



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:53 AM UTC

PDB ID : 6T46 / pdb_00006t46
Title : Structure of the Rap conjugation gene regulator of the plasmid pLS20 in complex with the Phr* peptide
Authors : Crespo, I.; Bernardo, N.; Meijer, W.J.J.; Boer, D.R.
Deposited on : 2019-10-12
Resolution : 2.45 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

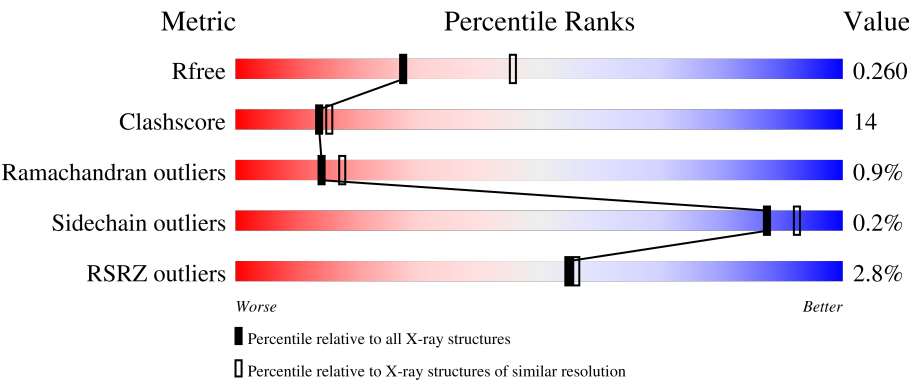
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	376	2% 72% 22% • 5%
1	C	376	% 70% 25% • •
1	E	376	6% 67% 27% • •
1	G	376	2% 67% 28% • •
2	B	44	9% 89%

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Mol	Chain	Length	Quality of chain
2	D	44	 9% • 89%
2	F	44	 9% • 89%
2	H	44	 7% 5% 89%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12274 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 Response regulator aspartate phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2998	1932	494	562	10			
1	C	363	Total	C	N	O	S	0	0	0
			3027	1951	500	566	10			
1	E	361	Total	C	N	O	S	0	0	0
			3009	1939	496	564	10			
1	G	365	Total	C	N	O	S	0	0	0
			3045	1962	503	570	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	369	LEU	-	expression tag	UNP E9RIY6
A	370	GLU	-	expression tag	UNP E9RIY6
A	371	HIS	-	expression tag	UNP E9RIY6
A	372	HIS	-	expression tag	UNP E9RIY6
A	373	HIS	-	expression tag	UNP E9RIY6
A	374	HIS	-	expression tag	UNP E9RIY6
A	375	HIS	-	expression tag	UNP E9RIY6
A	376	HIS	-	expression tag	UNP E9RIY6
C	369	LEU	-	expression tag	UNP E9RIY6
C	370	GLU	-	expression tag	UNP E9RIY6
C	371	HIS	-	expression tag	UNP E9RIY6
C	372	HIS	-	expression tag	UNP E9RIY6
C	373	HIS	-	expression tag	UNP E9RIY6
C	374	HIS	-	expression tag	UNP E9RIY6
C	375	HIS	-	expression tag	UNP E9RIY6
C	376	HIS	-	expression tag	UNP E9RIY6
E	369	LEU	-	expression tag	UNP E9RIY6
E	370	GLU	-	expression tag	UNP E9RIY6
E	371	HIS	-	expression tag	UNP E9RIY6
E	372	HIS	-	expression tag	UNP E9RIY6
E	373	HIS	-	expression tag	UNP E9RIY6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	374	HIS	-	expression tag	UNP E9RIY6
E	375	HIS	-	expression tag	UNP E9RIY6
E	376	HIS	-	expression tag	UNP E9RIY6
G	369	LEU	-	expression tag	UNP E9RIY6
G	370	GLU	-	expression tag	UNP E9RIY6
G	371	HIS	-	expression tag	UNP E9RIY6
G	372	HIS	-	expression tag	UNP E9RIY6
G	373	HIS	-	expression tag	UNP E9RIY6
G	374	HIS	-	expression tag	UNP E9RIY6
G	375	HIS	-	expression tag	UNP E9RIY6
G	376	HIS	-	expression tag	UNP E9RIY6

