



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2017 – 04:30 PM EST

PDB ID : 5SVF  
Title : IDH1 R132H in complex with IDH125  
Authors : Xie, X.; Kulathila, R.  
Deposited on : 2016-08-05  
Resolution : 2.34 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20028442

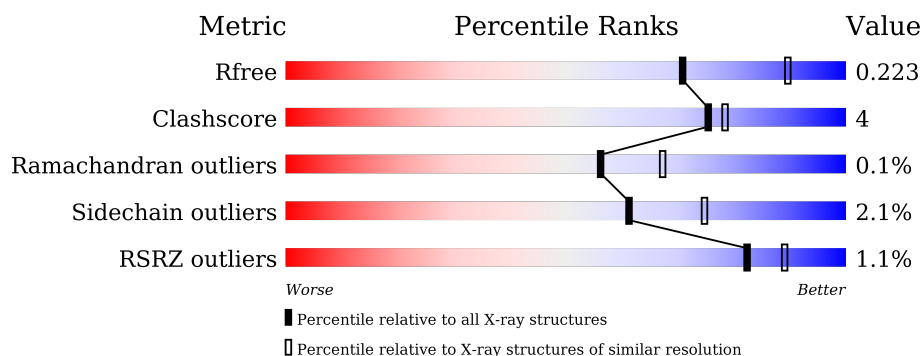
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
$R_{free}$	91344	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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  $\geq 3$ , 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	417	
1	B	417	
1	C	417	
1	D	417	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FLC	B	503	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13375 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.

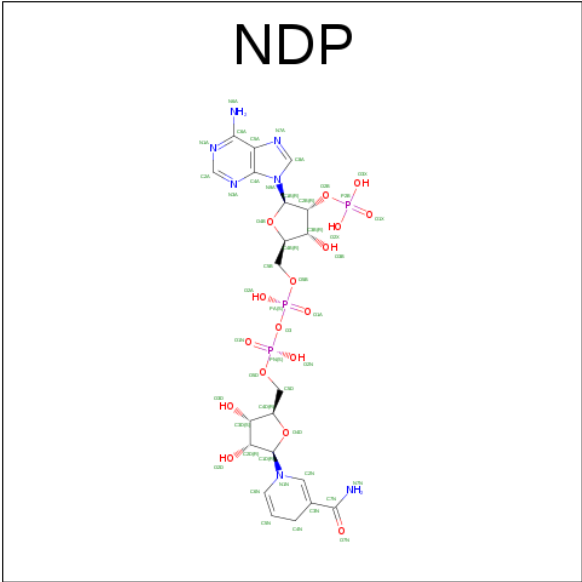
- Molecule 1 is a protein called Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	2	0
			3156	2008	533	597	18			
1	C	399	Total	C	N	O	S	0	0	0
			3155	2009	536	592	18			
1	B	397	Total	C	N	O	S	0	2	0
			3158	2010	540	590	18			
1	D	402	Total	C	N	O	S	0	1	0
			3194	2032	543	601	18			

There are 16 discrepancies between the modelled and reference sequences:

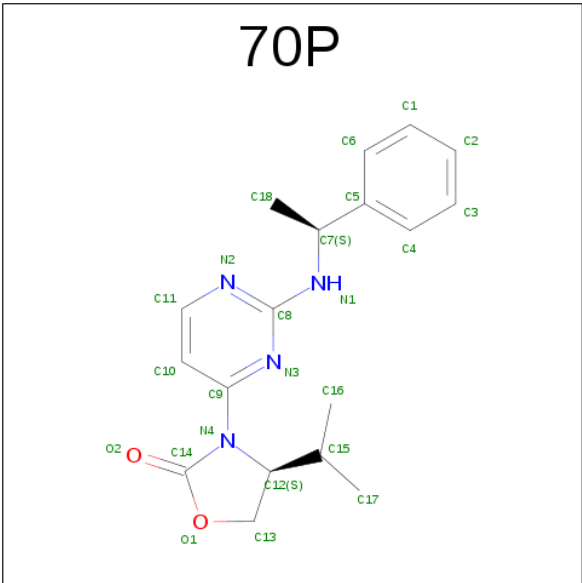
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O75874
A	-1	PRO	-	expression tag	UNP O75874
A	0	GLY	-	expression tag	UNP O75874
A	132	HIS	ARG	engineered mutation	UNP O75874
C	-2	GLY	-	expression tag	UNP O75874
C	-1	PRO	-	expression tag	UNP O75874
C	0	GLY	-	expression tag	UNP O75874
C	132	HIS	ARG	engineered mutation	UNP O75874
B	-2	GLY	-	expression tag	UNP O75874
B	-1	PRO	-	expression tag	UNP O75874
B	0	GLY	-	expression tag	UNP O75874
B	132	HIS	ARG	engineered mutation	UNP O75874
D	-2	GLY	-	expression tag	UNP O75874
D	-1	PRO	-	expression tag	UNP O75874
D	0	GLY	-	expression tag	UNP O75874
D	132	HIS	ARG	engineered mutation	UNP O75874

