



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:01 PM GMT

PDB ID : 3CSD  
Title : Actinorhodin Polyketide Ketoreductase Mutant P94L bound to NADPH and the Inhibitor Emodin  
Authors : Javidpour, P.  
Deposited on : 2008-04-09  
Resolution : 2.29 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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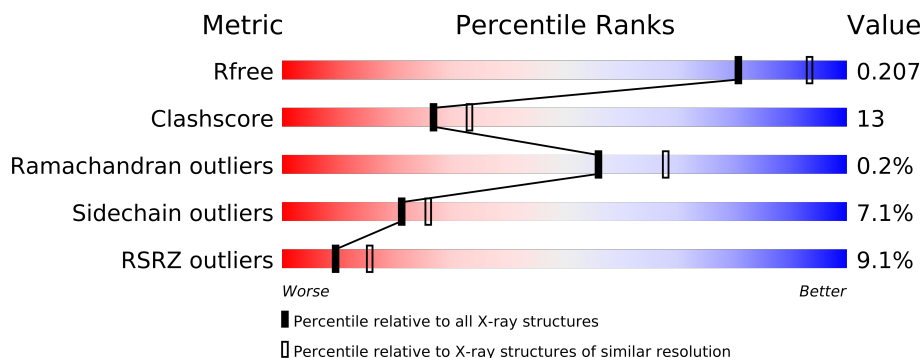
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.29 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	281	
1	B	281	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	EMO	B	302	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4110 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Putative ketoacyl reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	257	Total	C	N	O	S	0	0	0
			1875	1165	342	360	8			
1	A	256	Total	C	N	O	S	0	0	0
			1877	1173	336	361	7			

There are 42 discrepancies between the modelled and reference sequences:

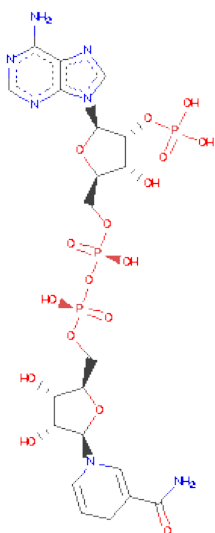
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP P16544
B	-18	GLY	-	EXPRESSION TAG	UNP P16544
B	-17	SER	-	EXPRESSION TAG	UNP P16544
B	-16	SER	-	EXPRESSION TAG	UNP P16544
B	-15	HIS	-	EXPRESSION TAG	UNP P16544
B	-14	HIS	-	EXPRESSION TAG	UNP P16544
B	-13	HIS	-	EXPRESSION TAG	UNP P16544
B	-12	HIS	-	EXPRESSION TAG	UNP P16544
B	-11	HIS	-	EXPRESSION TAG	UNP P16544
B	-10	HIS	-	EXPRESSION TAG	UNP P16544
B	-9	SER	-	EXPRESSION TAG	UNP P16544
B	-8	SER	-	EXPRESSION TAG	UNP P16544
B	-7	GLY	-	EXPRESSION TAG	UNP P16544
B	-6	LEU	-	EXPRESSION TAG	UNP P16544
B	-5	VAL	-	EXPRESSION TAG	UNP P16544
B	-4	PRO	-	EXPRESSION TAG	UNP P16544
B	-3	ARG	-	EXPRESSION TAG	UNP P16544
B	-2	GLY	-	EXPRESSION TAG	UNP P16544
B	-1	SER	-	EXPRESSION TAG	UNP P16544
B	0	HIS	-	EXPRESSION TAG	UNP P16544
B	94	LEU	PRO	ENGINEERED	UNP P16544
A	-19	MET	-	EXPRESSION TAG	UNP P16544
A	-18	GLY	-	EXPRESSION TAG	UNP P16544
A	-17	SER	-	EXPRESSION TAG	UNP P16544
A	-16	SER	-	EXPRESSION TAG	UNP P16544

