



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 4, 2017 – 12:57 PM EST

PDB ID : 5WT5  
Title : L-homocysteine-bound NifS from Helicobacter pylori  
Authors : Fujishiro, T.; Takahashi, Y.  
Deposited on : unknown  
Resolution : 1.90 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

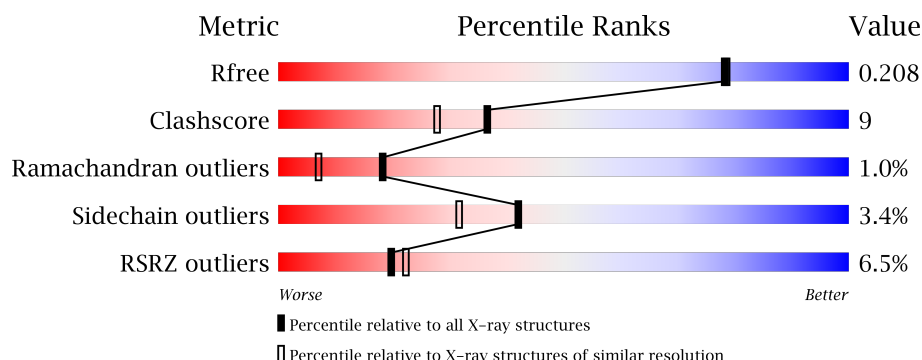
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	401	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>9%</div> </div> </div>
1	B	401	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>9%</div> </div> </div>
1	C	401	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>9%</div> </div> </div>
1	D	401	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>9%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IPA	A	501	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12116 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 Cysteine desulfurase IscS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	P	S	0	1	0
			2826	1782	494	537	1	12			
1	B	363	Total	C	N	O	P	S	0	0	0
			2822	1780	494	535	1	12			
1	C	364	Total	C	N	O	P	S	0	0	0
			2829	1783	495	538	1	12			
1	D	365	Total	C	N	O	P	S	0	0	0
			2834	1786	496	539	1	12			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP O25008
A	138	ARG	LYS	engineered mutation	UNP O25008
A	388	VAL	-	expression tag	UNP O25008
A	389	ASP	-	expression tag	UNP O25008
A	390	LEU	-	expression tag	UNP O25008
A	391	VAL	-	expression tag	UNP O25008
A	392	PRO	-	expression tag	UNP O25008
A	393	ARG	-	expression tag	UNP O25008
A	394	GLY	-	expression tag	UNP O25008
A	395	SER	-	expression tag	UNP O25008
A	396	HIS	-	expression tag	UNP O25008
A	397	HIS	-	expression tag	UNP O25008
A	398	HIS	-	expression tag	UNP O25008
A	399	HIS	-	expression tag	UNP O25008
A	400	HIS	-	expression tag	UNP O25008
A	401	HIS	-	expression tag	UNP O25008
B	2	VAL	LEU	engineered mutation	UNP O25008
B	138	ARG	LYS	engineered mutation	UNP O25008
B	388	VAL	-	expression tag	UNP O25008
B	389	ASP	-	expression tag	UNP O25008
B	390	LEU	-	expression tag	UNP O25008