- Molecule 2 is a protein called Quorum-sensing secretion protein (processed).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	S	0	0	0
			43	27	7	8	1			
2	D	5	Total	C	N	O	S	0	0	0
			43	27	7	8	1			
2	F	5	Total	C	N	O	S	0	0	0
			43	27	7	8	1			
2	H	5	Total	C	N	O	S	0	0	0
			43	27	7	8	1			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Na	0	0
			1	1		

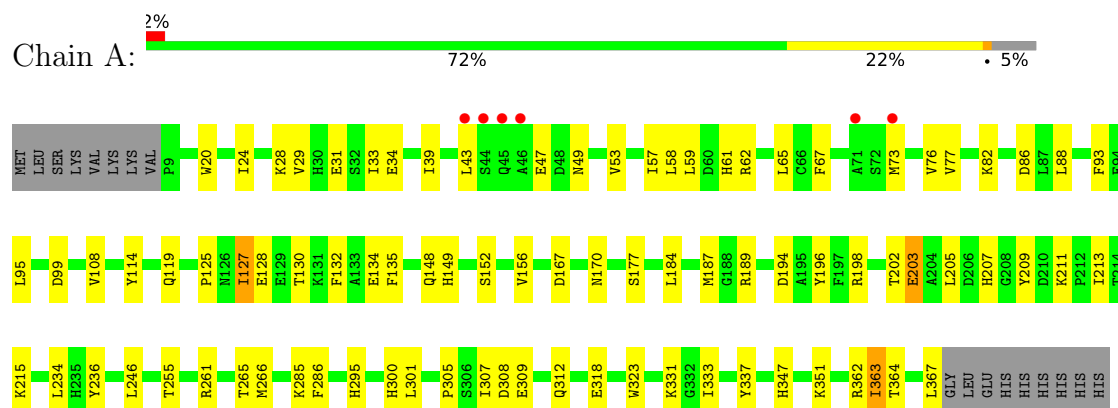
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total 11	O 11	0	0
5	B	1	Total 1	O 1	0	0
5	C	6	Total 6	O 6	0	0
5	G	1	Total 1	O 1	0	0

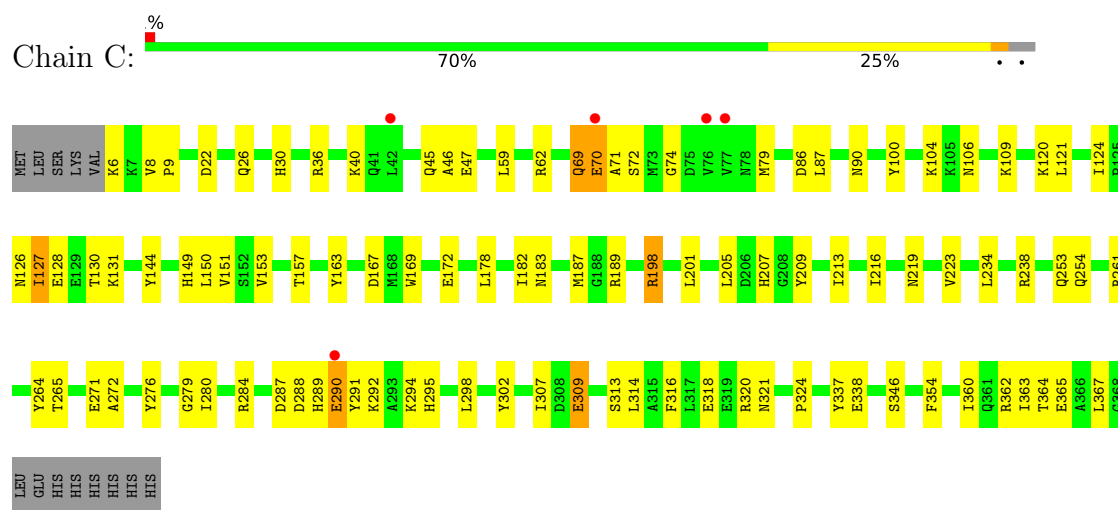
3 Residue-property plots [i](#)

