



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1X86  
Title : Crystal Structure of the DH/PH domains of Leukemia-associated RhoGEF in complex with RhoA  
Authors : Kristelly, R.; Gao, G.; Tesmer, J.J.  
Deposited on : 2004-08-17  
Resolution : 3.22 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

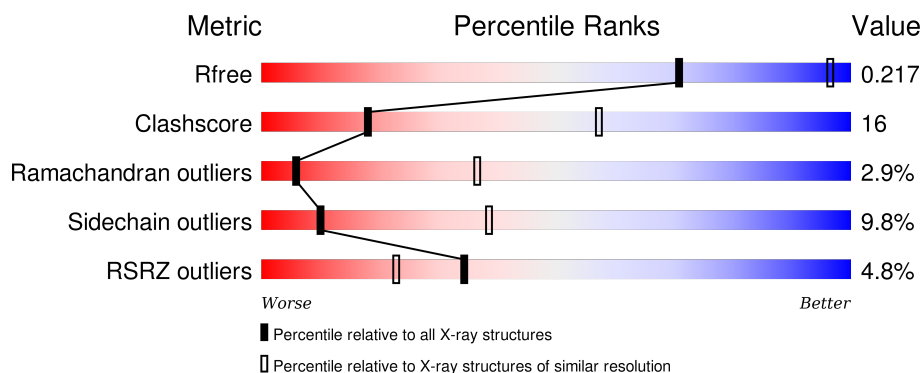
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 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	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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	385	<div> <div>52%</div> <div>35%</div> <div>7%</div> <div>6%</div> </div>
1	C	385	<div>4%</div> <div>59%</div> <div>31%</div> <div>•</div> <div>6%</div>
1	E	385	<div>7%</div> <div>48%</div> <div>33%</div> <div>6%</div> <div>•</div> <div>13%</div>
1	G	385	<div>9%</div> <div>44%</div> <div>32%</div> <div>5%</div> <div>18%</div>
2	B	196	<div>50%</div> <div>37%</div> <div>•</div> <div>•</div> <div>8%</div>

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Mol	Chain	Length	Quality of chain
2	D	196	
2	F	196	
2	H	196	