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



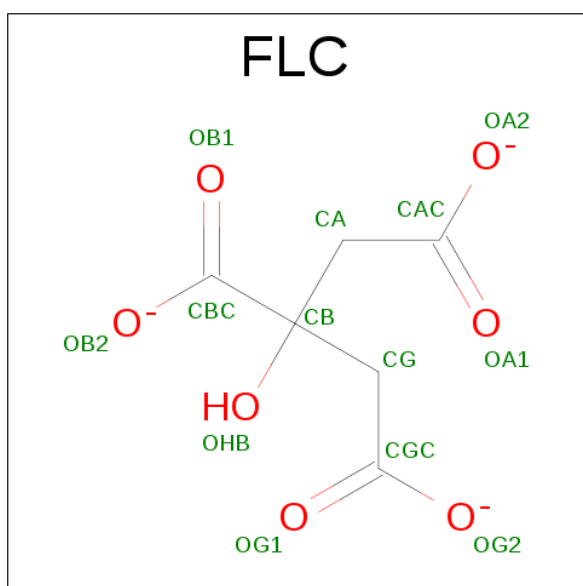
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is (4S)-3-(2-{[(1S)-1-phenylethyl]amino}pyrimidin-4-yl)-4-(propan-2-yl)-1,3-oxazolidin-2-one (three-letter code: 70P) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	18	4	2		
3	C	1	Total	C	N	O	0	0
			24	18	4	2		
3	B	1	Total	C	N	O	0	0
			24	18	4	2		
3	D	1	Total	C	N	O	0	0
			24	18	4	2		

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		
5	C	64	Total	O	0	0
			64	64		

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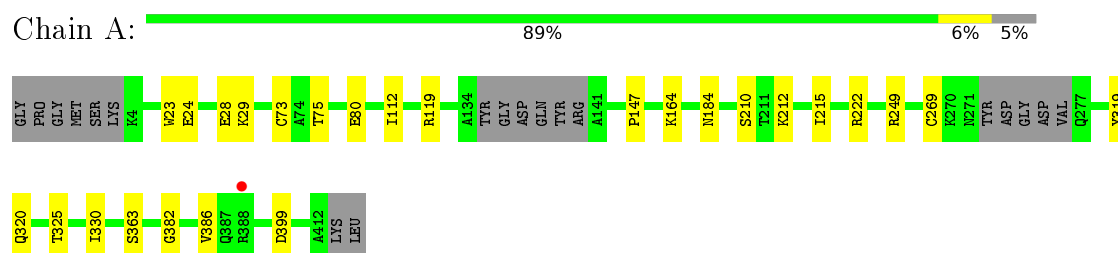
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	134	Total 134	O 134	0	0
5	D	49	Total 49	O 49	0	0

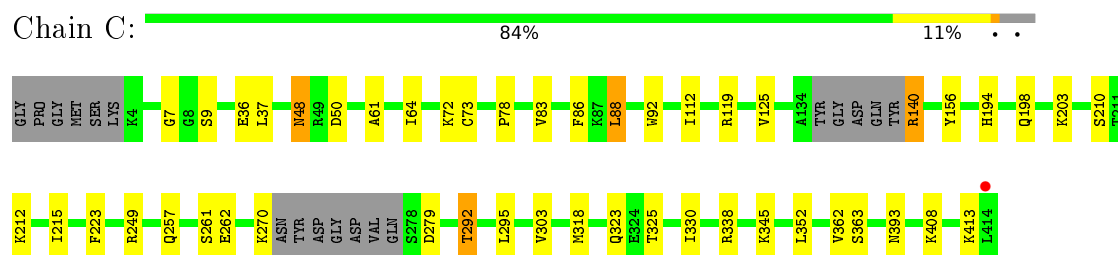
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

