



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:30 PM GMT

PDB ID : 4IJV  
Title : Crystal structure of 11b-HSD1 double mutant (L262R, F278E) in complex with 3-[1-(4-chlorophenyl)cyclopropyl]-8-(2-fluorophenoxy)[1,2,4]triazolo[4,3-a]pyridine  
Authors : Sheriff, S.  
Deposited on : 2012-12-23  
Resolution : 2.35 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

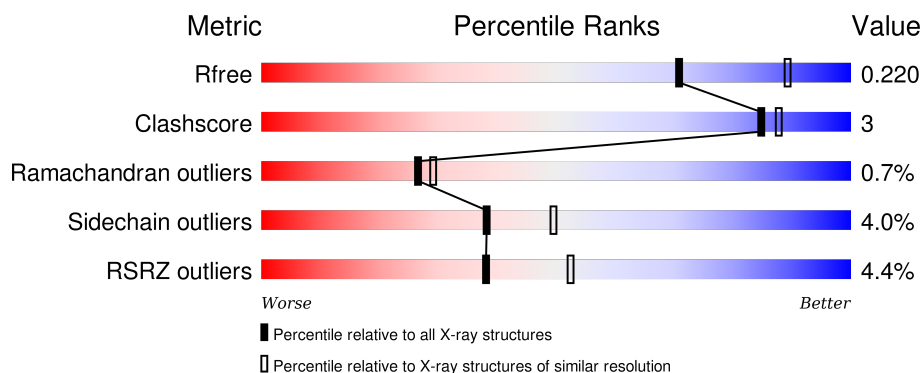
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




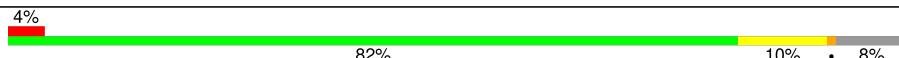
The reported resolution of this entry is 2.35 Å.

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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	286	
1	B	286	
1	D	286	
1	E	286	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8918 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	1	0
			2055	1307	352	379	17			
1	B	281	Total	C	N	O	S	0	0	0
			2133	1351	365	397	20			
1	D	275	Total	C	N	O	S	0	1	0
			2089	1324	358	388	19			
1	E	264	Total	C	N	O	S	0	0	0
			2029	1290	346	376	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLY	-	EXPRESSION TAG	UNP P28845
A	8	SER	-	EXPRESSION TAG	UNP P28845
A	9	HIS	-	EXPRESSION TAG	UNP P28845
A	10	MET	-	EXPRESSION TAG	UNP P28845
A	12	SER	-	EXPRESSION TAG	UNP P28845
A	13	MET	-	EXPRESSION TAG	UNP P28845
A	14	THR	-	EXPRESSION TAG	UNP P28845
A	15	GLY	-	EXPRESSION TAG	UNP P28845
A	16	GLY	-	EXPRESSION TAG	UNP P28845
A	17	GLN	-	EXPRESSION TAG	UNP P28845
A	18	GLN	-	EXPRESSION TAG	UNP P28845
A	19	MET	-	EXPRESSION TAG	UNP P28845
A	20	GLY	-	EXPRESSION TAG	UNP P28845
A	21	ARG	-	EXPRESSION TAG	UNP P28845
A	22	GLY	-	EXPRESSION TAG	UNP P28845
A	23	SER	-	EXPRESSION TAG	UNP P28845
A	262	ARG	LEU	ENGINEERED MUTATION	UNP P28845
A	278	GLU	PHE	ENGINEERED MUTATION	UNP P28845
B	7	GLY	-	EXPRESSION TAG	UNP P28845
B	8	SER	-	EXPRESSION TAG	UNP P28845
B	9	HIS	-	EXPRESSION TAG	UNP P28845

