



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:33 PM GMT

PDB ID : 4Y5X  
Title : Diabody 305 complex with EpoR  
Authors : Moraga, I.; Guo, F.; Ozkan, E.; Jude, K.M.; Garcia, K.C.  
Deposited on : 2015-02-12  
Resolution : 3.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

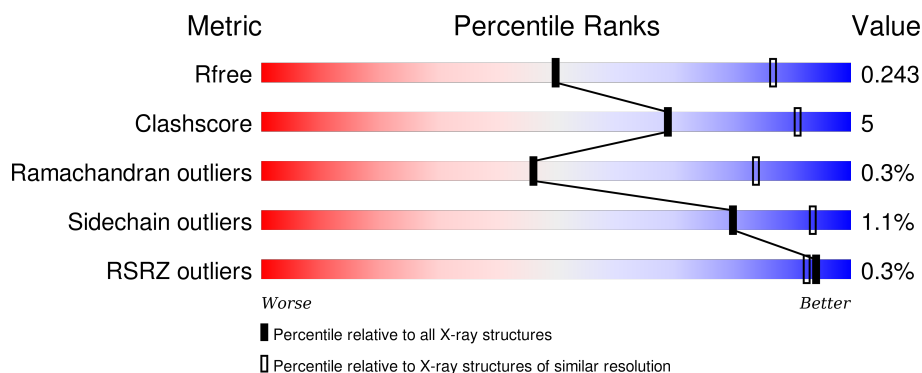
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	136	<div> <div></div> <div>79%12%9%</div> </div>
1	D	136	<div> <div>%</div> <div>76%15%9%</div> </div>
1	G	136	<div> <div></div> <div>76%15%9%</div> </div>
1	J	136	<div> <div></div> <div>82%10%9%</div> </div>
2	B	116	<div> <div>%</div> <div>84%10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	116	
2	H	116	
2	K	116	
3	C	229	
3	F	229	
3	I	229	
3	L	229	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	A	201	-	-	-	X
4	PEG	B	202	-	-	-	X
4	PEG	B	203	-	-	-	X
4	PEG	J	201	-	-	-	X
4	PEG	K	201	-	-	-	X
4	PEG	L	301	-	-	-	X
5	FLC	K	202	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13334 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 diabody 310 VL domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			925	580	157	184	4			
1	D	124	Total	C	N	O	S	0	0	0
			913	573	154	182	4			
1	G	124	Total	C	N	O	S	0	0	0
			913	572	154	183	4			
1	J	124	Total	C	N	O	S	0	0	0
			925	580	157	184	4			

- Molecule 2 is a protein called diabody 310 VH domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	111	Total	C	N	O	S	0	0	0
			809	504	132	171	2			
2	E	111	Total	C	N	O	S	0	0	0
			813	507	133	171	2			
2	H	109	Total	C	N	O	S	0	0	0
			780	490	128	160	2			
2	K	111	Total	C	N	O	S	0	0	0
			812	507	133	170	2			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	GLY	ARG	conflict	UNP Q5NV67
B	21	ALA	SER	conflict	UNP Q5NV67
B	35	SER	ASN	conflict	UNP Q5NV67
B	46	THR	LYS	conflict	UNP Q5NV67
B	53	ASN	ASP	conflict	UNP Q5NV67
B	98	ASP	-	expression tag	UNP Q5NV67
B	99	TRP	-	expression tag	UNP Q5NV67
B	100	VAL	-	expression tag	UNP Q5NV67