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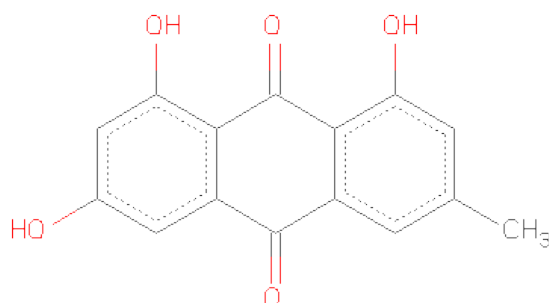
Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	EXPRESSION TAG	UNP P16544
A	-14	HIS	-	EXPRESSION TAG	UNP P16544
A	-13	HIS	-	EXPRESSION TAG	UNP P16544
A	-12	HIS	-	EXPRESSION TAG	UNP P16544
A	-11	HIS	-	EXPRESSION TAG	UNP P16544
A	-10	HIS	-	EXPRESSION TAG	UNP P16544
A	-9	SER	-	EXPRESSION TAG	UNP P16544
A	-8	SER	-	EXPRESSION TAG	UNP P16544
A	-7	GLY	-	EXPRESSION TAG	UNP P16544
A	-6	LEU	-	EXPRESSION TAG	UNP P16544
A	-5	VAL	-	EXPRESSION TAG	UNP P16544
A	-4	PRO	-	EXPRESSION TAG	UNP P16544
A	-3	ARG	-	EXPRESSION TAG	UNP P16544
A	-2	GLY	-	EXPRESSION TAG	UNP P16544
A	-1	SER	-	EXPRESSION TAG	UNP P16544
A	0	HIS	-	EXPRESSION TAG	UNP P16544
A	94	LEU	PRO	ENGINEERED	UNP P16544

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



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

- Molecule 3 is 3-METHYL-1,6,8-TRIHIDROXYANTHRAQUINONE (three-letter code: EMO) (formula: C<sub>15</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			20	15	5		
3	B	1	Total	C	O	0	0
			20	15	5		
3	A	1	Total	C	O	0	0
			20	15	5		
3	A	1	Total	C	O	0	0
			20	15	5		

- Molecule 4 is water.

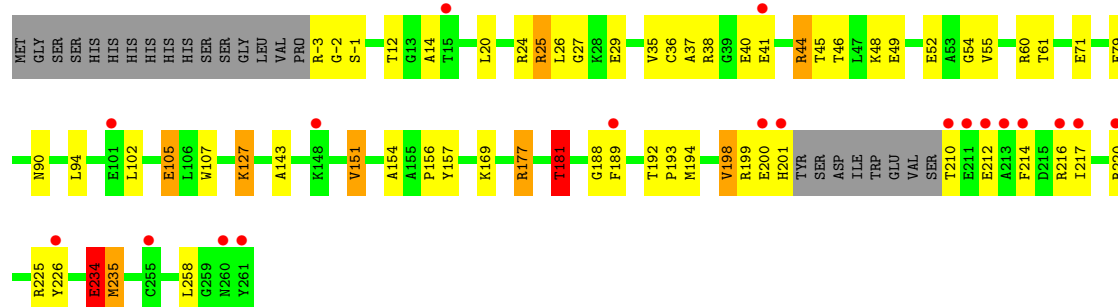
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	90	Total	O	0	0
			90	90		
4	A	92	Total	O	0	0
			92	92		

### 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.

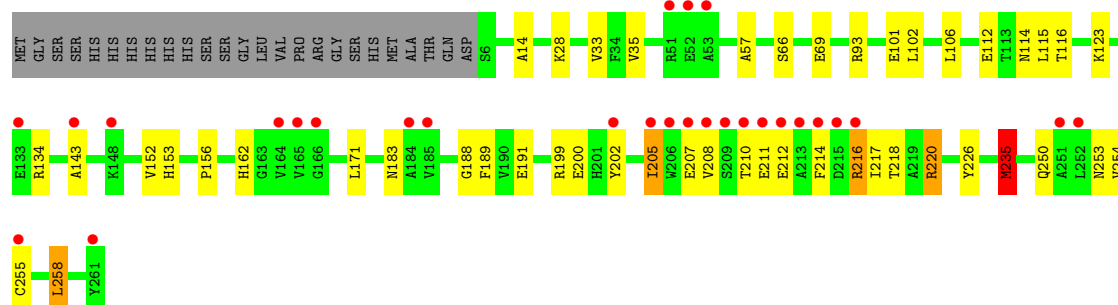
- Molecule 1: Putative ketoacyl reductase