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
3	PO4	B	401	-	-	-	X
3	PO4	F	403	-	-	-	X
3	PO4	H	404	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16981 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 Rho guanine nucleotide exchange factor 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2964	1873	528	551	12			
1	C	362	Total	C	N	O	S	0	0	0
			2964	1873	528	551	12			
1	E	336	Total	C	N	O	S	0	0	0
			2767	1754	494	509	10			
1	G	314	Total	C	N	O	S	0	0	0
			2584	1643	460	471	10			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	764	GLY	THR	CLONING ARTIFACT	UNP Q9NZN5
A	765	SER	ASP	CLONING ARTIFACT	UNP Q9NZN5
A	973	PHE	TYR	ENGINEERED	UNP Q9NZN5
A	1139	VAL	-	CLONING ARTIFACT	UNP Q9NZN5
A	1140	ASP	-	CLONING ARTIFACT	UNP Q9NZN5
A	1141	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
A	1142	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
A	1143	HIS	-	EXPRESSION TAG	UNP Q9NZN5
A	1144	HIS	-	EXPRESSION TAG	UNP Q9NZN5
A	1145	HIS	-	EXPRESSION TAG	UNP Q9NZN5
A	1146	HIS	-	EXPRESSION TAG	UNP Q9NZN5
A	1147	HIS	-	EXPRESSION TAG	UNP Q9NZN5
A	1148	HIS	-	EXPRESSION TAG	UNP Q9NZN5
C	764	GLY	THR	CLONING ARTIFACT	UNP Q9NZN5
C	765	SER	ASP	CLONING ARTIFACT	UNP Q9NZN5
C	973	PHE	TYR	ENGINEERED	UNP Q9NZN5
C	1139	VAL	-	CLONING ARTIFACT	UNP Q9NZN5
C	1140	ASP	-	CLONING ARTIFACT	UNP Q9NZN5
C	1141	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
C	1142	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
C	1143	HIS	-	EXPRESSION TAG	UNP Q9NZN5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1144	HIS	-	EXPRESSION TAG	UNP Q9NZN5
C	1145	HIS	-	EXPRESSION TAG	UNP Q9NZN5
C	1146	HIS	-	EXPRESSION TAG	UNP Q9NZN5
C	1147	HIS	-	EXPRESSION TAG	UNP Q9NZN5
C	1148	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	764	GLY	THR	CLONING ARTIFACT	UNP Q9NZN5
E	765	SER	ASP	CLONING ARTIFACT	UNP Q9NZN5
E	973	PHE	TYR	ENGINEERED	UNP Q9NZN5
E	1139	VAL	-	CLONING ARTIFACT	UNP Q9NZN5
E	1140	ASP	-	CLONING ARTIFACT	UNP Q9NZN5
E	1141	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
E	1142	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
E	1143	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	1144	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	1145	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	1146	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	1147	HIS	-	EXPRESSION TAG	UNP Q9NZN5
E	1148	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	764	GLY	THR	CLONING ARTIFACT	UNP Q9NZN5
G	765	SER	ASP	CLONING ARTIFACT	UNP Q9NZN5
G	973	PHE	TYR	ENGINEERED	UNP Q9NZN5
G	1139	VAL	-	CLONING ARTIFACT	UNP Q9NZN5
G	1140	ASP	-	CLONING ARTIFACT	UNP Q9NZN5
G	1141	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
G	1142	GLY	-	CLONING ARTIFACT	UNP Q9NZN5
G	1143	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	1144	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	1145	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	1146	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	1147	HIS	-	EXPRESSION TAG	UNP Q9NZN5
G	1148	HIS	-	EXPRESSION TAG	UNP Q9NZN5

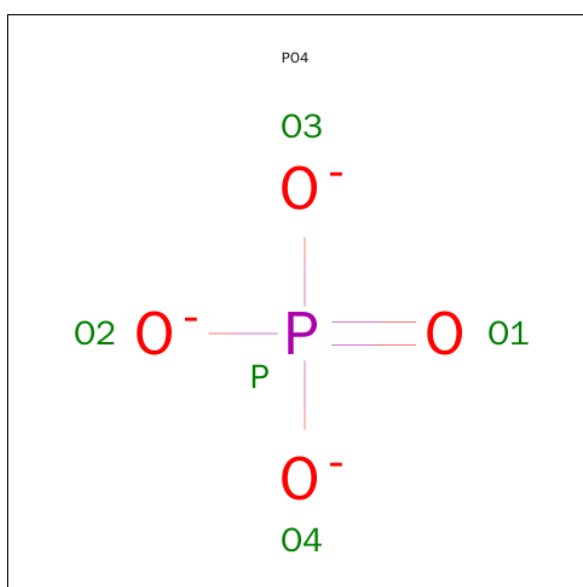
- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1423	900	241	272	10			
2	D	180	Total	C	N	O	S	0	0	0
			1423	900	241	272	10			
2	F	179	Total	C	N	O	S	0	0	0
			1418	897	240	271	10			
2	H	179	Total	C	N	O	S	0	0	0
			1418	897	240	271	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	CLONING ARTIFACT	UNP P61586
B	-1	GLU	-	CLONING ARTIFACT	UNP P61586
B	0	PHE	-	CLONING ARTIFACT	UNP P61586
D	-2	GLY	-	CLONING ARTIFACT	UNP P61586
D	-1	GLU	-	CLONING ARTIFACT	UNP P61586
D	0	PHE	-	CLONING ARTIFACT	UNP P61586
F	-2	GLY	-	CLONING ARTIFACT	UNP P61586
F	-1	GLU	-	CLONING ARTIFACT	UNP P61586
F	0	PHE	-	CLONING ARTIFACT	UNP P61586
H	-2	GLY	-	CLONING ARTIFACT	UNP P61586
H	-1	GLU	-	CLONING ARTIFACT	UNP P61586
H	0	PHE	-	CLONING ARTIFACT	UNP P61586