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Chain	Residue	Modelled	Actual	Comment	Reference
B	101	PHE	-	expression tag	UNP Q5NV67
B	102	GLY	-	expression tag	UNP Q5NV67
B	103	GLY	-	expression tag	UNP Q5NV67
B	104	GLY	-	expression tag	UNP Q5NV67
B	105	THR	-	expression tag	UNP Q5NV67
B	106	LYS	-	expression tag	UNP Q5NV67
B	107	VAL	-	expression tag	UNP Q5NV67
B	108	THR	-	expression tag	UNP Q5NV67
B	109	VAL	-	expression tag	UNP Q5NV67
B	110	LEU	-	expression tag	UNP Q5NV67
B	111	ALA	-	expression tag	UNP Q5NV67
B	112	ALA	-	expression tag	UNP Q5NV67
B	113	ALA	-	expression tag	UNP Q5NV67
B	114	GLY	-	expression tag	UNP Q5NV67
B	115	GLY	-	expression tag	UNP Q5NV67
B	116	GLY	-	expression tag	UNP Q5NV67
E	15	GLY	ARG	conflict	UNP Q5NV67
E	21	ALA	SER	conflict	UNP Q5NV67
E	35	SER	ASN	conflict	UNP Q5NV67
E	46	THR	LYS	conflict	UNP Q5NV67
E	53	ASN	ASP	conflict	UNP Q5NV67
E	98	ASP	-	expression tag	UNP Q5NV67
E	99	TRP	-	expression tag	UNP Q5NV67
E	100	VAL	-	expression tag	UNP Q5NV67
E	101	PHE	-	expression tag	UNP Q5NV67
E	102	GLY	-	expression tag	UNP Q5NV67
E	103	GLY	-	expression tag	UNP Q5NV67
E	104	GLY	-	expression tag	UNP Q5NV67
E	105	THR	-	expression tag	UNP Q5NV67
E	106	LYS	-	expression tag	UNP Q5NV67
E	107	VAL	-	expression tag	UNP Q5NV67
E	108	THR	-	expression tag	UNP Q5NV67
E	109	VAL	-	expression tag	UNP Q5NV67
E	110	LEU	-	expression tag	UNP Q5NV67
E	111	ALA	-	expression tag	UNP Q5NV67
E	112	ALA	-	expression tag	UNP Q5NV67
E	113	ALA	-	expression tag	UNP Q5NV67
E	114	GLY	-	expression tag	UNP Q5NV67
E	115	GLY	-	expression tag	UNP Q5NV67
E	116	GLY	-	expression tag	UNP Q5NV67
H	15	GLY	ARG	conflict	UNP Q5NV67
H	21	ALA	SER	conflict	UNP Q5NV67

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Chain	Residue	Modelled	Actual	Comment	Reference
H	35	SER	ASN	conflict	UNP Q5NV67
H	46	THR	LYS	conflict	UNP Q5NV67
H	53	ASN	ASP	conflict	UNP Q5NV67
H	98	ASP	-	expression tag	UNP Q5NV67
H	99	TRP	-	expression tag	UNP Q5NV67
H	100	VAL	-	expression tag	UNP Q5NV67
H	101	PHE	-	expression tag	UNP Q5NV67
H	102	GLY	-	expression tag	UNP Q5NV67
H	103	GLY	-	expression tag	UNP Q5NV67
H	104	GLY	-	expression tag	UNP Q5NV67
H	105	THR	-	expression tag	UNP Q5NV67
H	106	LYS	-	expression tag	UNP Q5NV67
H	107	VAL	-	expression tag	UNP Q5NV67
H	108	THR	-	expression tag	UNP Q5NV67
H	109	VAL	-	expression tag	UNP Q5NV67
H	110	LEU	-	expression tag	UNP Q5NV67
H	111	ALA	-	expression tag	UNP Q5NV67
H	112	ALA	-	expression tag	UNP Q5NV67
H	113	ALA	-	expression tag	UNP Q5NV67
H	114	GLY	-	expression tag	UNP Q5NV67
H	115	GLY	-	expression tag	UNP Q5NV67
H	116	GLY	-	expression tag	UNP Q5NV67
K	15	GLY	ARG	conflict	UNP Q5NV67
K	21	ALA	SER	conflict	UNP Q5NV67
K	35	SER	ASN	conflict	UNP Q5NV67
K	46	THR	LYS	conflict	UNP Q5NV67
K	53	ASN	ASP	conflict	UNP Q5NV67
K	98	ASP	-	expression tag	UNP Q5NV67
K	99	TRP	-	expression tag	UNP Q5NV67
K	100	VAL	-	expression tag	UNP Q5NV67
K	101	PHE	-	expression tag	UNP Q5NV67
K	102	GLY	-	expression tag	UNP Q5NV67
K	103	GLY	-	expression tag	UNP Q5NV67
K	104	GLY	-	expression tag	UNP Q5NV67
K	105	THR	-	expression tag	UNP Q5NV67
K	106	LYS	-	expression tag	UNP Q5NV67
K	107	VAL	-	expression tag	UNP Q5NV67
K	108	THR	-	expression tag	UNP Q5NV67
K	109	VAL	-	expression tag	UNP Q5NV67
K	110	LEU	-	expression tag	UNP Q5NV67
K	111	ALA	-	expression tag	UNP Q5NV67
K	112	ALA	-	expression tag	UNP Q5NV67