Chain B: 



- Molecule 1: Putative ketoacyl reductase

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.09Å 105.09Å 123.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.29 48.36 – 2.29	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.29) 100.0 (48.36-2.29)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.93 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.173 , 0.207 0.173 , 0.207	Depositor DCC
$R_{free}$ test set	1795 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 41.8	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 35932 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4110	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, EMO

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	0.97	0/1902	0.85	1/2582 (0.0%)
1	B	1.08	4/1897 (0.2%)	0.94	7/2570 (0.3%)
All	All	1.03	4/3799 (0.1%)	0.90	8/5152 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	234	GLU	CG-CD	7.66	1.63	1.51
1	B	79	GLU	CG-CD	6.42	1.61	1.51
1	B	105	GLU	CG-CD	6.20	1.61	1.51
1	B	234	GLU	CB-CG	6.10	1.63	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	MET	CG-SD-CE	-8.89	85.97	100.20
1	B	235	MET	CG-SD-CE	-8.78	86.15	100.20
1	B	177	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	177	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	B	225	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	44	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	B	181	THR	N-CA-CB	-5.11	100.58	110.30
1	B	225	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1877	0	1900	39	0
1	B	1875	0	1904	59	0
2	A	48	0	26	6	0
2	B	48	0	26	7	0
3	A	40	0	14	6	0
3	B	40	0	14	17	0
4	A	92	0	0	2	0
4	B	90	0	0	3	0
All	All	4110	0	3884	102	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (102) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:25:ARG:NH2	1:B:234:GLU:HG3	1.60	1.15
1:B:194:MET:CE	3:B:303:EMO:H2	1.78	1.12
1:A:220:ARG:HA	1:A:220:ARG:HE	1.22	1.03
1:B:107:TRP:HE1	1:A:116:THR:HG22	1.21	1.01
1:B:151:VAL:HG22	1:B:154:ALA:HB3	1.43	0.97
1:A:216:ARG:CB	1:A:216:ARG:HH11	1.77	0.97
1:B:-3:ARG:N	1:B:-2:GLY:HA2	1.88	0.88
1:B:217:ILE:HG23	3:B:303:EMO:H16	1.59	0.85
1:B:25:ARG:NH2	1:B:234:GLU:CG	2.41	0.84
1:B:181:THR:HG21	4:B:336:HOH:O	1.78	0.83
1:B:25:ARG:HH22	1:B:234:GLU:HG3	1.39	0.83
1:A:93:ARG:H	1:A:114:ASN:HD21	1.26	0.83
2:B:301:NDP:H41N	3:B:303:EMO:C3	2.10	0.82
1:B:189:PHE:CZ	1:B:226:TYR:CE1	2.68	0.81
2:A:301:NDP:H41N	3:A:302:EMO:C3	2.10	0.81
1:A:216:ARG:HB2	1:A:216:ARG:HH11	1.47	0.79
1:B:102:LEU:HD21	1:B:156:PRO:HG3	1.63	0.79
1:B:25:ARG:HH21	1:B:234:GLU:CG	1.98	0.75
1:B:214:PHE:HE1	1:B:226:TYR:CE2	2.05	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:301:NDP:C5N	3:A:302:EMO:O3	2.35	0.74
1:B:-3:ARG:H3	1:B:-2:GLY:HA2	1.53	0.73
1:B:25:ARG:HH21	1:B:234:GLU:CD	1.92	0.73
1:B:107:TRP:HE1	1:A:116:THR:CG2	2.02	0.72
1:B:194:MET:HE2	3:B:303:EMO:H2	1.67	0.72
1:B:38:ARG:HB2	2:B:301:NDP:O2X	1.89	0.72
1:A:183:ASN:HD22	1:A:250:GLN:H	1.37	0.71
1:B:24:ARG:NH1	1:B:49:GLU:OE1	2.24	0.70
1:B:194:MET:HE3	3:B:303:EMO:H2	1.73	0.70
1:B:217:ILE:CG2	3:B:303:EMO:H16	2.25	0.67