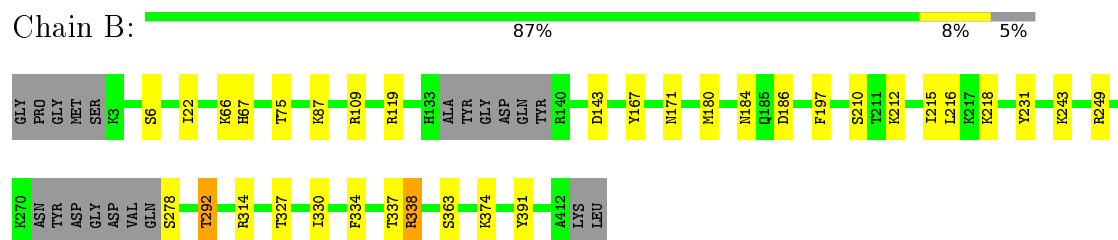
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



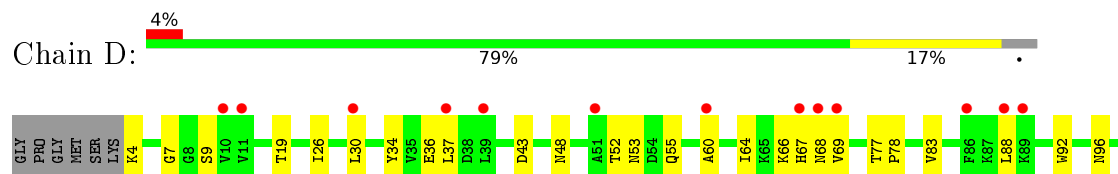
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



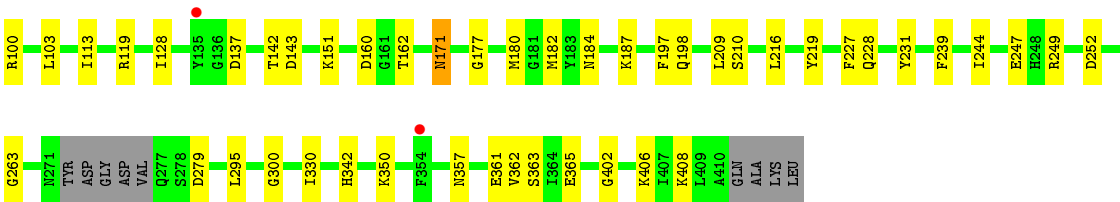
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.98Å 154.99Å 162.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.75 – 2.34 112.32 – 2.34	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.75-2.34) 96.1 (112.32-2.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.41 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.179 , 0.223 0.179 , 0.223	Depositor DCC
$R_{free}$ test set	4256 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NDP, FLC, 70P

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	0.49	1/3226 (0.0%)	0.59	0/4348
1	B	0.49	0/3228	0.56	0/4347
1	C	0.43	0/3219	0.55	1/4337 (0.0%)
1	D	0.46	0/3264	0.57	0/4400
All	All	0.47	1/12937 (0.0%)	0.57	1/17432 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	CYS	CB-SG	-7.09	1.70	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	LEU	CA-CB-CG	5.47	127.89	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	3156	0	3131	12	1
1	B	3158	0	3152	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3155	0	3142	30	1
1	D	3194	0	3166	43	2
2	A	48	0	26	1	0
2	B	48	0	26	2	0
2	C	48	0	26	1	0
2	D	48	0	26	1	0
3	A	24	0	0	0	0
3	B	24	0	0	0	0
3	C	24	0	0	0	0
3	D	24	0	0	0	0
4	A	13	0	5	0	0
4	B	13	0	5	2	0
4	C	13	0	5	1	0
4	D	13	0	5	2	0
5	A	125	0	0	0	0
5	B	134	0	0	0	0
5	C	64	0	0	2	0
5	D	49	0	0	1	0
All	All	13375	0	12715	101	2

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 4.