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

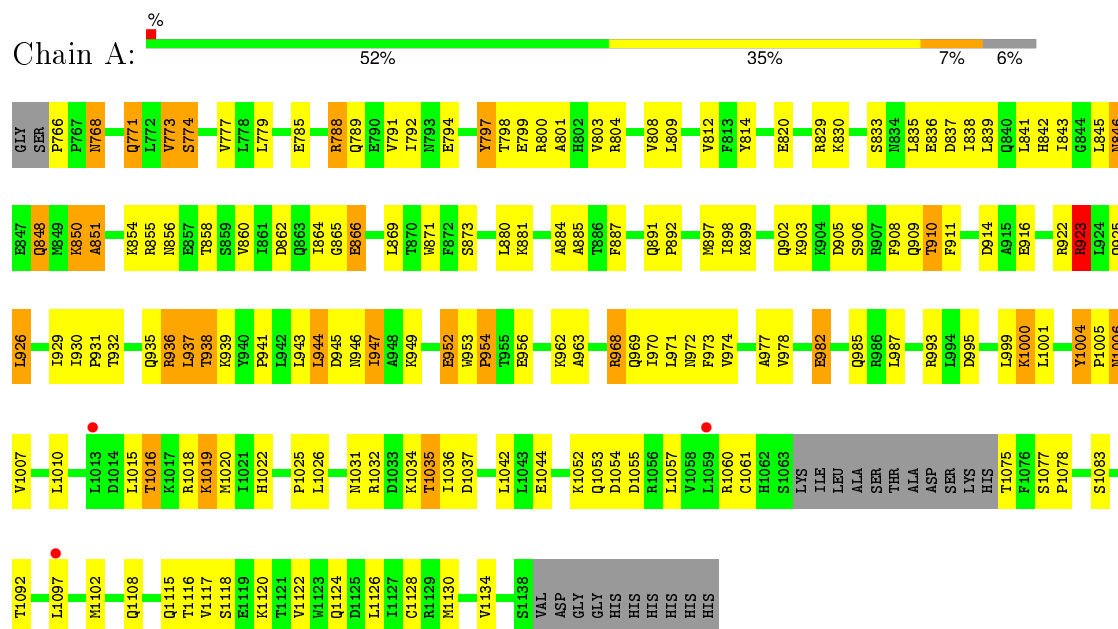


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0

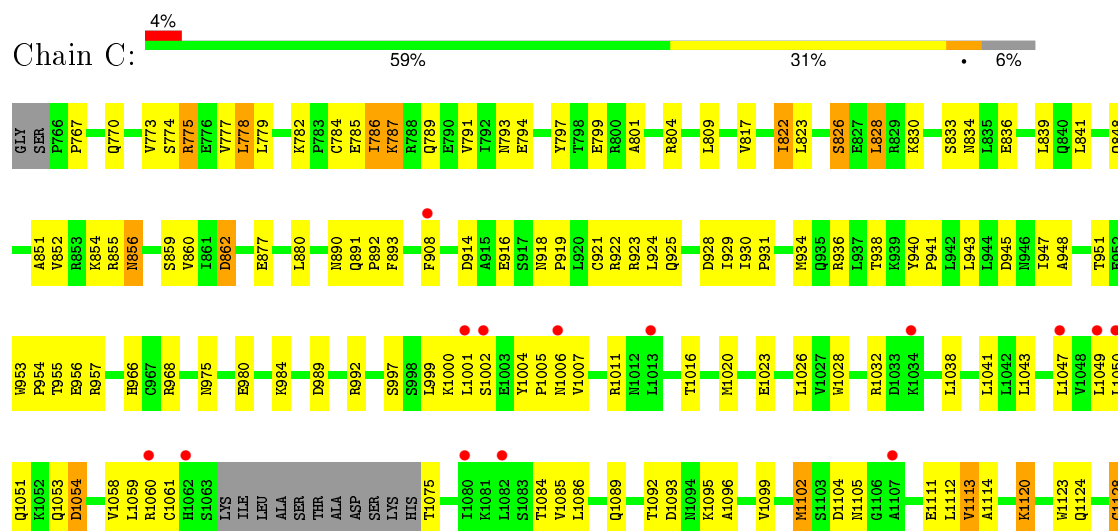
### 3 Residue-property plots [i](#)

