A:32:ASN:OD1	1:A:35:LYS:NZ	2.44	0.45
1:B:195:ASP:OD1	1:B:196[B]:TYR:HD2	2.01	0.44
1:D:82:ALA:HB1	1:D:85:LEU:HB2	1.99	0.44
1:D:311:HIS:HD2	3:D:2121:HOH:O	1.99	0.44
1:B:201:LYS:HD3	1:B:201:LYS:HA	1.41	0.44
1:C:82:ALA:HB1	1:C:85:LEU:HB2	1.99	0.44
1:B:2:LYS:HE3	1:B:42:ILE:CD1	2.48	0.44
1:B:241:LYS:NZ	1:B:242:GLU:OE2	2.51	0.43
1:C:112:VAL:C	1:C:113:LEU:HD22	2.43	0.43
1:D:301:LYS:HD2	3:D:2408:HOH:O	2.18	0.43
1:B:42:ILE:HD12	1:B:42:ILE:N	2.33	0.43
1:B:119:ASN:ND2	3:B:2243:HOH:O	2.50	0.43
1:D:287:GLN:HA	1:D:288:PRO:C	2.43	0.43
1:B:282:ASP:HB2	1:B:310:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:CZ	1:D:317:LEU:HD12	2.54	0.42
1:B:58:ILE:N	1:B:59:PRO:CD	2.82	0.42
1:C:92:GLY:HA2	1:C:323:TYR:CE2	2.54	0.42
1:A:82:ALA:HB1	1:A:85:LEU:HB2	2.02	0.42
1:D:92:GLY:HA2	1:D:323:TYR:CD2	2.55	0.42
1:B:19:LYS:HG2	1:B:19:LYS:O	2.20	0.42
1:D:174:ARG:O	1:D:178:ARG:CG	2.68	0.42
1:D:284:TRP:CZ3	1:D:295:TRP:HB2	2.55	0.42
1:C:189:LYS:HE2	3:C:2330:HOH:O	2.19	0.41
1:D:167:ILE:HG12	1:D:224:ILE:HD12	2.02	0.41
1:B:314:GLY:O	1:B:323:TYR:OH	2.36	0.41
3:B:2478:HOH:O	1:C:152:VAL:HG21	2.20	0.41
1:B:120:VAL:HG21	1:B:178:ARG:HE	1.81	0.41
1:C:58:ILE:HB	1:C:59:PRO:HD3	2.01	0.41
1:C:328:VAL:HG21	2:C:1354:PG4:H52	2.03	0.41
1:A:163:GLU:HG3	1:A:187:ASN:HB3	2.02	0.41
1:B:284:TRP:CZ3	1:B:295:TRP:HB2	2.56	0.41
1:B:19:LYS:HE2	3:B:2487:HOH:O	2.21	0.41
1:B:82:ALA:HB1	1:B:85:LEU:HB2	2.02	0.41
1:C:113:LEU:HB3	1:C:330:ILE:HD13	2.03	0.41
1:D:139:VAL:N	1:D:140:PRO:HD2	2.36	0.41
1:D:199:LEU:HA	1:D:200:PRO:HD2	1.67	0.41
1:C:178:ARG:CZ	3:C:2339:HOH:O	2.69	0.41
1:D:120:VAL:CG1	1:D:178:ARG:HG3	2.51	0.41
1:B:232:HIS:O	1:B:233:ALA:C	2.65	0.40
1:B:2:LYS:HE3	1:B:42:ILE:HD11	2.02	0.40
1:A:58:ILE:HG23	1:A:82:ALA:HB2	2.04	0.40
1:D:216[C]:GLU:HG2	3:D:2339:HOH:O	2.21	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	353/364 (97%)	342 (97%)	11 (3%)	0	100	100
1	B	353/364 (97%)	340 (96%)	13 (4%)	0	100	100
1	C	350/364 (96%)	341 (97%)	9 (3%)	0	100	100
1	D	352/364 (97%)	339 (96%)	12 (3%)	1 (0%)	36	18
All	All	1408/1456 (97%)	1362 (97%)	45 (3%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	200	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/296 (98%)	286 (99%)	4 (1%)	59	33
1	B	290/296 (98%)	284 (98%)	6 (2%)	47	19
1	C	290/296 (98%)	285 (98%)	5 (2%)	53	25
1	D	292/296 (99%)	280 (96%)	12 (4%)	27	4
All	All	1162/1184 (98%)	1135 (98%)	27 (2%)	44	16

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	58	ILE
1	A	101	ASP
1	A	249	LYS
1	B	12	LYS
1	B	58	ILE
1	B	178	ARG
1	B	189	LYS
1	B	201	LYS
1	B	213	GLU

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Mol	Chain	Res	Type
1	C	16	ASP
1	C	51	ASN
1	C	249	LYS
1	C	344	GLN
1	C	349	LEU
1	D	12	LYS
1	D	18[A]	GLU
1	D	18[B]	GLU
1	D	35	LYS
1	D	47	LYS
1	D	58	ILE
1	D	96	ASP
1	D	119	ASN
1	D	178	ARG
1	D	202	ASP
1	D	213	GLU
1	D	301	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	287	GLN
1	A	311	HIS
1	A	350	ASN
1	B	32	ASN
1	B	37	GLN
1	B	147	ASN
1	B	197	GLN
1	B	228	ASN
1	B	275	GLN
1	B	311	HIS
1	C	51	ASN
1	C	97	HIS
1	C	126	HIS
1	C	148	HIS
1	C	228	ASN
1	C	311	HIS
1	C	325	GLN
1	C	329	ASN
1	C	344	GLN
1	C	350	ASN

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Mol	Chain	Res	Type
1	D	51	ASN
1	D	104	ASN
1	D	119	ASN
1	D	126	HIS
1	D	214	ASN
1	D	232	HIS
1	D	311	HIS
1	D	325	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
2	PG4	A	1354	-	12,12,12	0.45	0	11,11,11	0.33	0
2	PG4	D	1354	-	12,12,12	0.48	0	11,11,11	0.28	0
2	PG4	C	1354	-	12,12,12	0.48	0	11,11,11	0.22	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	PG4	A	1354	-	-	4/10/10/10	-
2	PG4	D	1354	-	-	6/10/10/10	-
2	PG4	C	1354	-	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1354	PG4	O2-C3-C4-O3
2	C	1354	PG4	O1-C1-C2-O2
2	C	1354	PG4	O4-C7-C8-O5
2	C	1354	PG4	O3-C5-C6-O4
2	D	1354	PG4	C3-C4-O3-C5
2	A	1354	PG4	C3-C4-O3-C5
2	D	1354	PG4	C8-C7-O4-C6
2	D	1354	PG4	O4-C7-C8-O5
2	A	1354	PG4	C8-C7-O4-C6
2	D	1354	PG4	C1-C2-O2-C3
2	D	1354	PG4	C6-C5-O3-C4
2	C	1354	PG4	C4-C3-O2-C2
2	A	1354	PG4	C6-C5-O3-C4
2	D	1354	PG4	O2-C3-C4-O3
2	A	1354	PG4	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1354	PG4	1	0

5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.