All (101) 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:B:501:NDP:H42N	4:B:503:FLC:HA2	1.60	0.84
1:B:180:MET:HE1	1:D:216:LEU:HD22	1.67	0.77
1:D:7:GLY:HA3	1:D:37:LEU:HD23	1.69	0.74
1:C:7:GLY:HA3	1:C:37:LEU:HD23	1.71	0.73
2:D:501:NDP:H42N	4:D:503:FLC:HA2	1.75	0.68
1:D:100:ARG:NH1	4:D:503:FLC:OA1	2.31	0.64
1:C:86:PHE:HB2	1:C:88:LEU:HD22	1.79	0.64
1:B:212:LYS:HG2	1:B:215:ILE:HD12	1.83	0.61
1:D:151:LYS:HE2	1:D:171:ASN:OD1	2.02	0.60
1:C:72:LYS:HG2	1:C:73:CYS:O	2.03	0.59
2:C:501:NDP:H42N	4:C:503:FLC:HA1	1.86	0.57
1:A:24:GLU:O	1:A:28[A]:GLU:HG2	2.04	0.57
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.87	0.56
1:D:113:ILE:HG23	1:D:119:ARG:HD3	1.86	0.56
1:A:319:TYR:HB2	1:A:325:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HE2	1:A:399:ASP:OD1	2.05	0.55
1:D:137:ASP:HA	1:D:182:MET:HG3	1.86	0.55
1:C:330:ILE:HD12	1:C:363:SER:HB3	1.88	0.55
1:D:52:THR:O	1:D:55:GLN:HB2	2.07	0.55
1:C:125:VAL:HG22	1:C:262:GLU:HG2	1.89	0.53
1:D:160:ASP:N	1:D:160:ASP:OD1	2.26	0.52
1:C:325:THR:O	1:C:393:ASN:HB2	2.10	0.52
1:B:374:LYS:HD2	1:B:391:TYR:CZ	2.44	0.51
1:C:362:VAL:HG23	1:C:408:LYS:HD2	1.92	0.51
1:C:210:SER:HA	1:C:249:ARG:O	2.11	0.50
1:D:34:TYR:OH	1:D:406:LYS:HG2	2.12	0.49
1:D:361:GLU:O	1:D:365:GLU:HG3	2.13	0.49
1:D:210:SER:HA	1:D:249:ARG:O	2.12	0.49
1:D:357:ASN:O	1:D:361:GLU:HG3	2.12	0.49
1:D:96:ASN:O	1:D:100:ARG:HG3	2.13	0.49
1:D:330:ILE:HD12	1:D:363:SER:HB3	1.95	0.49
1:B:216:LEU:HD22	1:D:180:MET:HE1	1.94	0.48
1:C:112:ILE:HD13	1:C:330:ILE:HG22	1.94	0.48
1:B:243:LYS:HD3	1:B:243:LYS:N	2.28	0.47
1:D:128:ILE:HG12	1:D:263:GLY:HA2	1.96	0.47
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.96	0.47
1:B:22:ILE:HD11	1:B:327:THR:HB	1.96	0.47
1:D:53:ASN:HA	1:D:92:TRP:CH2	2.50	0.47
1:C:212:LYS:HG2	1:C:215:ILE:HD12	1.97	0.47
1:D:187:LYS:HD2	1:D:187:LYS:HA	1.82	0.46
1:C:61:ALA:HA	1:C:64:ILE:HD12	1.96	0.46
1:D:60:ALA:O	1:D:64:ILE:HG13	2.15	0.46
1:D:83:VAL:HA	1:D:88:LEU:HD12	1.98	0.46
1:B:197:PHE:CZ	1:B:231:TYR:HB2	2.51	0.46
1:B:75:THR:O	2:B:501:NDP:H2N	2.15	0.46
1:C:203:LYS:NZ	1:C:203:LYS:HB3	2.32	0.45
1:D:209:LEU:HD22	1:D:227:PHE:CG	2.52	0.45
1:D:43:ASP:HB3	1:D:48:ASN:HD22	1.81	0.45
1:C:194:HIS:O	1:C:198:GLN:HG2	2.17	0.45
1:D:198:GLN:HG3	1:D:300:GLY:HA2	1.99	0.45