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: Rho guanine nucleotide exchange factor 12

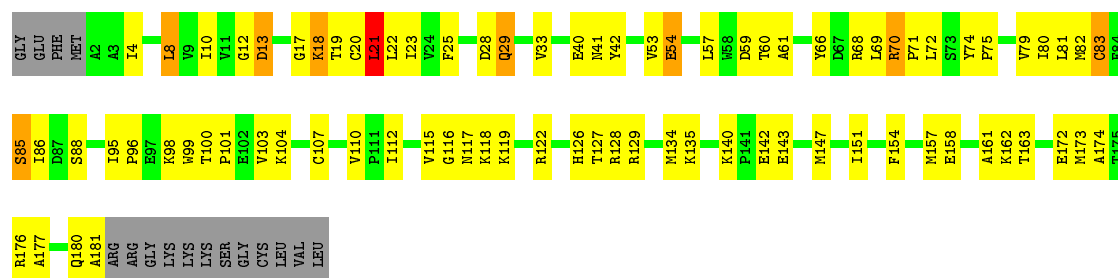


- Molecule 1: Rho guanine nucleotide exchange factor 12



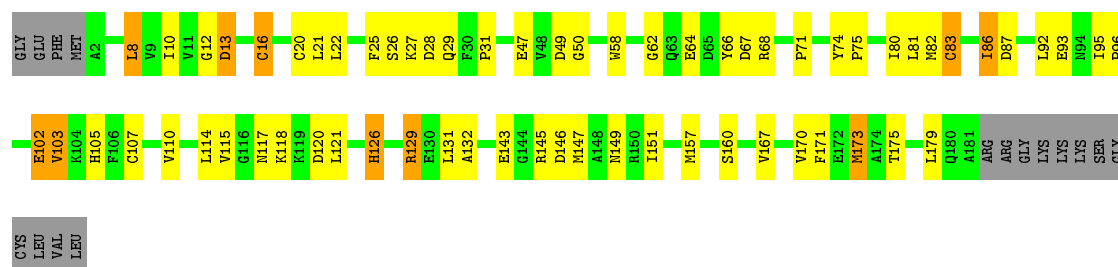






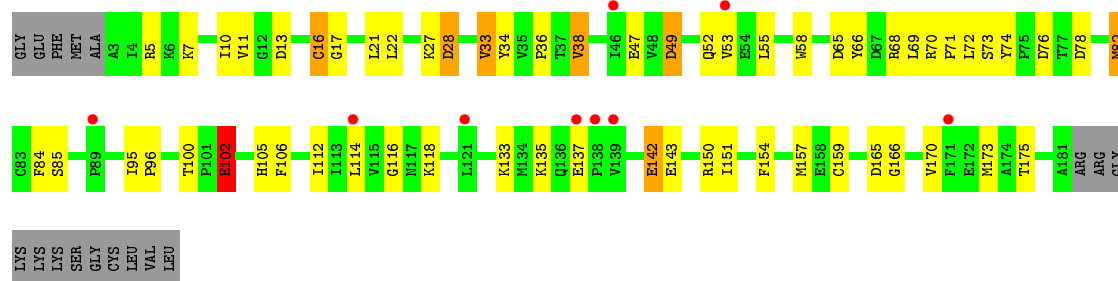
• Molecule 2: Transforming protein RhoA

Chain D: 59% 28% 5% 8%



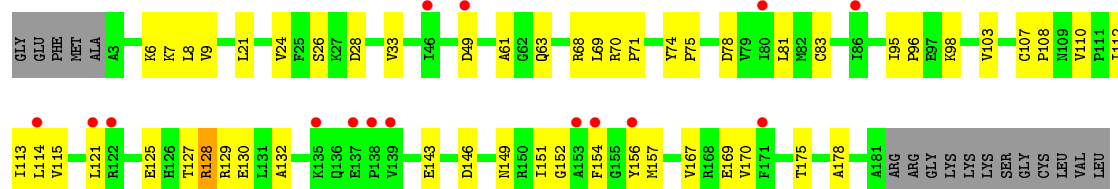
• Molecule 2: Transforming protein RhoA

Chain F: 5% 61% 27% 9%



• Molecule 2: Transforming protein RhoA

Chain H: 8% 65% 26% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	296.42Å 95.24Å 157.34Å 90.00° 94.19° 90.00°	Depositor
Resolution (Å)	15.00 – 3.22 47.00 – 3.19	Depositor EDS
% Data completeness (in resolution range)	90.4 (15.00-3.22) 88.9 (47.00-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.227 , 0.279 0.221 , 0.217	Depositor DCC
$R_{free}$ test set	3205 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.6	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 77.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 64999 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16981	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 4.12% 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: PO4

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	3/3010 (0.1%)	0.97	6/4060 (0.1%)
1	C	0.63	1/3010 (0.0%)	0.73	0/4060
1	E	0.73	3/2806 (0.1%)	0.75	0/3779
1	G	0.88	9/2622 (0.3%)	0.77	3/3532 (0.1%)
2	B	1.09	1/1451 (0.1%)	1.05	2/1963 (0.1%)
2	D	0.73	2/1451 (0.1%)	0.78	0/1963