1:A:116:THR:HG21	4:A:361:HOH:O	1.94	0.67
1:B:25:ARG:HH21	1:B:234:GLU:HG3	1.49	0.67
1:B:198:VAL:HG21	3:B:303:EMO:O19	1.95	0.66
1:A:202:TYR:OH	1:A:216:ARG:NH1	2.28	0.66
1:B:127:LYS:NZ	1:A:101:GLU:OE2	2.24	0.66
1:B:-3:ARG:N	1:B:-2:GLY:CA	2.60	0.64
2:B:301:NDP:H41N	3:B:303:EMO:C4	2.28	0.64
1:B:194:MET:HE1	3:B:303:EMO:H2	1.77	0.62
1:A:220:ARG:HA	1:A:220:ARG:NE	2.03	0.61
1:B:258:LEU:HD21	3:B:303:EMO:H8	1.82	0.61
1:B:14:ALA:HB3	1:B:35:VAL:HB	1.83	0.61
1:A:217:ILE:HG23	3:A:302:EMO:H16	1.83	0.60
2:B:301:NDP:C5N	3:B:303:EMO:O3	2.50	0.59
1:B:25:ARG:O	1:B:29:GLU:HG2	2.03	0.59
2:A:301:NDP:H41N	3:A:302:EMO:C4	2.32	0.58
1:B:-3:ARG:H2	1:B:-2:GLY:HA2	1.69	0.58
2:B:301:NDP:C4N	3:B:303:EMO:C3	2.83	0.56
1:A:183:ASN:ND2	1:A:250:GLN:H	2.03	0.56
1:B:-3:ARG:H2	1:B:-2:GLY:CA	2.20	0.55
1:B:25:ARG:HD2	1:B:29:GLU:OE2	2.07	0.55
1:A:216:ARG:HH11	1:A:216:ARG:HB3	1.69	0.54
1:B:41:GLU:O	1:B:45:THR:HG23	2.08	0.54
1:B:217:ILE:HG23	3:B:303:EMO:C16	2.37	0.53
1:B:189:PHE:CE2	1:B:226:TYR:CE1	2.96	0.53
2:A:301:NDP:C4N	3:A:302:EMO:C3	2.85	0.52
1:A:216:ARG:HB2	1:A:216:ARG:NH1	2.20	0.51
1:A:216:ARG:CB	1:A:216:ARG:NH1	2.61	0.50
1:B:157:TYR:OH	3:B:303:EMO:O3	2.21	0.50
1:B:105:GLU:CD	1:B:105:GLU:H	2.15	0.50
1:B:27:GLY:HA3	1:B:55:VAL:HG13	1.94	0.50
1:B:169:LYS:NZ	1:A:162:HIS:HE1	2.09	0.50
1:A:189:PHE:CZ	1:A:226:TYR:CE1	3.00	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:40:GLU:O	1:B:44:ARG:HD3	2.12	0.49
1:B:20:LEU:HD13	1:B:46:THR:HG23	1.93	0.49
1:A:220:ARG:HE	1:A:220:ARG:CA	2.09	0.48
1:A:216:ARG:HH11	1:A:216:ARG:CG	2.25	0.48
1:B:198:VAL:CG2	3:B:303:EMO:O19	2.60	0.48
4:B:309:HOH:O	1:A:123:LYS:HE2	2.14	0.48
1:A:189:PHE:CE2	1:A:226:TYR:CE1	3.02	0.48
1:B:189:PHE:CZ	1:B:226:TYR:CZ	3.02	0.48
1:B:216:ARG:HG2	1:B:220:ARG:HH21	1.77	0.48
1:B:143:ALA:O	2:B:301:NDP:H6N	2.14	0.47
1:B:189:PHE:CE1	1:B:226:TYR:CE1	3.03	0.47
1:B:181:THR:HG22	4:B:335:HOH:O	2.14	0.47
1:B:12:THR:O	1:B:90:ASN:HB3	2.14	0.47
1:B:48:LYS:NZ	1:B:52:GLU:OE2	2.39	0.47
1:A:258:LEU:HD22	4:A:310:HOH:O	2.15	0.47
1:B:94:LEU:CD1	1:B:198:VAL:HG12	2.45	0.46
1:A:14:ALA:HB3	1:A:35:VAL:HB	1.96	0.46
1:B:37:ALA:O	1:B:61:THR:HA	2.14	0.46
1:A:102:LEU:HD21	1:A:156:PRO:HG3	1.99	0.45
1:B:151:VAL:CG2	1:B:154:ALA:HB3	2.31	0.45
1:A:33:VAL:O	1:A:57:ALA:HA	2.17	0.44
1:B:192:THR:HB	1:B:193:PRO:HD2	2.00	0.44
1:B:188:GLY:O	2:B:301:NDP:H42N	2.17	0.44
1:A:143:ALA:O	2:A:301:NDP:H6N	2.18	0.44
1:A:205:ILE:HG23	1:A:205:ILE:O	2.18	0.43
1:A:112:GLU:HA	1:A:116:THR:OG1	2.18	0.43
1:A:199:ARG:HD2	1:A:210:THR:HG23	1.99	0.43
1:A:188:GLY:O	2:A:301:NDP:H42N	2.19	0.42
1:A:191:GLU:HG3	1:A:226:TYR:CE2	2.54	0.42
1:A:152:VAL:O	1:A:153:HIS:HB2	2.19	0.42
1:B:199:ARG:NH1	1:B:226:TYR:OH	2.47	0.42
1:A:212:GLU:O	1:A:216:ARG:HG3	2.20	0.42
1:B:-1:SER:CB	1:B:54:GLY:O	2.66	0.42
1:B:194:MET:CE	3:B:303:EMO:C2	2.72	0.41
1:B:194:MET:HE2	3:B:303:EMO:C2	2.45	0.41
1:A:235:MET:HE2	1:A:254:VAL:CG2	2.51	0.41
1:A:253:ASN:HB3	1:A:255:CYS:SG	2.61	0.41
1:B:200:GLU:HA	1:B:201:HIS:HA	1.75	0.41
1:A:258:LEU:HD21	3:A:302:EMO:H8	2.04	0.40
1:A:66:SER:OG	1:A:69:GLU:HG3	2.22	0.40
1:A:214:PHE:CZ	1:A:218:THR:HG21	2.57	0.40