1:D:197:PHE:CZ	1:D:231:TYR:HB2	2.51	0.45
1:C:295:LEU:O	1:C:303:VAL:HA	2.17	0.44
1:A:112:ILE:HD13	1:A:330:ILE:HG22	1.98	0.44
1:C:140:ARG:HH11	1:C:140:ARG:HG3	1.82	0.44
1:C:257:GLN:NE2	5:C:603:HOH:O	2.34	0.44
1:A:80:GLU:CD	1:A:80:GLU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TRP:CD2	1:A:73:CYS:HB2	2.53	0.43
1:B:292:THR:HG21	1:B:338[A]:ARG:NH1	2.34	0.43
1:B:210:SER:HA	1:B:249:ARG:O	2.18	0.43
1:B:334:PHE:HA	1:B:337:THR:OG1	2.19	0.43
1:C:292:THR:HG21	1:C:338:ARG:HH11	1.84	0.43
1:B:143:ASP:HB2	1:D:219:TYR:HB2	2.00	0.43
1:D:26:ILE:HG23	1:D:30:LEU:HD12	2.01	0.43
1:D:279:ASP:N	1:D:279:ASP:OD1	2.45	0.43
1:D:402:GLY:O	1:D:406:LYS:HG3	2.19	0.43
4:B:503:FLC:OG1	4:B:503:FLC:OHB	2.33	0.43
1:D:113:ILE:CG2	1:D:119:ARG:HD3	2.49	0.43
1:B:216:LEU:HD22	1:D:180:MET:CE	2.49	0.43
1:A:75:THR:O	2:A:501:NDP:H2N	2.19	0.42
1:C:48:ASN:C	1:C:48:ASN:HD22	2.22	0.42
1:C:50:ASP:CG	1:C:88:LEU:HB2	2.39	0.42
1:C:318:MET:HB3	1:C:323:GLN:HB3	2.01	0.42
1:D:362:VAL:HG23	1:D:408:LYS:HD2	2.01	0.42
1:D:239:PHE:CD2	1:D:244:ILE:HG13	2.54	0.42
1:D:67:HIS:O	1:D:68:ASN:HB2	2.20	0.42
1:A:210:SER:HA	1:A:249:ARG:O	2.19	0.42
1:B:180:MET:HG2	1:D:219:TYR:CE2	2.54	0.42
1:B:167:TYR:HB3	1:D:142:THR:HG21	2.02	0.42
1:D:77:THR:HA	1:D:78:PRO:HD3	1.92	0.42
1:B:66:LYS:HE3	1:B:67:HIS:CE1	2.55	0.42
1:C:203:LYS:HZ2	1:C:203:LYS:HB3	1.84	0.41
1:C:257:GLN:HB2	5:C:638:HOH:O	2.19	0.41
1:C:261:SER:OG	1:C:262:GLU:N	2.53	0.41
1:D:69:VAL:HG22	1:D:342:HIS:HD2	1.85	0.41
1:B:186:ASP:OD1	1:D:177:GLY:HA2	2.20	0.41
1:C:83:VAL:HA	1:C:88:LEU:CD2	2.50	0.41
1:A:382:GLY:O	1:A:386:VAL:HG23	2.21	0.41
1:C:7:GLY:HA2	1:C:352:LEU:HD22	2.02	0.41
1:B:314:ARG:NH1	1:B:314:ARG:HG2	2.34	0.41
1:D:228:GLN:HG2	5:D:613:HOH:O	2.19	0.41
1:A:147:PRO:HD2	1:C:156:TYR:CE2	2.56	0.41
1:A:212:LYS:HE3	1:A:215:ILE:HD12	2.03	0.41
1:B:314:ARG:CG	1:B:314:ARG:HH11	2.34	0.41
1:C:83:VAL:HA	1:C:88:LEU:HD23	2.01	0.41
1:D:357:ASN:ND2	1:D:361:GLU:OE1	2.53	0.41
1:D:143:ASP:HB3	1:D:180:MET:HE3	2.03	0.41
1:D:103:LEU:HD12	1:D:295:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ARG:HG2	1:C:140:ARG:O	2.20	0.40
1:C:223:PHE:CE2	1:C:270:LYS:HG3	2.57	0.40
1:D:247:GLU:OE2	1:D:249:ARG:NH2	2.50	0.40
1:C:78:PRO:HD2	1:C:92:TRP:O	2.22	0.40