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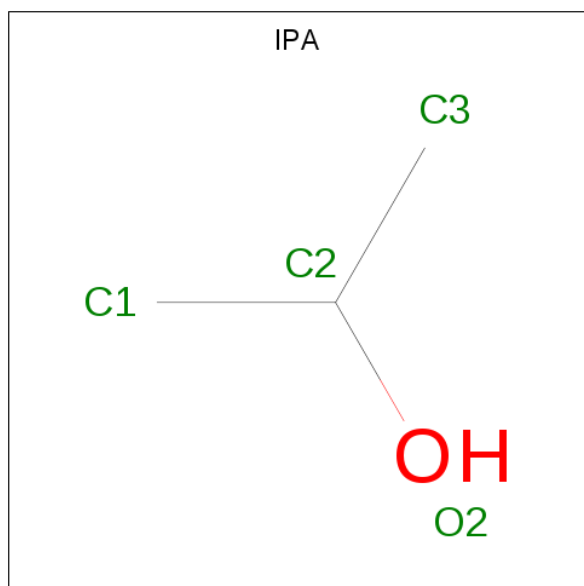
Chain	Residue	Modelled	Actual	Comment	Reference
B	391	VAL	-	expression tag	UNP O25008
B	392	PRO	-	expression tag	UNP O25008
B	393	ARG	-	expression tag	UNP O25008
B	394	GLY	-	expression tag	UNP O25008
B	395	SER	-	expression tag	UNP O25008
B	396	HIS	-	expression tag	UNP O25008
B	397	HIS	-	expression tag	UNP O25008
B	398	HIS	-	expression tag	UNP O25008
B	399	HIS	-	expression tag	UNP O25008
B	400	HIS	-	expression tag	UNP O25008
B	401	HIS	-	expression tag	UNP O25008
C	2	VAL	LEU	engineered mutation	UNP O25008
C	138	ARG	LYS	engineered mutation	UNP O25008
C	388	VAL	-	expression tag	UNP O25008
C	389	ASP	-	expression tag	UNP O25008
C	390	LEU	-	expression tag	UNP O25008
C	391	VAL	-	expression tag	UNP O25008
C	392	PRO	-	expression tag	UNP O25008
C	393	ARG	-	expression tag	UNP O25008
C	394	GLY	-	expression tag	UNP O25008
C	395	SER	-	expression tag	UNP O25008
C	396	HIS	-	expression tag	UNP O25008
C	397	HIS	-	expression tag	UNP O25008
C	398	HIS	-	expression tag	UNP O25008
C	399	HIS	-	expression tag	UNP O25008
C	400	HIS	-	expression tag	UNP O25008
C	401	HIS	-	expression tag	UNP O25008
D	2	VAL	LEU	engineered mutation	UNP O25008
D	138	ARG	LYS	engineered mutation	UNP O25008
D	388	VAL	-	expression tag	UNP O25008
D	389	ASP	-	expression tag	UNP O25008
D	390	LEU	-	expression tag	UNP O25008
D	391	VAL	-	expression tag	UNP O25008
D	392	PRO	-	expression tag	UNP O25008
D	393	ARG	-	expression tag	UNP O25008
D	394	GLY	-	expression tag	UNP O25008
D	395	SER	-	expression tag	UNP O25008
D	396	HIS	-	expression tag	UNP O25008
D	397	HIS	-	expression tag	UNP O25008
D	398	HIS	-	expression tag	UNP O25008
D	399	HIS	-	expression tag	UNP O25008
D	400	HIS	-	expression tag	UNP O25008

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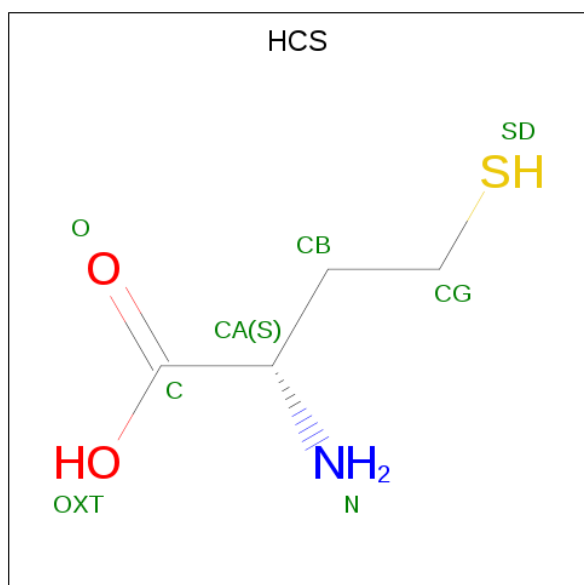
Chain	Residue	Modelled	Actual	Comment	Reference
D	401	HIS	-	expression tag	UNP O25008

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula:  $C_3H_8O$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 3 1	0	0

- Molecule 3 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (three-letter code: HCS) (formula:  $C_4H_9NO_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			8	4	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			8	4	1	2	1		
3	C	1	Total	C	N	O	S	0	0
			8	4	1	2	1		
3	D	1	Total	C	N	O	S	0	0
			8	4	1	2	1		