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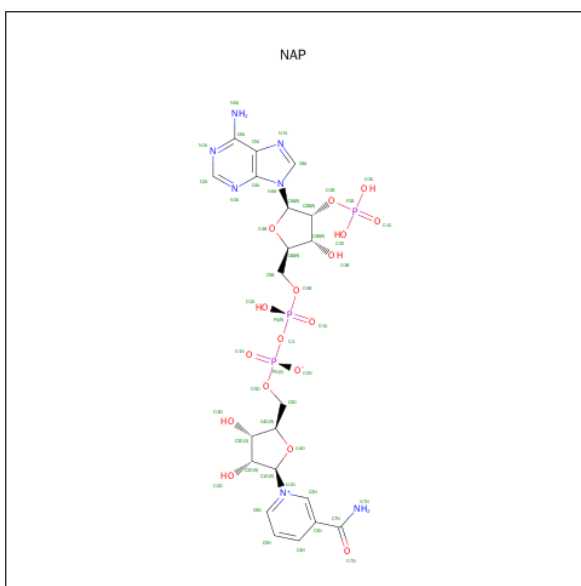
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	MET	-	EXPRESSION TAG	UNP P28845
B	12	SER	-	EXPRESSION TAG	UNP P28845
B	13	MET	-	EXPRESSION TAG	UNP P28845
B	14	THR	-	EXPRESSION TAG	UNP P28845
B	15	GLY	-	EXPRESSION TAG	UNP P28845
B	16	GLY	-	EXPRESSION TAG	UNP P28845
B	17	GLN	-	EXPRESSION TAG	UNP P28845
B	18	GLN	-	EXPRESSION TAG	UNP P28845
B	19	MET	-	EXPRESSION TAG	UNP P28845
B	20	GLY	-	EXPRESSION TAG	UNP P28845
B	21	ARG	-	EXPRESSION TAG	UNP P28845
B	22	GLY	-	EXPRESSION TAG	UNP P28845
B	23	SER	-	EXPRESSION TAG	UNP P28845
B	262	ARG	LEU	ENGINEERED MUTATION	UNP P28845
B	278	GLU	PHE	ENGINEERED MUTATION	UNP P28845
D	7	GLY	-	EXPRESSION TAG	UNP P28845
D	8	SER	-	EXPRESSION TAG	UNP P28845
D	9	HIS	-	EXPRESSION TAG	UNP P28845
D	10	MET	-	EXPRESSION TAG	UNP P28845
D	12	SER	-	EXPRESSION TAG	UNP P28845
D	13	MET	-	EXPRESSION TAG	UNP P28845
D	14	THR	-	EXPRESSION TAG	UNP P28845
D	15	GLY	-	EXPRESSION TAG	UNP P28845
D	16	GLY	-	EXPRESSION TAG	UNP P28845
D	17	GLN	-	EXPRESSION TAG	UNP P28845
D	18	GLN	-	EXPRESSION TAG	UNP P28845
D	19	MET	-	EXPRESSION TAG	UNP P28845
D	20	GLY	-	EXPRESSION TAG	UNP P28845
D	21	ARG	-	EXPRESSION TAG	UNP P28845
D	22	GLY	-	EXPRESSION TAG	UNP P28845
D	23	SER	-	EXPRESSION TAG	UNP P28845
D	262	ARG	LEU	ENGINEERED MUTATION	UNP P28845
D	278	GLU	PHE	ENGINEERED MUTATION	UNP P28845
E	7	GLY	-	EXPRESSION TAG	UNP P28845
E	8	SER	-	EXPRESSION TAG	UNP P28845
E	9	HIS	-	EXPRESSION TAG	UNP P28845
E	10	MET	-	EXPRESSION TAG	UNP P28845
E	12	SER	-	EXPRESSION TAG	UNP P28845
E	13	MET	-	EXPRESSION TAG	UNP P28845
E	14	THR	-	EXPRESSION TAG	UNP P28845
E	15	GLY	-	EXPRESSION TAG	UNP P28845
E	16	GLY	-	EXPRESSION TAG	UNP P28845