2	F	0.67	2/1446 (0.1%)	0.71	1/1956 (0.1%)
2	H	0.47	0/1446	0.61	0/1956
All	All	0.80	21/17242 (0.1%)	0.81	12/23269 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	E	0	1
1	G	0	2
All	All	0	5

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	982	GLU	CD-OE2	19.11	1.46	1.25
1	G	980	GLU	CD-OE2	13.09	1.40	1.25
1	G	980	GLU	CD-OE1	8.76	1.35	1.25
1	G	1108	GLN	CD-NE2	8.74	1.54	1.32
2	B	83	CYS	CB-SG	-8.64	1.67	1.82

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	968	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	G	982	GLU	OE1-CD-OE2	6.60	131.22	123.30
2	F	142	GLU	OE1-CD-OE2	-6.45	115.56	123.30
1	A	809	LEU	CB-CG-CD2	-5.90	100.97	111.00
2	B	21	LEU	CA-CB-CG	5.47	127.88	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1006	ASN	Peptide
1	A	766	PRO	Peptide
1	E	766	PRO	Peptide
1	G	1038	LEU	Peptide
1	G	1108	GLN	Sidechain

## 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	2964	0	3047	87	0
1	C	2964	0	3047	78	0
1	E	2767	0	2861	104	0
1	G	2584	0	2671	101	0
2	B	1423	0	1415	69	0
2	D	1423	0	1415	47	0
2	F	1418	0	1410	35	0
2	H	1418	0	1410	38	0
3	B	5	0	0	1	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
All	All	16981	0	17276	536	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 16.

The worst 5 of 536 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:A:929:ILE:O	1:A:932:THR:HG23	1.54	1.06
1:G:975:ASN:OD1	2:H:68:ARG:HB2	1.56	1.05
2:F:10:ILE:HG21	2:F:22:LEU:HD11	1.52	0.88
1:A:848:GLN:O	1:A:851:ALA:HB3	1.75	0.85
2:D:8:LEU:HD21	2:D:81:LEU:HD12	1.62	0.81