All (2) 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:C:9:SER:OG	1:D:36:GLU:OE2[1_556]	2.13	0.07
1:A:320:GLN:O	1:D:350:LYS:NZ[2_555]	2.15	0.05

## 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	394/417 (94%)	385 (98%)	9 (2%)	0	100	100
1	B	393/417 (94%)	383 (98%)	10 (2%)	0	100	100
1	C	393/417 (94%)	381 (97%)	12 (3%)	0	100	100
1	D	399/417 (96%)	380 (95%)	18 (4%)	1 (0%)	46	54
All	All	1579/1668 (95%)	1529 (97%)	49 (3%)	1 (0%)	56	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	162	THR

### 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	338/351 (96%)	334 (99%)	4 (1%)	78	88
1	B	338/351 (96%)	327 (97%)	11 (3%)	45	57
1	C	337/351 (96%)	329 (98%)	8 (2%)	57	69
1	D	341/351 (97%)	334 (98%)	7 (2%)	61	75
All	All	1354/1404 (96%)	1324 (98%)	30 (2%)	61	73

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ARG
1	A	164	LYS
1	A	184	ASN
1	A	222	ARG
1	C	36	GLU
1	C	48	ASN
1	C	119	ARG
1	C	140	ARG
1	C	279	ASP
1	C	292	THR
1	C	345	LYS
1	C	413	LYS
1	B	6	SER
1	B	87	LYS
1	B	109	ARG
1	B	119	ARG
1	B	171	ASN
1	B	184	ASN
1	B	218	LYS
1	B	278	SER
1	B	292	THR
1	B	338[A]	ARG
1	B	338[B]	ARG
1	D	4	LYS

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Mol	Chain	Res	Type
1	D	9	SER
1	D	19	THR
1	D	66	LYS
1	D	171	ASN
1	D	184	ASN
1	D	252	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	D	55	GLN
1	D	67	HIS
1	D	323	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	NDP	A	501	-	44,52,52	1.11	3 (6%)	55,80,80	1.58	4 (7%)
3	70P	A	502	-	26,26,26	1.24	2 (7%)	35,36,36	1.57	8 (22%)
4	FLC	A	503	-	3,12,12	0.90	0	3,17,17	2.92	2 (66%)
2	NDP	B	501	-	44,52,52	1.19	3 (6%)	55,80,80	1.77	6 (10%)
3	70P	B	502	-	26,26,26	1.28	3 (11%)	35,36,36	1.37	6 (17%)
4	FLC	B	503	-	3,12,12	0.65	0	3,17,17	1.76	1 (33%)
2	NDP	C	501	-	44,52,52	1.10	2 (4%)	55,80,80	1.80	7 (12%)
3	70P	C	502	-	26,26,26	1.30	2 (7%)	35,36,36	1.59	8 (22%)
4	FLC	C	503	-	3,12,12	0.56	0	3,17,17	0.31	0
2	NDP	D	501	-	44,52,52	1.11	3 (6%)	55,80,80	1.68	3 (5%)
3	70P	D	502	-	26,26,26	1.41	2 (7%)	35,36,36	1.79	8 (22%)
4	FLC	D	503	-	3,12,12	0.94	0	3,17,17	1.86	1 (33%)