There are no symmetry-related clashes.

## 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	254/281 (90%)	244 (96%)	9 (4%)	1 (0%)	43	52
1	B	253/281 (90%)	244 (96%)	9 (4%)	0	100	100
All	All	507/562 (90%)	488 (96%)	18 (4%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ARG

### 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	191/212 (90%)	178 (93%)	13 (7%)	22	28
1	B	190/212 (90%)	176 (93%)	14 (7%)	20	24
All	All	381/424 (90%)	354 (93%)	27 (7%)	21	26

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

Mol	Chain	Res	Type
1	B	25	ARG
1	B	26	LEU
1	B	36	CYS
1	B	60	ARG
1	B	71	GLU
1	B	127	LYS
1	B	151	VAL
1	B	177	ARG

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Mol	Chain	Res	Type
1	B	181	THR
1	B	198	VAL
1	B	210	THR
1	B	212	GLU
1	B	234	GLU
1	B	235	MET
1	A	28	LYS
1	A	106	LEU
1	A	115	LEU
1	A	171	LEU
1	A	200	GLU
1	A	205	ILE
1	A	207	GLU
1	A	208	VAL
1	A	211	GLU
1	A	216	ARG
1	A	220	ARG
1	A	235	MET
1	A	258	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	89	ASN
1	B	162	HIS
1	B	183	ASN
1	A	89	ASN
1	A	114	ASN
1	A	162	HIS
1	A	183	ASN
1	A	228	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry

6 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	301	-	52,52,52	1.39	8 (15%)	80,80,80	1.74	18 (22%)
3	EMO	A	302	-	22,22,22	1.98	4 (18%)	34,34,34	0.95	1 (2%)
3	EMO	A	303	-	22,22,22	1.98	4 (18%)	34,34,34	0.95	1 (2%)
2	NDP	B	301	-	52,52,52	1.48	8 (15%)	80,80,80	1.62	14 (17%)
3	EMO	B	302	-	22,22,22	1.99	4 (18%)	34,34,34	0.95	1 (2%)
3	EMO	B	303	-	22,22,22	1.99	4 (18%)	34,34,34	0.95	1 (2%)