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Chain	Residue	Modelled	Actual	Comment	Reference
K	113	ALA	-	expression tag	UNP Q5NV67
K	114	GLY	-	expression tag	UNP Q5NV67
K	115	GLY	-	expression tag	UNP Q5NV67
K	116	GLY	-	expression tag	UNP Q5NV67

- Molecule 3 is a protein called Erythropoietin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	205	Total	C	N	O	S	0	0	0
			1570	1007	269	287	7			
3	F	206	Total	C	N	O	S	0	0	0
			1564	999	271	287	7			
3	I	207	Total	C	N	O	S	0	0	0
			1569	1008	268	286	7			
3	L	206	Total	C	N	O	S	0	0	0
			1581	1012	275	287	7			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	PHE	-	expression tag	UNP P19235
C	4	ALA	-	expression tag	UNP P19235
C	5	GLY	-	expression tag	UNP P19235
C	6	SER	-	expression tag	UNP P19235
C	7	ALA	-	expression tag	UNP P19235
C	52	GLN	ASN	engineered mutation	UNP P19235
C	164	GLN	ASN	engineered mutation	UNP P19235
C	226	LYS	-	expression tag	UNP P19235
C	227	GLU	-	expression tag	UNP P19235
C	228	LYS	-	expression tag	UNP P19235
C	229	ALA	-	expression tag	UNP P19235
C	230	ALA	-	expression tag	UNP P19235
C	231	ALA	-	expression tag	UNP P19235
F	3	PHE	-	expression tag	UNP P19235
F	4	ALA	-	expression tag	UNP P19235
F	5	GLY	-	expression tag	UNP P19235
F	6	SER	-	expression tag	UNP P19235
F	7	ALA	-	expression tag	UNP P19235
F	52	GLN	ASN	engineered mutation	UNP P19235
F	164	GLN	ASN	engineered mutation	UNP P19235
F	226	LYS	-	expression tag	UNP P19235
F	227	GLU	-	expression tag	UNP P19235

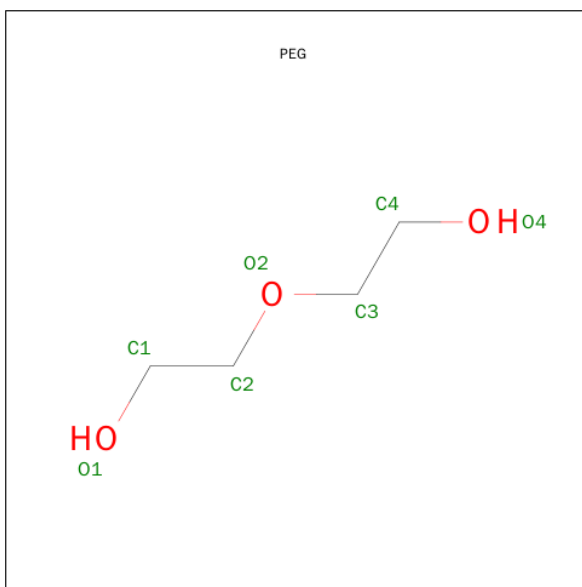
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Chain	Residue	Modelled	Actual	Comment	Reference
F	228	LYS	-	expression tag	UNP P19235
F	229	ALA	-	expression tag	UNP P19235
F	230	ALA	-	expression tag	UNP P19235
F	231	ALA	-	expression tag	UNP P19235
I	3	PHE	-	expression tag	UNP P19235
I	4	ALA	-	expression tag	UNP P19235
I	5	GLY	-	expression tag	UNP P19235
I	6	SER	-	expression tag	UNP P19235
I	7	ALA	-	expression tag	UNP P19235
I	52	GLN	ASN	engineered mutation	UNP P19235
I	164	GLN	ASN	engineered mutation	UNP P19235
I	226	LYS	-	expression tag	UNP P19235
I	227	GLU	-	expression tag	UNP P19235
I	228	LYS	-	expression tag	UNP P19235
I	229	ALA	-	expression tag	UNP P19235
I	230	ALA	-	expression tag	UNP P19235
I	231	ALA	-	expression tag	UNP P19235
L	3	PHE	-	expression tag	UNP P19235
L	4	ALA	-	expression tag	UNP P19235
L	5	GLY	-	expression tag	UNP P19235
L	6	SER	-	expression tag	UNP P19235
L	7	ALA	-	expression tag	UNP P19235
L	52	GLN	ASN	engineered mutation	UNP P19235
L	164	GLN	ASN	engineered mutation	UNP P19235
L	226	LYS	-	expression tag	UNP P19235
L	227	GLU	-	expression tag	UNP P19235
L	228	LYS	-	expression tag	UNP P19235
L	229	ALA	-	expression tag	UNP P19235
L	230	ALA	-	expression tag	UNP P19235
L	231	ALA	-	expression tag	UNP P19235