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	NDP	A	501	-	-	0/30/77/77	0/5/5/5
3	70P	A	502	-	-	0/16/29/29	0/3/3/3
4	FLC	A	503	-	-	0/6/16/16	0/0/0/0
2	NDP	B	501	-	-	0/30/77/77	0/5/5/5
3	70P	B	502	-	-	0/16/29/29	0/3/3/3
4	FLC	B	503	-	-	0/6/16/16	0/0/0/0
2	NDP	C	501	-	-	0/30/77/77	0/5/5/5
3	70P	C	502	-	-	0/16/29/29	0/3/3/3
4	FLC	C	503	-	-	0/6/16/16	0/0/0/0
2	NDP	D	501	-	-	0/30/77/77	0/5/5/5
3	70P	D	502	-	-	0/16/29/29	0/3/3/3
4	FLC	D	503	-	-	0/6/16/16	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NDP	C4N-C5N	-4.31	1.39	1.49
2	D	501	NDP	C4N-C5N	-4.27	1.39	1.49
2	B	501	NDP	C4N-C5N	-3.89	1.40	1.49
2	A	501	NDP	C4N-C5N	-3.76	1.40	1.49
3	C	502	70P	C12-N4	-2.25	1.46	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	70P	C6-C5	2.01	1.42	1.39
3	B	502	70P	C8-N1	2.08	1.37	1.34
3	A	502	70P	C14-N4	2.12	1.39	1.36
3	C	502	70P	C14-N4	2.31	1.39	1.36
3	A	502	70P	C8-N1	2.36	1.37	1.34
2	D	501	NDP	O4B-C1B	2.42	1.44	1.41
2	A	501	NDP	O4B-C1B	2.51	1.44	1.41
3	D	502	70P	C8-N1	2.53	1.37	1.34
2	B	501	NDP	O4B-C1B	2.73	1.45	1.41
3	B	502	70P	C14-N4	2.84	1.39	1.36
3	D	502	70P	C14-N4	3.21	1.40	1.36
2	C	501	NDP	C6N-C5N	3.66	1.40	1.33
2	D	501	NDP	C6N-C5N	3.83	1.40	1.33
2	A	501	NDP	C6N-C5N	3.95	1.40	1.33
2	B	501	NDP	C6N-C5N	3.95	1.40	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NDP	N3A-C2A-N1A	-9.95	121.06	128.87
2	D	501	NDP	N3A-C2A-N1A	-9.69	121.26	128.87
2	B	501	NDP	N3A-C2A-N1A	-9.60	121.33	128.87
2	A	501	NDP	N3A-C2A-N1A	-8.94	121.84	128.87
4	A	503	FLC	CB-CA-CAC	-4.12	108.51	114.95
2	B	501	NDP	O2B-P2B-O1X	-4.07	97.75	107.48
3	C	502	70P	O1-C13-C12	-3.57	102.40	105.45
3	C	502	70P	O1-C14-N4	-3.47	105.91	108.80
3	D	502	70P	O1-C14-N4	-3.36	106.00	108.80
3	D	502	70P	C10-C9-N3	-3.24	118.14	123.38
4	D	503	FLC	CB-CG-CGC	-3.01	110.25	114.95
3	D	502	70P	O1-C13-C12	-2.99	102.90	105.45
2	C	501	NDP	C1B-N9A-C4A	-2.97	123.49	126.81
3	B	502	70P	C13-C12-C15	-2.88	110.23	115.16
4	A	503	FLC	CB-CG-CGC	-2.81	110.56	114.95
3	B	502	70P	C10-C9-N3	-2.81	118.85	123.38
2	B	501	NDP	C1D-N1N-C2N	-2.75	116.06	120.85
2	A	501	NDP	C1D-N1N-C2N	-2.71	116.14	120.85
3	A	502	70P	C10-C9-N3	-2.68	119.05	123.38
3	B	502	70P	O1-C14-N4	-2.63	106.61	108.80
3	A	502	70P	O1-C14-N4	-2.62	106.61	108.80
4	B	503	FLC	CB-CG-CGC	-2.58	110.92	114.95
3	C	502	70P	C13-C12-C15	-2.48	110.91	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	70P	C13-C12-C15	-2.44	110.99	115.16
3	A	502	70P	O1-C13-C12	-2.43	103.37	105.45
2	C	501	NDP	O2X-P2B-O2B	-2.40	99.44	106.62
2	C	501	NDP	C1D-N1N-C2N	-2.28	116.89	120.85
3	C	502	70P	C10-C9-N3	-2.26	119.73	123.38
3	B	502	70P	O1-C13-C12	-2.21	103.57	105.45
2	A	501	NDP	O2B-P2B-O1X	-2.17	102.29	107.48