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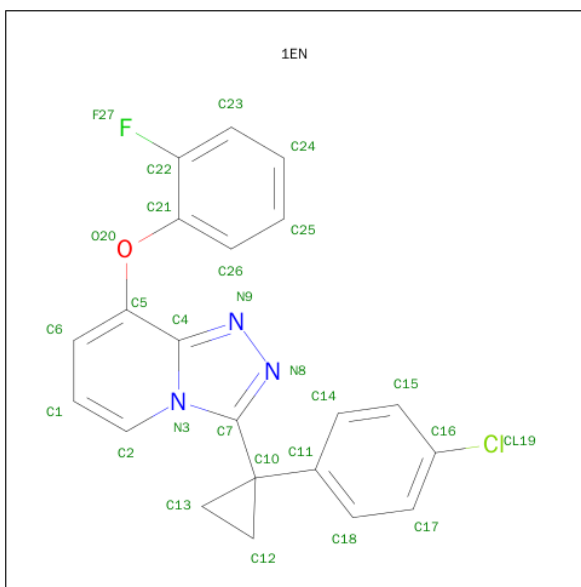
Chain	Residue	Modelled	Actual	Comment	Reference
E	17	GLN	-	EXPRESSION TAG	UNP P28845
E	18	GLN	-	EXPRESSION TAG	UNP P28845
E	19	MET	-	EXPRESSION TAG	UNP P28845
E	20	GLY	-	EXPRESSION TAG	UNP P28845
E	21	ARG	-	EXPRESSION TAG	UNP P28845
E	22	GLY	-	EXPRESSION TAG	UNP P28845
E	23	SER	-	EXPRESSION TAG	UNP P28845
E	262	ARG	LEU	ENGINEERED MUTATION	UNP P28845
E	278	GLU	PHE	ENGINEERED MUTATION	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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

- Molecule 3 is 3-[1-(4-CHLOROPHENYL)CYCLOPROPYL]-8-(2-FLUOROPHENOXY)[1,2,4]TRIAZOLO[4,3-A]PYRIDINE (three-letter code: 1EN) (formula:  $C_{21}H_{15}ClFN_3O$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 27	C 21	Cl 1	F 1	N 3	O 1	0	0
3	B	1	Total 27	C 21	Cl 1	F 1	N 3	O 1	0	0
3	D	1	Total 27	C 21	Cl 1	F 1	N 3	O 1	0	0
3	E	1	Total 27	C 21	Cl 1	F 1	N 3	O 1	0	0

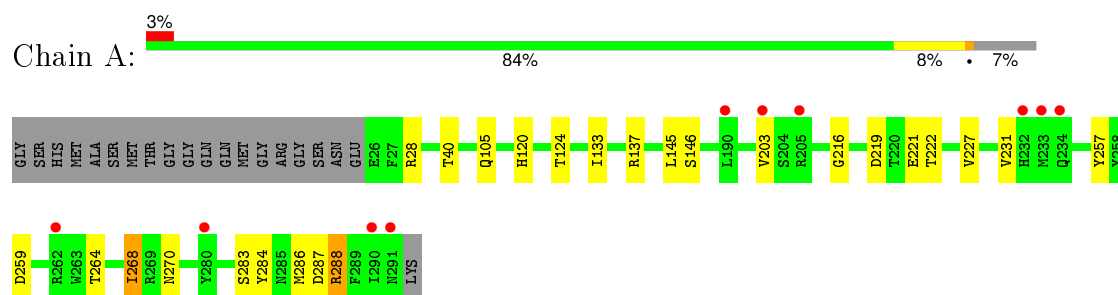
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	75	Total	O	0	0
			75	75		
4	D	97	Total	O	0	0
			97	97		
4	E	66	Total	O	0	0
			66	66		

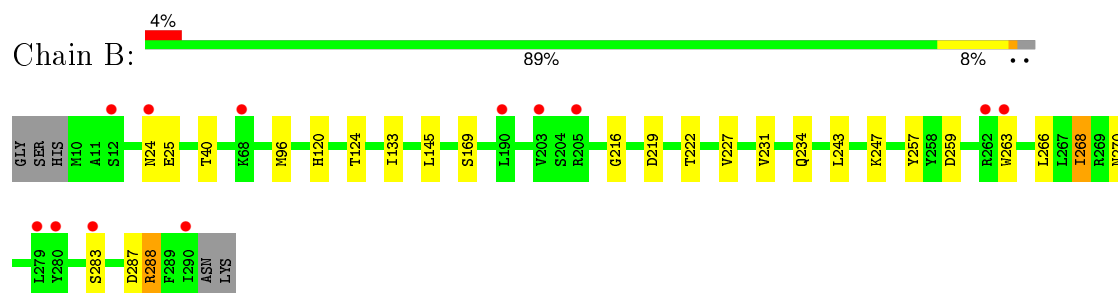
### 3 Residue-property plots [i](#)

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.