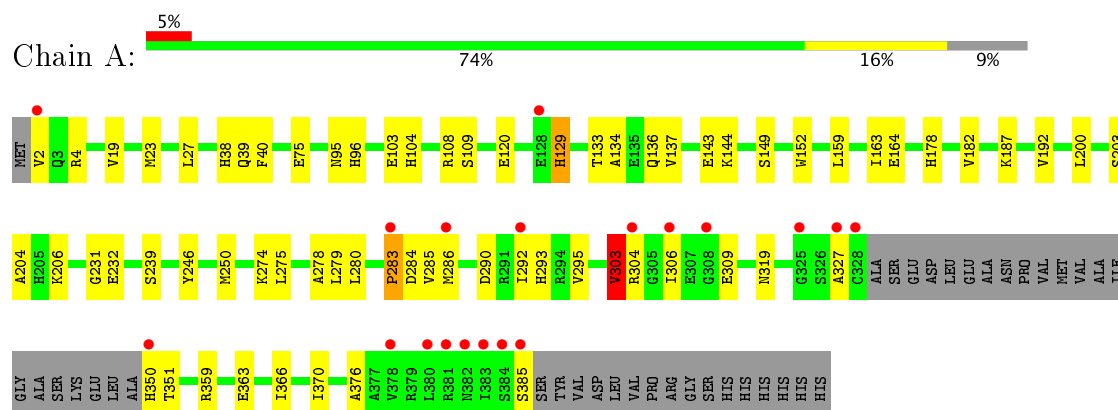
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		
4	B	175	Total	O	0	0
			175	175		
4	C	180	Total	O	0	0
			180	180		
4	D	199	Total	O	0	0
			199	199		

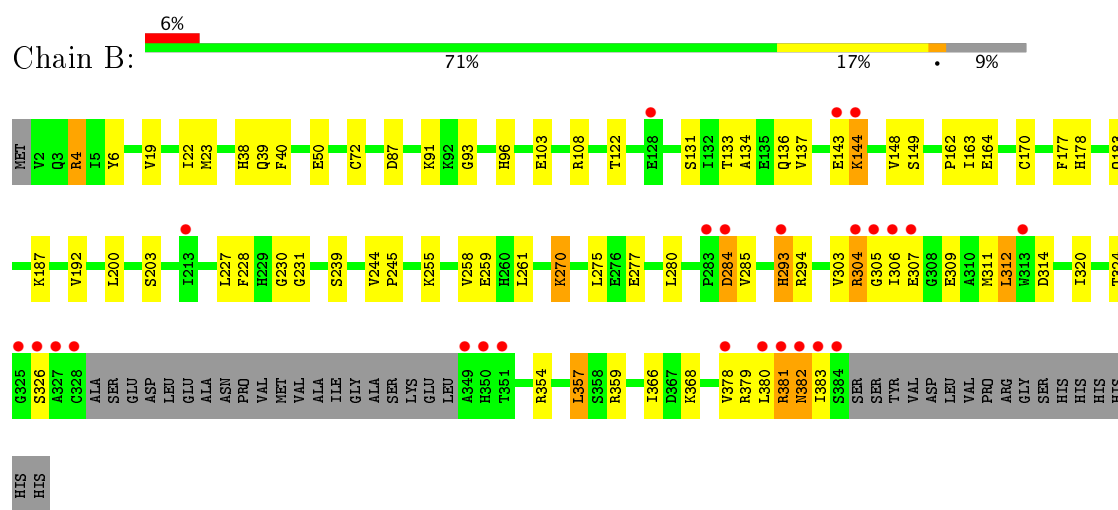
### 3 Residue-property plots

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

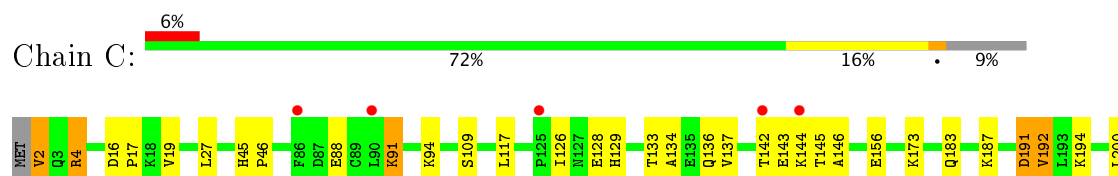
#### • Molecule 1: Cysteine desulfurase IscS



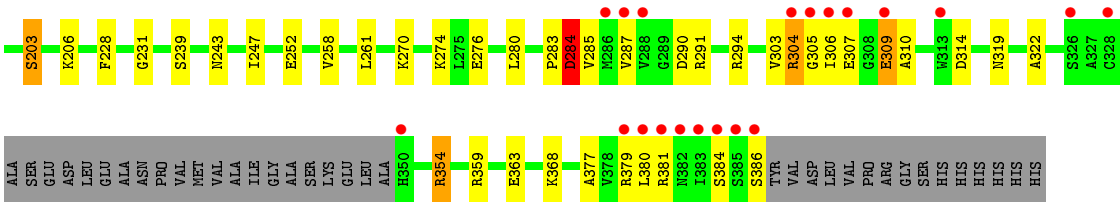
#### • Molecule 1: Cysteine desulfurase IscS