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

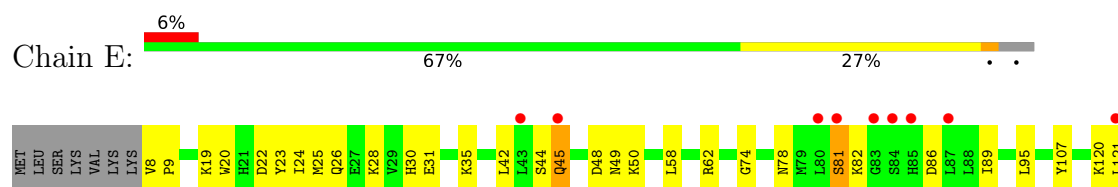
• Molecule 1: Response regulator aspartate phosphatase

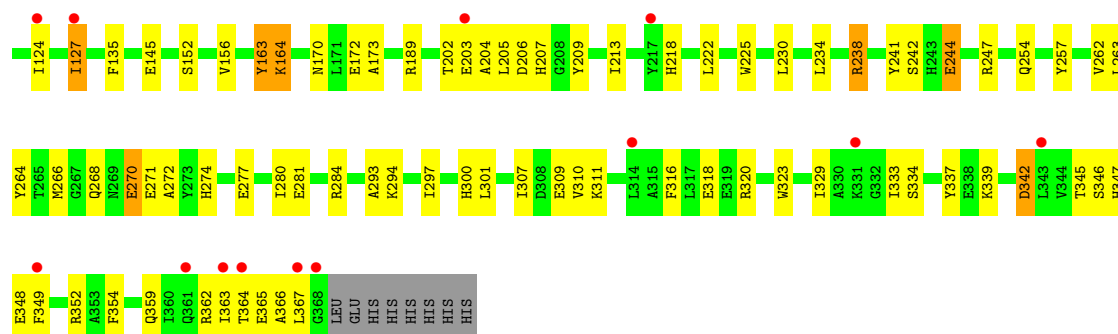


• Molecule 1: Response regulator aspartate phosphatase

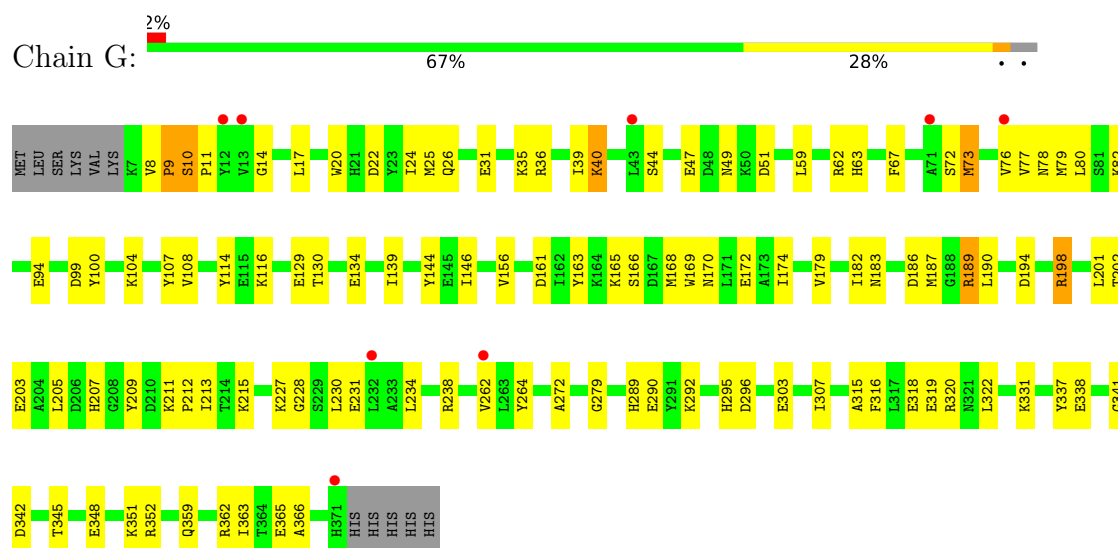


• Molecule 1: Response regulator aspartate phosphatase

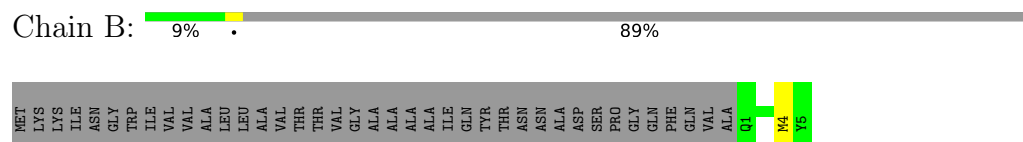




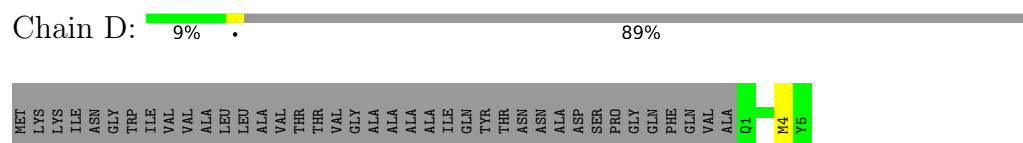
- Molecule 1: Response regulator aspartate phosphatase



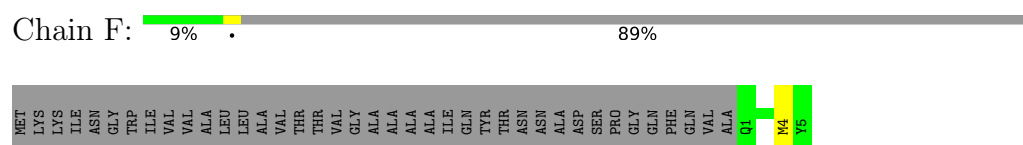
- Molecule 2: Quorum-sensing secretion protein (processed)



- Molecule 2: Quorum-sensing secretion protein (processed)



- Molecule 2: Quorum-sensing secretion protein (processed)



- Molecule 2: Quorum-sensing secretion protein (processed)

Chain H: 7% 5% 89%

MET	LYS	LYS	ILE	ILE	ASN	GLY	THR	ILE	VAL	VAL	ALA	LEU	LEU	ALA	VAL	THR	THR	VAL	GLY	ALA	ALA	ALA	ALA	ILE	ILE	GLN	TYR	THR	ASN	ASN	ALA	ASP	SER	PRO	GLY	GLN	PHE	GLN	GLN	VAL	ALA	ALA	Q1	K2	G3	M4	Y5
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.67Å 93.28Å 167.69Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	45.42 – 2.45 45.42 – 2.45	Depositor EDS