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).





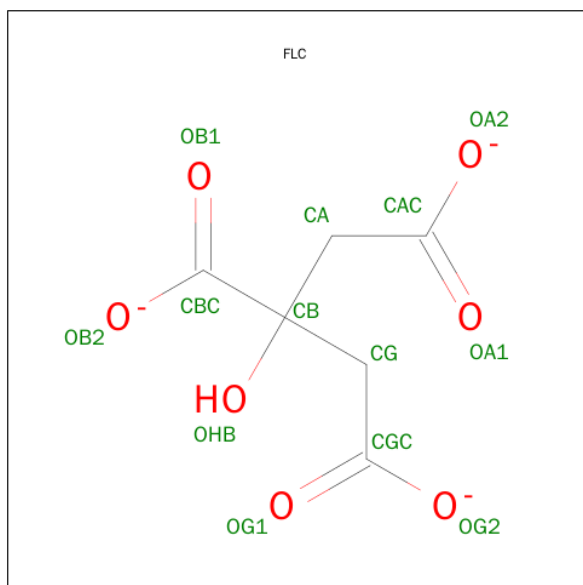
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	H	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	K	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			7	4	3		
4	L	1	Total	C	O	0	0
			7	4	3		
4	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7^-$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	C	3	Total	O	0	0
			3	3		
6	D	2	Total	O	0	0
			2	2		
6	E	5	Total	O	0	0
			5	5		
6	F	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	3	Total 3	O 3	0	0
6	H	1	Total 1	O 1	0	0
6	I	1	Total 1	O 1	0	0
6	J	4	Total 4	O 4	0	0
6	K	1	Total 1	O 1	0	0
6	L	5	Total 5	O 5	0	0

### 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: diabody 310 VL domain

Chain A: 



- Molecule 1: diabody 310 VL domain

Chain D: 




- Molecule 1: diabody 310 VL domain

Chain G: 




- Molecule 1: diabody 310 VL domain

Chain J: 



- Molecule 2: diabody 310 VH domain

Chain B: 

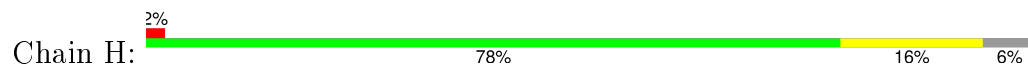


- Molecule 2: diabody 310 VH domain

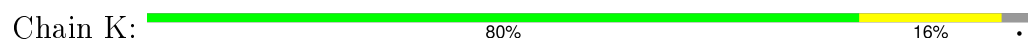
Chain E: 