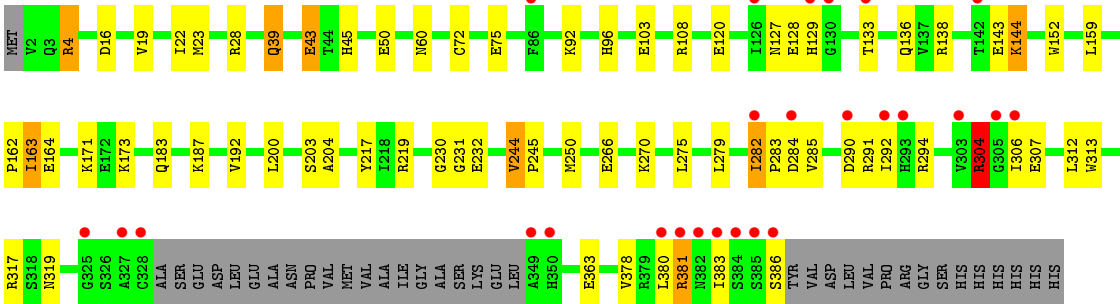
#### • Molecule 1: Cysteine desulfurase IscS







● Molecule 1: Cysteine desulfurase IscS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.44Å 102.32Å 132.05Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	47.78 – 1.90 47.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.78-1.90) 99.7 (47.78-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	23.88 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.184 , 0.209 0.182 , 0.208	Depositor DCC
$R_{free}$ test set	10777 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.146 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: HCS, LLP, IPA

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	0.93	2/2855 (0.1%)	0.97	7/3866 (0.2%)
1	B	0.92	4/2848 (0.1%)	0.97	7/3857 (0.2%)
1	C	0.94	4/2855 (0.1%)	0.98	9/3866 (0.2%)
1	D	0.86	3/2860 (0.1%)	0.92	7/3873 (0.2%)
All	All	0.91	13/11418 (0.1%)	0.96	30/15462 (0.2%)

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	1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	354	ARG	CZ-NH1	6.71	1.41	1.33
1	B	228	PHE	CD1-CE1	5.88	1.51	1.39
1	D	244	VAL	CB-CG2	5.50	1.64	1.52
1	A	75	GLU	CG-CD	5.46	1.60	1.51
1	B	228	PHE	CD2-CE2	5.46	1.50	1.39

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	359	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	B	359	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	354	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	C	359	ARG	NE-CZ-NH1	7.59	124.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	LEU	CB-CG-CD1	-7.58	98.12	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	143	GLU	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2826	0	2830	62	0
1	B	2822	0	2825	55	0
1	C	2829	0	2830	57	0
1	D	2834	0	2835	39	0
2	A	4	0	8	0	0
3	A	8	0	8	2	0
3	B	8	0	8	0	0
3	C	8	0	9	3	0
3	D	8	0	8	0	0
4	A	215	0	0	7	0
4	B	175	0	0	6	0
4	C	180	0	0	11	0
4	D	199	0	0	8	0
All	All	12116	0	11361	205	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 9.

The worst 5 of 205 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:4:ARG:HH11	1:B:39:GLN:HE22	0.96	0.92
1:B:148:VAL:HG11	1:B:170:CYS:SG	2.16	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:GLU:HG2	1:C:310:ALA:H	1.41	0.86
1:C:306:ILE:HD11	1:C:381:ARG:HG2	1.58	0.85
1:A:4:ARG:HH11	1:B:39:GLN:NE2	1.74	0.85

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	359/401 (90%)	347 (97%)	11 (3%)	1 (0%)	44	34
1	B	358/401 (89%)	346 (97%)	7 (2%)	5 (1%)	13	4
1	C	359/401 (90%)	346 (96%)	10 (3%)	3 (1%)	22	11
1	D	360/401 (90%)	347 (96%)	8 (2%)	5 (1%)	13	4
All	All	1436/1604 (90%)	1386 (96%)	36 (2%)	14 (1%)	18	7

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	PRO
1	B	304	ARG
1	C	304	ARG
1	D	163	ILE
1	D	304	ARG

### 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	306/336 (91%)	300 (98%)	6 (2%)	60	55
1	B	304/336 (90%)	292 (96%)	12 (4%)	37	26
1	C	306/336 (91%)	297 (97%)	9 (3%)	48	39
1	D	306/336 (91%)	292 (95%)	14 (5%)	31	20
All	All	1222/1344 (91%)	1181 (97%)	41 (3%)	42	32