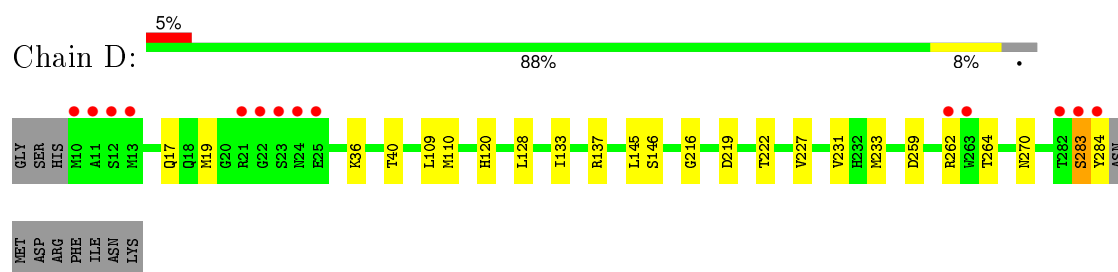
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



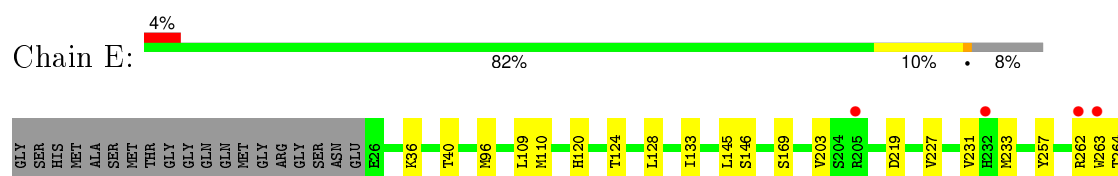
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

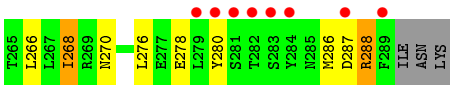


- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.40 Å 94.00 Å 167.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.98 – 2.35 35.98 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.4 (35.98-2.35) 98.4 (35.98-2.35)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.11 (at 2.34 Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.189 , 0.213 0.191 , 0.220	Depositor DCC
$R_{free}$ test set	1046 reflections (2.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 48992 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NAP, 1EN

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	0.45	0/2093	0.67	0/2824
1	B	0.46	0/2167	0.70	1/2921 (0.0%)
1	D	0.47	0/2126	0.67	0/2867
1	E	0.47	0/2063	0.69	0/2784
All	All	0.46	0/8449	0.68	1/11396 (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	B	24	ASN	C-N-CA	8.13	142.02	121.70

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	2055	0	2098	12	0
1	B	2133	0	2162	12	0
1	D	2089	0	2120	17	0
1	E	2029	0	2065	19	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	25	0	0
2	E	48	0	25	1	0
3	A	27	0	15	3	0
3	B	27	0	15	3	0
3	D	27	0	15	1	0
3	E	27	0	15	1	0
4	A	74	0	0	0	0
4	B	75	0	0	0	0
4	D	97	0	0	0	0
4	E	66	0	0	0	0
All	All	8918	0	8605	49	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 3.