% Data completeness (in resolution range)	67.9 (45.42-2.45) 68.0 (45.42-2.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.202 , 0.262 0.203 , 0.260	Depositor DCC
R_{free} test set	2339 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12274	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/3075	0.95	15/4149 (0.4%)
1	C	0.53	0/3104	0.97	16/4187 (0.4%)
1	E	0.48	1/3086 (0.0%)	0.96	12/4165 (0.3%)
1	G	0.48	0/3123	0.87	10/4214 (0.2%)
2	B	0.42	0/43	0.61	0/53
2	D	0.41	0/43	0.72	0/53
2	F	0.36	0/43	0.59	0/53
2	H	0.40	0/43	0.69	0/53
All	All	0.50	1/12560 (0.0%)	0.94	53/16927 (0.3%)

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	C	0	2
1	E	0	1
1	G	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	164	LYS	CG-CD	5.38	1.68	1.52

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	THR	CA-C-N	-12.03	102.70	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	THR	C-N-CA	-12.03	102.70	122.54
1	E	238	ARG	CB-CG-CD	11.27	137.22	111.30
1	A	127	ILE	CA-C-N	-10.55	104.16	123.05
1	A	127	ILE	C-N-CA	-10.55	104.16	123.05

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	198	ARG	Sidechain
1	C	46	ALA	Peptide
1	E	81	SER	Peptide
1	G	72	SER	Peptide