3	C	502	70P	C8-N1-C7	2.01	127.31	123.84
2	B	501	NDP	O3X-P2B-O1X	2.07	117.37	110.63
2	B	501	NDP	O4B-C1B-N9A	2.09	112.06	108.11
3	A	502	70P	N3-C9-N4	2.10	119.30	115.87
2	A	501	NDP	O2A-PA-O1A	2.12	123.57	112.56
3	A	502	70P	C8-N1-C7	2.18	127.61	123.84
3	D	502	70P	C8-N1-C7	2.21	127.66	123.84
3	A	502	70P	C13-C12-N4	2.22	101.78	100.19
2	B	501	NDP	C4N-C3N-C7N	2.23	124.23	118.19
2	D	501	NDP	O4D-C1D-N1N	2.32	112.52	108.09
2	C	501	NDP	C5N-C4N-C3N	2.42	118.67	112.41
2	C	501	NDP	O4D-C1D-N1N	2.52	112.89	108.09
2	D	501	NDP	C5N-C4N-C3N	2.57	119.06	112.41
3	C	502	70P	O2-C14-N4	2.71	131.41	128.83
2	C	501	NDP	O4B-C1B-N9A	2.79	113.39	108.11
3	B	502	70P	C13-O1-C14	2.87	113.25	109.99
3	D	502	70P	N3-C9-N4	2.91	120.63	115.87
3	B	502	70P	C18-C7-N1	2.96	113.60	109.08
3	C	502	70P	C18-C7-N1	3.27	114.07	109.08
3	A	502	70P	C13-O1-C14	3.67	114.15	109.99
3	D	502	70P	C13-O1-C14	3.71	114.19	109.99
3	C	502	70P	C13-O1-C14	3.76	114.25	109.99
3	D	502	70P	C18-C7-N1	4.69	116.24	109.08
3	A	502	70P	C18-C7-N1	4.78	116.38	109.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NDP	1	0
2	B	501	NDP	2	0
4	B	503	FLC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NDP	1	0
4	C	503	FLC	1	0
2	D	501	NDP	1	0
4	D	503	FLC	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	398/417 (95%)	-0.12	1 (0%) 94 97	31, 41, 60, 83	0
1	B	397/417 (95%)	-0.14	0 100 100	31, 42, 55, 80	0
1	C	399/417 (95%)	0.04	1 (0%) 94 97	33, 51, 81, 101	0
1	D	402/417 (96%)	0.18	15 (3%) 45 57	35, 58, 81, 92	0
All	All	1596/1668 (95%)	-0.01	17 (1%) 82 89	31, 47, 75, 101	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	414	LEU	4.4
1	D	86	PHE	3.8
1	D	88	LEU	3.2
1	D	10	VAL	3.1
1	D	68	ASN	2.9
1	D	135	TYR	2.8
1	A	388	ARG	2.8
1	D	89	LYS	2.7
1	D	11	VAL	2.6
1	D	67	HIS	2.5
1	D	354	PHE	2.3
1	D	30	LEU	2.2
1	D	51	ALA	2.1
1	D	60	ALA	2.1
1	D	69	VAL	2.1
1	D	37	LEU	2.1
1	D	39	LEU	2.1

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

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

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	FLC	B	503	13/13	0.90	0.25	5.09	54,62,71,82	0
4	FLC	C	503	13/13	0.90	0.22	1.12	79,83,85,86	0
3	70P	D	502	24/24	0.96	0.17	0.39	44,49,55,59	0
3	70P	B	502	24/24	0.97	0.14	-0.03	37,43,51,53	0
3	70P	C	502	24/24	0.97	0.15	-0.04	40,47,53,58	0
2	NDP	D	501	48/48	0.97	0.13	-0.16	44,54,61,64	0
2	NDP	B	501	48/48	0.98	0.13	-0.21	31,37,44,62	0
3	70P	A	502	24/24	0.98	0.14	-0.26	31,40,46,50	0
2	NDP	A	501	48/48	0.98	0.13	-0.56	33,40,46,50	0
2	NDP	C	501	48/48	0.97	0.11	-0.83	42,54,64,69	0
4	FLC	D	503	13/13	0.88	0.16	-	70,77,81,84	0
4	FLC	A	503	13/13	0.91	0.17	-	55,66,76,81	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.