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	301	-	-	0/35/77/77	0/3/5/5
3	EMO	A	302	-	-	0/0/16/16	0/0/3/3
3	EMO	A	303	-	-	0/0/16/16	0/0/3/3
2	NDP	B	301	-	-	0/35/77/77	0/3/5/5
3	EMO	B	302	-	-	0/0/16/16	0/0/3/3
3	EMO	B	303	-	-	0/0/16/16	0/0/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	EMO	C5-C20	4.90	1.49	1.41
3	A	303	EMO	C5-C20	4.88	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NDP	C4N-C3N	-4.88	1.40	1.50
3	B	303	EMO	C7-C18	4.87	1.49	1.41
3	A	302	EMO	C7-C18	4.86	1.48	1.41
3	B	302	EMO	C7-C18	4.85	1.48	1.41
3	A	303	EMO	C7-C18	4.85	1.48	1.41
3	B	302	EMO	C5-C20	4.85	1.48	1.41
3	A	302	EMO	C5-C20	4.81	1.48	1.41
3	B	302	EMO	C20-C1	4.11	1.49	1.41
3	B	303	EMO	C18-C17	4.10	1.49	1.41
3	A	302	EMO	C20-C1	4.09	1.49	1.41
3	B	302	EMO	C18-C17	4.09	1.49	1.41
3	A	303	EMO	C20-C1	4.08	1.49	1.41
3	A	303	EMO	C18-C17	4.04	1.48	1.41
3	B	303	EMO	C20-C1	4.03	1.48	1.41
2	B	301	NDP	C4N-C5N	-4.01	1.40	1.49
3	A	302	EMO	C18-C17	4.00	1.48	1.41
2	A	301	NDP	C4A-N9A	-3.99	1.31	1.37
2	A	301	NDP	C6N-C5N	3.81	1.41	1.33
2	A	301	NDP	C4N-C3N	-3.78	1.42	1.50
2	A	301	NDP	C4N-C5N	-3.66	1.41	1.49
2	B	301	NDP	C6N-C5N	3.16	1.40	1.33
2	A	301	NDP	PA-O3	2.87	1.65	1.59
2	B	301	NDP	C2N-C3N	2.84	1.40	1.34
2	B	301	NDP	O4B-C1B	2.78	1.45	1.41
2	A	301	NDP	C2N-C3N	2.50	1.39	1.34
2	A	301	NDP	O4B-C1B	2.48	1.45	1.41
2	B	301	NDP	PN-O3	2.38	1.64	1.59
2	B	301	NDP	C7N-C3N	2.37	1.52	1.47
2	B	301	NDP	PA-O3	2.05	1.63	1.59
2	A	301	NDP	PA-O2A	-2.01	1.46	1.55