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	358/385 (93%)	306 (86%)	40 (11%)	12 (3%)	5	31
1	C	358/385 (93%)	309 (86%)	40 (11%)	9 (2%)	7	41
1	E	326/385 (85%)	276 (85%)	41 (13%)	9 (3%)	6	38
1	G	304/385 (79%)	255 (84%)	41 (14%)	8 (3%)	7	40
2	B	178/196 (91%)	152 (85%)	24 (14%)	2 (1%)	17	62
2	D	178/196 (91%)	149 (84%)	21 (12%)	8 (4%)	3	24
2	F	177/196 (90%)	147 (83%)	24 (14%)	6 (3%)	5	31
2	H	177/196 (90%)	146 (82%)	26 (15%)	5 (3%)	6	38
All	All	2056/2324 (88%)	1740 (85%)	257 (12%)	59 (3%)	6	36

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	ASN
2	B	13	ASP
1	C	836	GLU
1	C	1001	LEU
1	C	1054	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	336/354 (95%)	284 (84%)	52 (16%)	3	15
1	C	336/354 (95%)	313 (93%)	23 (7%)	20	59
1	E	313/354 (88%)	274 (88%)	39 (12%)	6	26
1	G	290/354 (82%)	258 (89%)	32 (11%)	8	33
2	B	156/169 (92%)	145 (93%)	11 (7%)	18	57
2	D	156/169 (92%)	146 (94%)	10 (6%)	22	62
2	F	156/169 (92%)	143 (92%)	13 (8%)	14	49
2	H	156/169 (92%)	149 (96%)	7 (4%)	34	74
All	All	1899/2092 (91%)	1712 (90%)	187 (10%)	10	38

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1120	LYS
1	E	854	LYS
1	G	984	LYS
2	D	16	CYS
2	D	145	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	856	ASN
1	E	768	ASN
1	G	935	GLN
1	C	925	GLN
1	C	1012	ASN

### 5.3.3 RNA ⓘ

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](#)

4 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	$\# Z  > 2$
3	PO4	B	401	-	4,4,4	0.47	0	6,6,6	0.26	0
3	PO4	D	402	-	4,4,4	0.46	0	6,6,6	0.27	0
3	PO4	F	403	-	4,4,4	0.48	0	6,6,6	0.26	0
3	PO4	H	404	-	4,4,4	0.42	0	6,6,6	0.28	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
3	PO4	B	401	-	-	0/0/0/0	0/0/0/0
3	PO4	D	402	-	-	0/0/0/0	0/0/0/0
3	PO4	F	403	-	-	0/0/0/0	0/0/0/0
3	PO4	H	404	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	PO4	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	362/385 (94%)	-0.17	3 (0%) 87 80	15, 38, 57, 82	0
1	C	362/385 (94%)	0.05	14 (3%) 43 30	22, 42, 55, 61	0
1	E	336/385 (87%)	0.26	26 (7%) 16 10	14, 51, 67, 74	0
1	G	314/385 (81%)	0.40	33 (10%) 8 5	26, 48, 59, 63	0
2	B	180/196 (91%)	-0.34	0 100 100	15, 34, 51, 66	0
2	D	180/196 (91%)	-0.18	0 100 100	23, 43, 56, 63	0
2	F	179/196 (91%)	0.32	9 (5%) 32 21	39, 53, 62, 65	0
2	H	179/196 (91%)	0.39	15 (8%) 14 8	36, 46, 53, 55	0
All	All	2092/2324 (90%)	0.10	100 (4%) 34 23	14, 45, 60, 82	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1082	LEU	8.2
1	G	1113	VAL	6.1
1	G	1027	VAL	5.9
1	G	1114	ALA	5.6
1	G	994	LEU	5.4

### 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 ⓘ

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	PO4	B	401	5/5	0.84	0.35	3.47	169,169,169,170	0
3	PO4	F	403	5/5	0.89	0.34	3.12	124,124,125,125	0
3	PO4	H	404	5/5	0.68	0.39	2.98	123,123,123,123	0
3	PO4	D	402	5/5	0.90	0.20	0.54	135,135,135,135	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.