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	VAL
1	C	173	LYS
1	D	304	ARG
1	C	91	LYS
1	C	128	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	B	39	GLN
1	B	95	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	LLP	A	206	1	24,24,25	2.93	7 (29%)	28,32,34	1.60	8 (28%)
1	LLP	B	206	1	24,24,25	2.73	6 (25%)	28,32,34	2.12	11 (39%)
1	LLP	C	206	1	24,24,25	2.95	6 (25%)	28,32,34	2.30	14 (50%)
1	LLP	D	206	1	24,24,25	3.32	10 (41%)	28,32,34	1.82	7 (25%)

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
1	LLP	A	206	1	-	0/15/17/19	0/1/1/1
1	LLP	B	206	1	-	0/15/17/19	0/1/1/1
1	LLP	C	206	1	-	0/15/17/19	0/1/1/1
1	LLP	D	206	1	-	0/15/17/19	0/1/1/1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	LLP	CB-CA	-5.33	1.46	1.53
1	A	206	LLP	CA-C	-3.78	1.45	1.50
1	D	206	LLP	CB-CA	-3.54	1.48	1.53
1	B	206	LLP	P-OP3	-3.33	1.41	1.54
1	C	206	LLP	C4-C5	-2.57	1.38	1.42

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	LLP	OP3-P-OP4	-4.78	94.02	106.73
1	D	206	LLP	C3-C4-C5	-4.70	114.66	118.24
1	B	206	LLP	C5-C4-C4'	-4.22	115.05	121.36
1	B	206	LLP	C4-C3-C2	-3.90	117.75	120.15
1	C	206	LLP	C4-C4'-NZ	-3.71	106.64	124.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	206	LLP	1	0
1	C	206	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	IPA	A	501	-	3,3,3	0.53	0	3,3,3	0.52	0
3	HCS	A	502	-	2,7,7	1.61	1 (50%)	2,8,8	7.30	1 (50%)
3	HCS	B	501	-	2,7,7	0.61	0	2,8,8	2.91	1 (50%)
3	HCS	C	501	-	2,7,7	1.10	0	2,8,8	5.53	1 (50%)
3	HCS	D	501	-	2,7,7	0.51	0	2,8,8	1.98	1 (50%)

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	IPA	A	501	-	-	0/0/0/0	0/0/0/0
3	HCS	A	502	-	-	0/3/7/7	0/0/0/0
3	HCS	B	501	-	-	0/3/7/7	0/0/0/0
3	HCS	C	501	-	-	0/3/7/7	0/0/0/0
3	HCS	D	501	-	-	0/3/7/7	0/0/0/0

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	HCS	CB-CG	-2.08	1.50	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	HCS	CB-CG-SD	-10.16	103.16	113.74
3	C	501	HCS	CB-CG-SD	-7.75	105.67	113.74
3	B	501	HCS	CB-CG-SD	-3.92	109.65	113.74
3	D	501	HCS	CB-CG-SD	-2.79	110.83	113.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	HCS	2	0
3	C	501	HCS	3	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	362/401 (90%)	0.38	19 (5%) 28 31	19, 36, 66, 97	0
1	B	362/401 (90%)	0.42	25 (6%) 18 20	21, 35, 64, 79	0
1	C	363/401 (90%)	0.46	25 (6%) 18 20	19, 37, 64, 108	0
1	D	364/401 (90%)	0.52	26 (7%) 17 19	21, 39, 64, 81	0
All	All	1451/1604 (90%)	0.44	95 (6%) 20 22	19, 37, 65, 108	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	386	SER	8.9
1	D	384	SER	8.1
1	B	383	ILE	7.8
1	C	383	ILE	7.8
1	C	328	CYS	7.7

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

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
1	LLP	A	206	24/25	0.97	0.13	-	20,24,29,33	0
1	LLP	C	206	24/25	0.97	0.14	-	18,24,43,45	0
1	LLP	B	206	24/25	0.98	0.13	-	20,25,34,35	0
1	LLP	D	206	24/25	0.96	0.16	-	21,26,34,41	0

### 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( $\text{\AA}^2$ )	Q<0.9
2	IPA	A	501	4/4	0.82	0.23	6.37	60,64,65,67	0
3	HCS	B	501	8/8	0.93	0.15	1.49	37,43,48,50	0
3	HCS	C	501	8/8	0.82	0.13	0.77	44,46,51,54	0
3	HCS	A	502	8/8	0.84	0.13	0.29	44,48,50,55	0
3	HCS	D	501	8/8	0.89	0.11	-0.37	49,53,56,59	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.