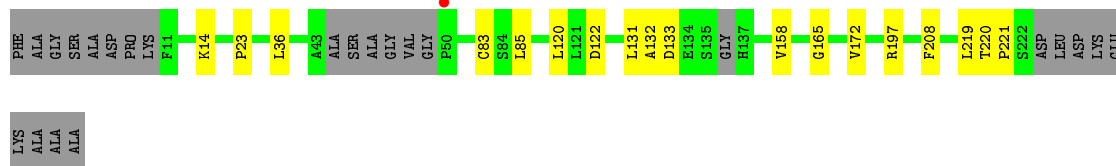
- Molecule 2: diabody 310 VH domain



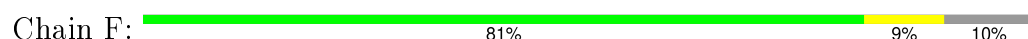
- Molecule 2: diabody 310 VH domain



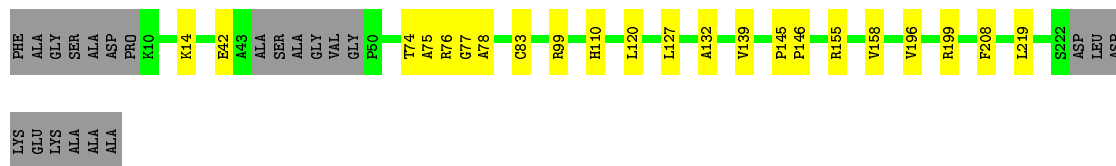
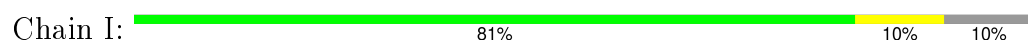
- Molecule 3: Erythropoietin receptor



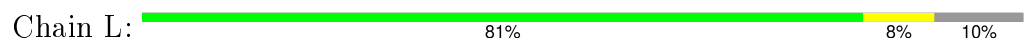
- Molecule 3: Erythropoietin receptor

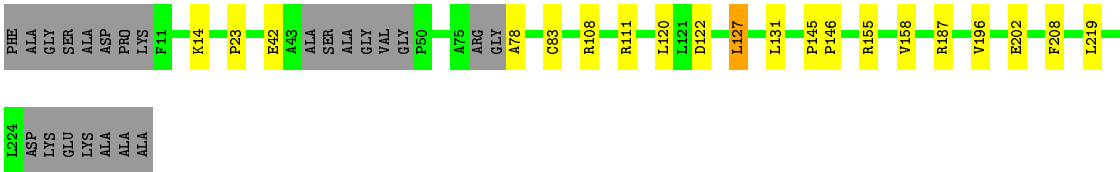


- Molecule 3: Erythropoietin receptor



- Molecule 3: Erythropoietin receptor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.54Å 239.54Å 132.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.94 – 3.15 24.94 – 3.15	Depositor EDS
% Data completeness (in resolution range)	94.8 (24.94-3.15) 94.9 (24.94-3.15)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 3.17Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, $R_{free}$	0.201 , 0.241 0.208 , 0.243	Depositor DCC
$R_{free}$ test set	4000 reflections (6.74%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.5	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 63357 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13334	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.42% 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

### 5.1 Standard geometry

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

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	0.24	0/944	0.38	0/1277
1	D	0.23	0/932	0.39	0/1263
1	G	0.22	0/932	0.36	0/1264
1	J	0.25	0/944	0.38	0/1277
2	B	0.22	0/827	0.40	0/1133
2	E	0.23	0/831	0.38	0/1137
2	H	0.21	0/798	0.38	0/1096
2	K	0.25	0/830	0.41	0/1136
3	C	0.22	0/1613	0.39	0/2204
3	F	0.22	0/1607	0.40	0/2196
3	I	0.22	0/1613	0.40	0/2204
3	L	0.23	0/1624	0.40	0/2217
All	All	0.23	0/13495	0.39	0/18404

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	925	0	888	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	913	0	865	13	0
1	G	913	0	860	13	0
1	J	925	0	888	7	0
2	B	809	0	755	8	0
2	E	813	0	766	9	0
2	H	780	0	710	11	0
2	K	812	0	763	13	0
3	C	1570	0	1508	8	0
3	F	1564	0	1479	11	0
3	I	1569	0	1495	11	0
3	L	1581	0	1519	10	0
4	A	7	0	9	0	0
4	B	21	0	27	1	0
4	C	21	0	27	0	0
4	E	7	0	9	2	0
4	F	7	0	9	0	0
4	G	14	0	18	0	0
4	H	7	0	9	1	0
4	J	7	0	9	0	0
4	K	7	0	9	0	0
4	L	21	0	27	0	0
5	K	13	0	5	0	0
6	A	1	0	0	0	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
6	E	5	0	0	0	0
6	F	2	0	0	0	0
6	G	3	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	4	0	0	0	0
6	K	1	0	0	0	0
6	L	5	0	0	0	0
All	All	13334	0	12654	120	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 5.