All (49) 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:E:227:VAL:HB	1:E:231:VAL:HB	1.61	0.82
1:B:227:VAL:HB	1:B:231:VAL:HB	1.77	0.67
1:D:283:SER:HB3	1:E:233:MET:HG2	1.79	0.65
1:D:222:THR:HG22	3:D:302:1EN:H13	1.82	0.60
1:B:222:THR:HG22	3:B:302:1EN:H12	1.89	0.55
1:E:124:THR:O	3:E:302:1EN:H14	2.07	0.54
1:B:124:THR:O	3:B:302:1EN:H14	2.07	0.54
1:B:263:TRP:HH2	1:E:278:GLU:HG2	1.73	0.54
1:E:264:THR:O	1:E:268:ILE:HG13	2.09	0.52
1:E:203:VAL:HG21	1:E:286:MET:SD	2.50	0.52
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.93	0.52
1:D:284:TYR:HB3	1:E:231:VAL:HG22	1.92	0.51
1:D:231:VAL:HG12	1:D:233:MET:HG2	1.92	0.51
1:E:40:THR:OG1	1:E:120:HIS:HD2	1.94	0.51
1:D:227:VAL:HB	1:D:231:VAL:HB	1.93	0.51
1:D:283:SER:HB3	1:E:233:MET:CG	2.41	0.51
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.94	0.50
1:E:120:HIS:HE1	1:E:146:SER:OG	1.96	0.49
1:A:120:HIS:HE1	1:A:146:SER:OG	1.96	0.49
1:A:203:VAL:HG11	1:A:286:MET:HE3	1.96	0.48
1:D:264:THR:HG23	1:E:280:TYR:OH	2.12	0.48
1:B:222:THR:HG22	3:B:302:1EN:C23	2.44	0.47
1:E:36:LYS:HG2	1:E:110:MET:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.96	0.47
1:D:128:LEU:HD21	1:E:286:MET:CE	2.45	0.47
1:D:264:THR:HA	1:E:276:LEU:HD21	1.97	0.47
1:B:257:TYR:CD1	1:B:268:ILE:HD13	2.50	0.47
1:E:257:TYR:CD1	1:E:268:ILE:HD13	2.51	0.45
1:D:231:VAL:CG1	1:D:233:MET:HG2	2.46	0.45
1:B:169:SER:O	2:B:301:NAP:H6N	2.17	0.45
1:A:227:VAL:HB	1:A:231:VAL:HB	1.99	0.45
1:D:36:LYS:HG2	1:D:110:MET:HB3	1.99	0.45
1:A:264:THR:O	1:A:268:ILE:HG13	2.18	0.44
1:A:137:ARG:HH22	1:B:96:MET:HG3	1.83	0.44
1:D:216:GLY:HA3	1:D:259:ASP:OD1	2.18	0.43
1:D:128:LEU:HD21	1:E:286:MET:HE2	2.01	0.43
1:B:216:GLY:HA3	1:B:259:ASP:OD1	2.20	0.42
1:B:263:TRP:CH2	1:E:278:GLU:HG2	2.52	0.42
1:A:284:TYR:CE1	1:A:286:MET:HE2	2.54	0.42
1:D:17:GLN:HE21	1:D:19:MET:HB2	1.85	0.42
1:A:216:GLY:HA3	1:A:259:ASP:OD1	2.19	0.42
1:A:222:THR:HG22	3:A:302:1EN:H12	2.02	0.41
1:E:169:SER:O	2:E:301:NAP:H6N	2.21	0.41
1:D:137:ARG:HH22	1:E:96:MET:HG3	1.84	0.41
1:A:124:THR:HG23	3:A:302:1EN:C25	2.49	0.41
1:B:243:LEU:HG	1:B:247:LYS:HE3	2.03	0.40
1:D:120:HIS:HE1	1:D:146:SER:OG	2.05	0.40
1:A:257:TYR:CD1	1:A:268:ILE:HD13	2.57	0.40
1:A:124:THR:O	3:A:302:1EN:H14	2.22	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	265/286 (93%)	256 (97%)	7 (3%)	2 (1%)	24	26
1	B	279/286 (98%)	265 (95%)	11 (4%)	3 (1%)	17	17
1	D	274/286 (96%)	265 (97%)	8 (3%)	1 (0%)	39	46
1	E	262/286 (92%)	252 (96%)	8 (3%)	2 (1%)	24	26
All	All	1080/1144 (94%)	1038 (96%)	34 (3%)	8 (1%)	26	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	GLU
1	B	288	ARG
1	E	288	ARG
1	A	288	ARG
1	A	219	ASP
1	B	219	ASP
1	D	219	ASP
1	E	219	ASP

### 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	224/237 (94%)	214 (96%)	10 (4%)	34	43
1	B	229/237 (97%)	220 (96%)	9 (4%)	39	51
1	D	224/237 (94%)	218 (97%)	6 (3%)	52	67
1	E	220/237 (93%)	209 (95%)	11 (5%)	30	37
All	All	897/948 (95%)	861 (96%)	36 (4%)	38	49