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	2998	0	2902	89	0
1	C	3027	0	2939	82	1
1	E	3009	0	2913	102	1
1	G	3045	0	2950	95	0
2	B	43	0	44	1	0
2	D	43	0	44	1	0
2	F	43	0	44	1	0
2	H	43	0	44	3	0
3	A	1	0	0	1	0
3	C	1	0	0	1	0
3	E	1	0	0	0	0
4	C	1	0	0	0	0
5	A	11	0	0	3	1
5	B	1	0	0	0	0
5	C	6	0	0	0	1
5	G	1	0	0	1	0
All	All	12274	0	11880	350	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 350 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:28:LYS:NZ	1:A:31:GLU:CD	1.76	1.44
1:G:194:ASP:CG	1:G:198:ARG:HH21	1.30	1.37
1:A:127:ILE:HD12	1:A:127:ILE:O	1.27	1.27
1:A:28:LYS:NZ	1:A:31:GLU:OE2	1.69	1.21
1:E:62:ARG:NH1	1:E:81:SER:OG	1.73	1.20

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:GLU:OE2	1:E:30:HIS:NE2[4_645]	2.05	0.15
5:A:511:HOH:O	5:C:506:HOH:O[2_654]	2.18	0.02

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	357/376 (95%)	346 (97%)	8 (2%)	3 (1%)	16	20
1	C	361/376 (96%)	350 (97%)	8 (2%)	3 (1%)	16	20
1	E	359/376 (96%)	342 (95%)	13 (4%)	4 (1%)	11	12
1	G	363/376 (96%)	342 (94%)	18 (5%)	3 (1%)	16	20
2	B	3/44 (7%)	3 (100%)	0	0	100	100
2	D	3/44 (7%)	3 (100%)	0	0	100	100
2	F	3/44 (7%)	3 (100%)	0	0	100	100
2	H	3/44 (7%)	3 (100%)	0	0	100	100
All	All	1452/1680 (86%)	1392 (96%)	47 (3%)	13 (1%)	14	17

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	ILE
1	E	45	GLN
1	G	9	PRO
1	G	10	SER
1	C	47	GLU

5.3.2 Protein sidechains [i](#)

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	321/337 (95%)	321 (100%)	0	100	100
1	C	324/337 (96%)	322 (99%)	2 (1%)	78	86
1	E	322/337 (96%)	321 (100%)	1 (0%)	86	91
1	G	326/337 (97%)	326 (100%)	0	100	100
2	B	4/32 (12%)	4 (100%)	0	100	100
2	D	4/32 (12%)	4 (100%)	0	100	100
2	F	4/32 (12%)	4 (100%)	0	100	100
2	H	4/32 (12%)	4 (100%)	0	100	100
All	All	1309/1476 (89%)	1306 (100%)	3 (0%)	87	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	313	SER
1	C	367	LEU
1	E	342	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	78	ASN
1	E	289	HIS

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Mol	Chain	Res	Type
1	E	170	ASN
1	G	21	HIS
1	A	300	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q < 0.9
1	A	359/376 (95%)	-0.13	6 (1%) 69 71	28, 55, 98, 174	0
1	C	363/376 (96%)	-0.01	5 (1%) 73 75	28, 59, 111, 190	0
1	E	361/376 (96%)	0.35	22 (6%) 27 24	44, 80, 126, 174	0
1	G	365/376 (97%)	0.04	8 (2%) 62 64	41, 66, 111, 160	0
2	B	5/44 (11%)	-0.68	0 100 100	40, 42, 48, 53	0
2	D	5/44 (11%)	-0.34	0 100 100	36, 47, 55, 55	0
2	F	5/44 (11%)	-0.59	0 100 100	55, 61, 64, 75	0
2	H	5/44 (11%)	-0.36	0 100 100	42, 53, 59, 63	0
All	All	1468/1680 (87%)	0.06	41 (2%) 55 56	28, 64, 116, 190	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	84	SER	4.5
1	E	367	LEU	4.0
1	C	70	GLU	3.7
1	A	73	MET	3.7
1	G	262	VAL	3.6

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
4	NA	C	402	1/1	0.85	0.21	38,38,38,38	0
3	CL	E	401	1/1	0.95	0.06	71,71,71,71	0
3	CL	A	401	1/1	0.96	0.09	64,64,64,64	0
3	CL	C	401	1/1	0.97	0.08	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.