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NDP	N3A-C2A-N1A	-8.40	121.68	128.71
2	B	301	NDP	N3A-C2A-N1A	-6.98	122.88	128.71
2	B	301	NDP	O4B-C1B-C2B	-4.19	103.03	106.95
2	A	301	NDP	O4B-C1B-N9A	4.04	112.20	108.44
2	B	301	NDP	N3A-C4A-N9A	3.49	131.73	125.43
2	A	301	NDP	N3A-C4A-N9A	3.03	130.90	125.43
2	A	301	NDP	O2A-PA-O1A	2.89	128.35	112.21
2	B	301	NDP	C5A-C4A-N3A	-2.88	119.43	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	EMO	C16-C9-C8	2.84	121.92	118.10
2	B	301	NDP	C4N-C3N-C2N	-2.83	118.23	121.68
3	A	303	EMO	C16-C9-C8	2.83	121.90	118.10
2	A	301	NDP	C4A-C5A-N7A	-2.81	107.11	109.52
2	B	301	NDP	C5N-C4N-C3N	2.80	120.19	112.60
2	A	301	NDP	C5N-C4N-C3N	2.80	120.19	112.60
3	B	303	EMO	C16-C9-C8	2.80	121.86	118.10
3	A	302	EMO	C16-C9-C8	2.80	121.85	118.10
2	A	301	NDP	C6N-N1N-C2N	2.74	123.03	119.44
2	A	301	NDP	C3N-C2N-N1N	-2.61	119.34	123.05
2	B	301	NDP	O3D-C3D-C4D	-2.42	103.96	111.08
2	A	301	NDP	C5A-C4A-N3A	-2.40	120.48	125.70
2	B	301	NDP	O2D-C2D-C3D	2.38	119.59	111.83
2	B	301	NDP	C1D-N1N-C6N	-2.33	115.64	120.79
2	A	301	NDP	C1D-N1N-C6N	-2.32	115.66	120.79
2	B	301	NDP	C4A-C5A-N7A	-2.30	107.55	109.52
2	B	301	NDP	O2N-PN-O1N	2.25	124.75	112.21
2	B	301	NDP	C2D-C1D-N1N	2.24	118.91	113.21
2	A	301	NDP	C4N-C5N-C6N	-2.22	118.53	122.61
2	A	301	NDP	N7A-C8A-N9A	-2.19	108.15	114.36
2	A	301	NDP	O3D-C3D-C4D	-2.18	104.65	111.08
2	A	301	NDP	O5B-PA-O1A	-2.18	100.84	109.37
2	A	301	NDP	C4N-C3N-C2N	-2.15	119.07	121.68
2	B	301	NDP	O3X-P2B-O2B	-2.14	100.94	107.09
2	A	301	NDP	C2A-N3A-C4A	2.07	119.91	114.01
2	B	301	NDP	C4N-C5N-C6N	-2.06	118.82	122.61
2	A	301	NDP	O3B-C3B-C4B	-2.05	105.04	111.08
2	A	301	NDP	O2A-PA-O3	2.01	114.67	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	256/281 (91%)	0.46	28 (10%) 6 10	26, 38, 70, 95	0
1	B	257/281 (91%)	0.30	19 (7%) 14 21	25, 40, 76, 105	0
All	All	513/562 (91%)	0.38	47 (9%) 9 15	25, 39, 74, 105	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	TRP	8.7
1	B	261	TYR	6.9
1	A	202	TYR	6.4
1	A	205	ILE	5.7
1	B	210	THR	5.1
1	B	216	ARG	4.7
1	A	216	ARG	4.5
1	B	211	GLU	4.5
1	B	189	PHE	4.4
1	B	213	ALA	4.3
1	A	208	VAL	4.3
1	A	261	TYR	4.1
1	A	211	GLU	4.1
1	B	217	ILE	4.1
1	B	212	GLU	3.8
1	A	207	GLU	3.8
1	B	41	GLU	3.4
1	B	226	TYR	3.1
1	A	210	THR	3.0
1	A	52	GLU	2.9
1	B	101	GLU	2.9
1	B	214	PHE	2.9
1	A	214	PHE	2.8
1	B	201	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	15	THR	2.7
1	A	213	ALA	2.6
1	A	165	VAL	2.6
1	A	252	LEU	2.6
1	A	164	VAL	2.6
1	B	200	GLU	2.6
1	A	209	SER	2.6
1	B	220	ARG	2.5
1	B	260	ASN	2.5
1	A	251	ALA	2.5
1	A	184	ALA	2.4
1	A	215	ASP	2.3
1	A	185	VAL	2.3
1	A	143	ALA	2.2
1	A	255	CYS	2.2
1	A	53	ALA	2.2
1	A	148	LYS	2.2
1	A	133	GLU	2.1
1	B	148	LYS	2.1
1	B	255	CYS	2.1
1	A	166	GLY	2.0
1	A	212	GLU	2.0
1	A	51	ARG	2.0

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EMO	B	302	20/20	0.39	2.92	97,99,99,99	0
3	EMO	B	303	20/20	0.32	1.53	85,85,87,88	0
2	NDP	B	301	48/48	0.18	0.70	50,56,60,62	0
2	NDP	A	301	48/48	0.13	-0.15	23,31,33,35	0
3	EMO	A	303	20/20	0.16	-0.30	48,49,54,58	0
3	EMO	A	302	20/20	0.14	-0.55	41,45,47,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.