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	105	GLN
1	A	133	ILE

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Mol	Chain	Res	Type
1	A	145	LEU
1	A	221	GLU
1	A	268	ILE
1	A	270	ASN
1	A	283	SER
1	A	287	ASP
1	A	288	ARG
1	B	133	ILE
1	B	145	LEU
1	B	234	GLN
1	B	266	LEU
1	B	268	ILE
1	B	270	ASN
1	B	283	SER
1	B	287	ASP
1	B	288	ARG
1	D	109	LEU
1	D	133	ILE
1	D	145	LEU
1	D	262	ARG
1	D	270	ASN
1	D	283	SER
1	E	109	LEU
1	E	128	LEU
1	E	133	ILE
1	E	145	LEU
1	E	262	ARG
1	E	263	TRP
1	E	266	LEU
1	E	268	ILE
1	E	270	ASN
1	E	287	ASP
1	E	288	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	120	HIS
1	B	119	ASN
1	B	120	HIS
1	B	285	ASN

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Mol	Chain	Res	Type
1	D	17	GLN
1	D	119	ASN
1	D	120	HIS
1	E	119	ASN
1	E	120	HIS

### 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](#)

8 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	NAP	A	301	-	42,52,52	0.57	0	54,80,80	1.05	4 (7%)
3	1EN	A	302	-	28,31,31	1.79	6 (21%)	33,46,46	0.95	2 (6%)
2	NAP	B	301	-	42,52,52	0.59	0	54,80,80	0.99	2 (3%)
3	1EN	B	302	-	28,31,31	1.75	4 (14%)	33,46,46	0.90	2 (6%)
2	NAP	D	301	-	42,52,52	0.57	0	54,80,80	1.01	3 (5%)
3	1EN	D	302	-	28,31,31	1.70	5 (17%)	33,46,46	0.92	1 (3%)
2	NAP	E	301	-	42,52,52	0.54	0	54,80,80	0.92	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	1EN	E	302	-	28,31,31	1.71	5 (17%)	33,46,46	0.83	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	NAP	A	301	-	-	0/27/67/67	0/5/5/5
3	1EN	A	302	-	-	0/10/20/20	0/4/5/5
2	NAP	B	301	-	-	0/27/67/67	0/5/5/5
3	1EN	B	302	-	-	0/10/20/20	0/4/5/5
2	NAP	D	301	-	-	0/27/67/67	0/5/5/5
3	1EN	D	302	-	-	0/10/20/20	0/4/5/5
2	NAP	E	301	-	-	0/27/67/67	0/5/5/5
3	1EN	E	302	-	-	0/10/20/20	0/4/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	1EN	C4-N9	-2.62	1.30	1.33
3	E	302	1EN	C12-C10	-2.40	1.48	1.52
3	D	302	1EN	C10-C11	-2.37	1.50	1.54
3	A	302	1EN	C12-C10	-2.13	1.49	1.52
3	A	302	1EN	C4-N9	-2.10	1.31	1.33
3	B	302	1EN	C10-C11	-2.04	1.51	1.54
3	A	302	1EN	C13-C10	-2.03	1.49	1.52
3	E	302	1EN	C10-C11	-2.00	1.51	1.54
3	E	302	1EN	N9-N8	2.69	1.43	1.37
3	E	302	1EN	C5-C4	2.87	1.46	1.42
3	B	302	1EN	N9-N8	3.04	1.43	1.37
3	D	302	1EN	N9-N8	3.15	1.44	1.37
3	A	302	1EN	N9-N8	3.52	1.44	1.37
3	D	302	1EN	C5-C4	3.69	1.47	1.42
3	B	302	1EN	C5-C4	3.92	1.47	1.42
3	A	302	1EN	C5-C4	4.24	1.47	1.42
3	D	302	1EN	C1-C6	4.37	1.47	1.38
3	A	302	1EN	C1-C6	4.71	1.48	1.38
3	E	302	1EN	C1-C6	4.79	1.48	1.38
3	B	302	1EN	C1-C6	4.87	1.48	1.38

