



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2022 – 07:08 pm BST

PDB ID : 7Z8N  
Title : GacS histidine kinase from *Pseudomonas aeruginosa*  
Authors : Fadel, F.; Bassim, V.; Francis, V.I.; Porter, S.L.; Botzanowski, T.; Legrand, P.; Bourne, Y.; Cianferani, S.; Vincent, F.  
Deposited on : 2022-03-17  
Resolution : 2.64 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

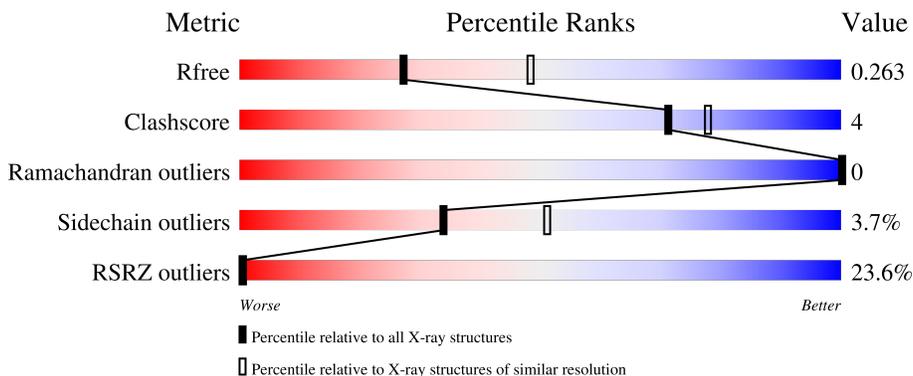
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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))
$R_{free}$	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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  $\geq 3$ , 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	317	 20% 80% 12% 8%
1	B	317	 9% 83% 8% 8%
1	C	317	 34% 81% 9% 8%
1	D	317	 22% 82% 9% 8%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9296 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 Histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	292	2269	1409	392	461	7	0	2	0
1	B	292	2299	1429	396	467	7	0	6	0
1	C	292	2269	1408	393	462	6	0	2	0
1	D	292	2263	1404	392	461	6	0	1	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	MSE	-	initiating methionine	UNP G3XD98
A	197	GLY	-	expression tag	UNP G3XD98
A	198	HIS	-	expression tag	UNP G3XD98
A	199	HIS	-	expression tag	UNP G3XD98
A	200	HIS	-	expression tag	UNP G3XD98
A	201	HIS	-	expression tag	UNP G3XD98
A	202	HIS	-	expression tag	UNP G3XD98
A	203	HIS	-	expression tag	UNP G3XD98
A	204	SER	-	expression tag	UNP G3XD98
A	205	SER	-	expression tag	UNP G3XD98
A	206	GLY	-	expression tag	UNP G3XD98
A	207	VAL	-	expression tag	UNP G3XD98
A	208	ASP	-	expression tag	UNP G3XD98
A	209	LEU	-	expression tag	UNP G3XD98
A	210	GLY	-	expression tag	UNP G3XD98
A	211	THR	-	expression tag	UNP G3XD98
A	212	GLU	-	expression tag	UNP G3XD98
A	213	ASN	-	expression tag	UNP G3XD98
A	214	LEU	-	expression tag	UNP G3XD98
A	215	TYR	-	expression tag	UNP G3XD98
A	216	PHE	-	expression tag	UNP G3XD98

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Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLN	-	expression tag	UNP G3XD98
A	218	SER	-	expression tag	UNP G3XD98
A	219	MSE	-	expression tag	UNP G3XD98
B	196	MSE	-	initiating methionine	UNP G3XD98
B	197	GLY	-	expression tag	UNP G3XD98
B	198	HIS	-	expression tag	UNP G3XD98
B	199	HIS	-	expression tag	UNP G3XD98
B	200	HIS	-	expression tag	UNP G3XD98
B	201	HIS	-	expression tag	UNP G3XD98
B	202	HIS	-	expression tag	UNP G3XD98
B	203	HIS	-	expression tag	UNP G3XD98
B	204	SER	-	expression tag	UNP G3XD98
B	205	SER	-	expression tag	UNP G3XD98
B	206	GLY	-	expression tag	UNP G3XD98
B	207	VAL	-	expression tag	UNP G3XD98
B	208	ASP	-	expression tag	UNP G3XD98
B	209	LEU	-	expression tag	UNP G3XD98
B	210	GLY	-	expression tag	UNP G3XD98
B	211	THR	-	expression tag	UNP G3XD98
B	212	GLU	-	expression tag	UNP G3XD98
B	213	ASN	-	expression tag	UNP G3XD98
B	214	LEU	-	expression tag	UNP G3XD98
B	215	TYR	-	expression tag	UNP G3XD98
B	216	PHE	-	expression tag	UNP G3XD98
B	217	GLN	-	expression tag	UNP G3XD98
B	218	SER	-	expression tag	UNP G3XD98
B	219	MSE	-	expression tag	UNP G3XD98
C	196	MSE	-	initiating methionine	UNP G3XD98
C	197	GLY	-	expression tag	UNP G3XD98
C	198	HIS	-	expression tag	UNP G3XD98
C	199	HIS	-	expression tag	UNP G3XD98
C	200	HIS	-	expression tag	UNP G3XD98
C	201	HIS	-	expression tag	UNP G3XD98
C	202	HIS	-	expression tag	UNP G3XD98
C	203	HIS	-	expression tag	UNP G3XD98
C	204	SER	-	expression tag	UNP G3XD98
C	205	SER	-	expression tag	UNP G3XD98
C	206	GLY	-	expression tag	UNP G3XD98
C	207	VAL	-	expression tag	UNP G3XD98
C	208	ASP	-	expression tag	UNP G3XD98
C	209	LEU	-	expression tag	UNP G3XD98
C	210	GLY	-	expression tag	UNP G3XD98