The worst 5 of 120 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:K:28:ASN:ND2	2:K:93:ASP:OD2	2.16	0.76
2:B:29:ILE:O	2:B:67:LYS:NZ	2.20	0.74
1:A:39:GLN:HB3	1:A:45:LEU:HD23	1.74	0.68
1:J:9:GLY:HA2	1:J:18:LEU:HD13	1.77	0.65
1:D:9:GLY:HA2	1:D:18:LEU:HD13	1.79	0.65

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	122/136 (90%)	117 (96%)	5 (4%)	0	100	100
1	D	122/136 (90%)	116 (95%)	6 (5%)	0	100	100
1	G	122/136 (90%)	117 (96%)	5 (4%)	0	100	100
1	J	122/136 (90%)	117 (96%)	5 (4%)	0	100	100
2	B	109/116 (94%)	100 (92%)	9 (8%)	0	100	100
2	E	109/116 (94%)	101 (93%)	8 (7%)	0	100	100
2	H	107/116 (92%)	100 (94%)	7 (6%)	0	100	100
2	K	109/116 (94%)	101 (93%)	8 (7%)	0	100	100
3	C	199/229 (87%)	188 (94%)	10 (5%)	1 (0%)	34	76
3	F	202/229 (88%)	190 (94%)	10 (5%)	2 (1%)	19	63
3	I	203/229 (89%)	192 (95%)	10 (5%)	1 (0%)	34	76
3	L	200/229 (87%)	189 (94%)	10 (5%)	1 (0%)	34	76
All	All	1726/1924 (90%)	1628 (94%)	93 (5%)	5 (0%)	46	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	75	ALA
3	F	75	ALA
3	C	23	PRO
3	F	23	PRO
3	L	23	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	97/103 (94%)	96 (99%)	1 (1%)	82	94
1	D	94/103 (91%)	94 (100%)	0	100	100
1	G	94/103 (91%)	94 (100%)	0	100	100
1	J	97/103 (94%)	97 (100%)	0	100	100
2	B	88/90 (98%)	87 (99%)	1 (1%)	80	93
2	E	89/90 (99%)	88 (99%)	1 (1%)	80	93
2	H	79/90 (88%)	79 (100%)	0	100	100
2	K	88/90 (98%)	88 (100%)	0	100	100
3	C	163/185 (88%)	160 (98%)	3 (2%)	66	89
3	F	157/185 (85%)	155 (99%)	2 (1%)	76	92
3	I	159/185 (86%)	157 (99%)	2 (1%)	76	92
3	L	163/185 (88%)	158 (97%)	5 (3%)	47	81
All	All	1368/1512 (90%)	1353 (99%)	15 (1%)	80	93

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	83	CYS
3	F	219	LEU
3	L	131	LEU
2	E	31	ASN
3	L	127	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	39	GLN
2	H	39	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