All (18) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAP	O4D-C1D-N1N	2.01	110.34	108.13
3	D	302	1EN	C26-C21-C22	2.03	121.09	117.90
2	E	301	NAP	O4D-C1D-N1N	2.07	110.40	108.13
2	E	301	NAP	O3-PA-O5B	2.11	108.52	102.94
3	A	302	1EN	C26-C21-C22	2.16	121.30	117.90
3	B	302	1EN	C12-C10-C13	2.23	60.06	58.68
3	B	302	1EN	C26-C21-C22	2.25	121.44	117.90
3	A	302	1EN	C12-C10-C13	2.38	60.15	58.68
2	D	301	NAP	O3-PA-O5B	2.41	109.33	102.94
2	A	301	NAP	O3-PA-O5B	2.67	110.03	102.94
2	E	301	NAP	P2B-O2B-C2B	3.19	129.20	121.56
2	D	301	NAP	O2B-P2B-O1X	3.21	115.12	107.11
2	E	301	NAP	O2B-P2B-O1X	3.24	115.19	107.11
2	D	301	NAP	P2B-O2B-C2B	3.72	130.47	121.56
2	B	301	NAP	O2B-P2B-O1X	3.87	116.78	107.11
2	A	301	NAP	O2B-P2B-O1X	3.93	116.92	107.11
2	A	301	NAP	P2B-O2B-C2B	4.08	131.34	121.56
2	B	301	NAP	P2B-O2B-C2B	4.20	131.64	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	1EN	3	0
2	B	301	NAP	1	0
3	B	302	1EN	3	0
3	D	302	1EN	1	0
2	E	301	NAP	1	0
3	E	302	1EN	1	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	266/286 (93%)	-0.05	10 (3%)	44 58	13, 24, 48, 105	0
1	B	281/286 (98%)	0.01	12 (4%)	39 53	13, 27, 54, 85	0
1	D	275/286 (96%)	-0.15	14 (5%)	32 46	10, 21, 53, 71	0
1	E	264/286 (92%)	-0.04	12 (4%)	37 52	11, 26, 61, 81	0
All	All	1086/1144 (94%)	-0.06	48 (4%)	38 52	10, 25, 54, 105	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	282	THR	6.0
1	E	263	TRP	5.3
1	D	282	THR	4.9
1	D	11	ALA	4.7
1	D	10	MET	4.4
1	A	291	ASN	4.3
1	D	263	TRP	4.3
1	B	290	ILE	4.2
1	B	262	ARG	4.2
1	E	280	TYR	4.1
1	B	280	TYR	4.0
1	A	290	ILE	3.9
1	D	24	ASN	3.8
1	A	233	MET	3.5
1	B	283	SER	3.5
1	E	205	ARG	3.5
1	E	283	SER	3.4
1	D	22	GLY	3.3
1	B	205	ARG	3.3
1	D	23	SER	3.1
1	B	263	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	279	LEU	3.1
1	E	262	ARG	3.1
1	D	262	ARG	3.0
1	B	12	SER	3.0
1	A	234	GLN	3.0
1	A	262	ARG	2.9
1	A	205	ARG	2.9
1	D	12	SER	2.7
1	E	287	ASP	2.7
1	E	289	PHE	2.6
1	E	279	LEU	2.6
1	E	232	HIS	2.5
1	D	25	GLU	2.5
1	B	68	LYS	2.5
1	A	232	HIS	2.5
1	B	24	ASN	2.5
1	B	203	VAL	2.4
1	D	21	ARG	2.4
1	D	284	TYR	2.3
1	A	203	VAL	2.3
1	B	190	LEU	2.2
1	E	284	TYR	2.2
1	A	190	LEU	2.2
1	D	283	SER	2.2
1	E	281	SER	2.1
1	A	280	TYR	2.1
1	D	13	MET	2.1

## 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 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(Å <sup>2</sup> )	Q<0.9
3	1EN	B	302	27/27	0.93	0.13	0.89	18,23,34,41	0
3	1EN	A	302	27/27	0.93	0.15	0.21	25,28,37,41	0
3	1EN	D	302	27/27	0.96	0.11	-0.03	15,17,22,38	0
3	1EN	E	302	27/27	0.96	0.10	-0.50	16,22,28,38	0
2	NAP	D	301	48/48	0.98	0.08	-1.00	10,15,22,25	0
2	NAP	E	301	48/48	0.98	0.08	-1.11	10,18,25,30	0
2	NAP	B	301	48/48	0.98	0.08	-1.12	12,19,25,32	0
2	NAP	A	301	48/48	0.98	0.08	-1.51	9,19,23,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.