18 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	$\# Z  > 2$
4	PEG	A	201	-	6,6,6	0.58	0	5,5,5	0.27	0
4	PEG	B	201	-	6,6,6	0.57	0	5,5,5	0.29	0
4	PEG	B	202	-	6,6,6	0.58	0	5,5,5	0.28	0
4	PEG	B	203	-	6,6,6	0.58	0	5,5,5	0.29	0
4	PEG	C	301	-	6,6,6	0.58	0	5,5,5	0.28	0
4	PEG	C	302	-	6,6,6	0.59	0	5,5,5	0.22	0
4	PEG	C	303	-	6,6,6	0.59	0	5,5,5	0.26	0
4	PEG	E	201	-	6,6,6	0.58	0	5,5,5	0.30	0
4	PEG	F	301	-	6,6,6	0.58	0	5,5,5	0.29	0
4	PEG	G	201	-	6,6,6	0.58	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PEG	G	202	-	6,6,6	0.58	0	5,5,5	0.26	0
4	PEG	H	201	-	6,6,6	0.56	0	5,5,5	0.31	0
4	PEG	J	201	-	6,6,6	0.57	0	5,5,5	0.27	0
4	PEG	K	201	-	6,6,6	0.58	0	5,5,5	0.26	0
5	FLC	K	202	-	3,12,12	1.59	0	3,17,17	1.78	1 (33%)
4	PEG	L	301	-	6,6,6	0.58	0	5,5,5	0.22	0
4	PEG	L	302	-	6,6,6	0.58	0	5,5,5	0.29	0
4	PEG	L	303	-	6,6,6	0.57	0	5,5,5	0.26	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
4	PEG	A	201	-	-	0/4/4/4	0/0/0/0
4	PEG	B	201	-	-	0/4/4/4	0/0/0/0
4	PEG	B	202	-	-	0/4/4/4	0/0/0/0
4	PEG	B	203	-	-	0/4/4/4	0/0/0/0
4	PEG	C	301	-	-	0/4/4/4	0/0/0/0
4	PEG	C	302	-	-	0/4/4/4	0/0/0/0
4	PEG	C	303	-	-	0/4/4/4	0/0/0/0
4	PEG	E	201	-	-	0/4/4/4	0/0/0/0
4	PEG	F	301	-	-	0/4/4/4	0/0/0/0
4	PEG	G	201	-	-	0/4/4/4	0/0/0/0
4	PEG	G	202	-	-	0/4/4/4	0/0/0/0
4	PEG	H	201	-	-	0/4/4/4	0/0/0/0
4	PEG	J	201	-	-	0/4/4/4	0/0/0/0
4	PEG	K	201	-	-	0/4/4/4	0/0/0/0
5	FLC	K	202	-	-	0/6/16/16	0/0/0/0
4	PEG	L	301	-	-	0/4/4/4	0/0/0/0
4	PEG	L	302	-	-	0/4/4/4	0/0/0/0
4	PEG	L	303	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	202	FLC	CB-CA-CAC	-2.65	110.72	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	201	PEG	1	0
4	E	201	PEG	2	0
4	H	201	PEG	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	124/136 (91%)	-0.44	0 100 100	38, 53, 85, 119	0
1	D	124/136 (91%)	-0.19	1 (0%) 87 79	47, 68, 88, 110	0
1	G	124/136 (91%)	-0.21	0 100 100	50, 72, 102, 134	0
1	J	124/136 (91%)	-0.51	0 100 100	31, 45, 66, 95	0
2	B	111/116 (95%)	-0.32	1 (0%) 85 77	43, 69, 93, 110	0
2	E	111/116 (95%)	-0.41	0 100 100	39, 59, 81, 120	0
2	H	109/116 (93%)	-0.06	2 (1%) 71 56	62, 93, 130, 149	0
2	K	111/116 (95%)	-0.56	0 100 100	30, 49, 67, 105	0
3	C	205/229 (89%)	-0.30	1 (0%) 91 87	45, 71, 122, 143	0
3	F	206/229 (89%)	-0.38	1 (0%) 91 87	43, 68, 117, 160	0
3	I	207/229 (90%)	-0.45	0 100 100	43, 70, 107, 136	0
3	L	206/229 (89%)	-0.55	0 100 100	36, 57, 94, 120	0
All	All	1762/1924 (91%)	-0.38	6 (0%) 94 92	30, 65, 109, 160	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	11	SER	3.0
3	F	76	ARG	2.7
2	B	1	GLN	2.6
1	D	35	SER	2.6
2	H	1	GLN	2.4

### 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(Å <sup>2</sup> )	Q<0.9
4	PEG	J	201	7/7	0.76	0.44	18.28	67,80,95,97	0
4	PEG	L	301	7/7	0.84	0.47	12.62	66,81,90,97	0
4	PEG	B	203	7/7	0.77	0.51	4.64	62,71,93,95	0
4	PEG	B	202	7/7	0.78	0.35	4.31	79,99,109,114	0
4	PEG	K	201	7/7	0.88	0.32	4.02	71,78,88,92	0
5	FLC	K	202	13/13	0.83	0.30	3.46	73,96,114,122	0
4	PEG	A	201	7/7	0.85	0.47	3.12	85,94,98,107	0
4	PEG	H	201	7/7	0.83	0.26	0.98	88,101,106,120	0
4	PEG	G	202	7/7	0.78	0.32	0.67	101,110,114,119	0
4	PEG	B	201	7/7	0.85	0.24	0.67	80,82,94,99	0
4	PEG	E	201	7/7	0.89	0.19	0.47	73,84,96,100	0
4	PEG	F	301	7/7	0.87	0.20	0.02	59,84,91,95	0
4	PEG	L	302	7/7	0.89	0.54	-	83,97,112,121	0
4	PEG	C	303	7/7	0.79	0.49	-	74,82,93,98	0
4	PEG	C	301	7/7	0.87	0.48	-	71,83,89,105	0
4	PEG	C	302	7/7	0.90	0.17	-	72,75,83,86	0
4	PEG	L	303	7/7	0.75	0.48	-	73,81,93,93	0
4	PEG	G	201	7/7	0.84	0.40	-	58,80,95,103	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.