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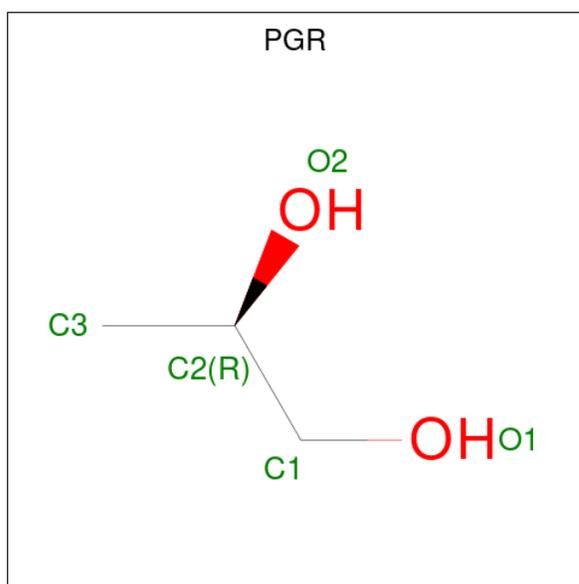
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Chain	Residue	Modelled	Actual	Comment	Reference
C	211	THR	-	expression tag	UNP G3XD98
C	212	GLU	-	expression tag	UNP G3XD98
C	213	ASN	-	expression tag	UNP G3XD98
C	214	LEU	-	expression tag	UNP G3XD98
C	215	TYR	-	expression tag	UNP G3XD98
C	216	PHE	-	expression tag	UNP G3XD98
C	217	GLN	-	expression tag	UNP G3XD98
C	218	SER	-	expression tag	UNP G3XD98
C	219	MSE	-	expression tag	UNP G3XD98
D	196	MSE	-	initiating methionine	UNP G3XD98
D	197	GLY	-	expression tag	UNP G3XD98
D	198	HIS	-	expression tag	UNP G3XD98
D	199	HIS	-	expression tag	UNP G3XD98
D	200	HIS	-	expression tag	UNP G3XD98
D	201	HIS	-	expression tag	UNP G3XD98
D	202	HIS	-	expression tag	UNP G3XD98
D	203	HIS	-	expression tag	UNP G3XD98
D	204	SER	-	expression tag	UNP G3XD98
D	205	SER	-	expression tag	UNP G3XD98
D	206	GLY	-	expression tag	UNP G3XD98
D	207	VAL	-	expression tag	UNP G3XD98
D	208	ASP	-	expression tag	UNP G3XD98
D	209	LEU	-	expression tag	UNP G3XD98
D	210	GLY	-	expression tag	UNP G3XD98
D	211	THR	-	expression tag	UNP G3XD98
D	212	GLU	-	expression tag	UNP G3XD98
D	213	ASN	-	expression tag	UNP G3XD98
D	214	LEU	-	expression tag	UNP G3XD98
D	215	TYR	-	expression tag	UNP G3XD98
D	216	PHE	-	expression tag	UNP G3XD98
D	217	GLN	-	expression tag	UNP G3XD98
D	218	SER	-	expression tag	UNP G3XD98
D	219	MSE	-	expression tag	UNP G3XD98

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	2	Total Ca 2 2	0	0

- Molecule 3 is R-1,2-PROPANEDIOL (three-letter code: PGR) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0

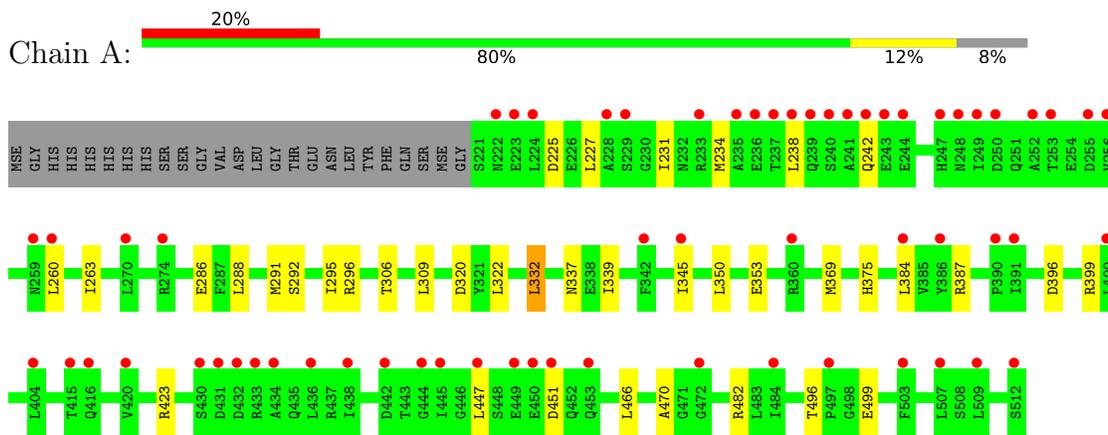
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	35	Total O 35 35	0	0
4	B	105	Total O 105 105	0	0
4	C	18	Total O 18 18	0	0
4	D	20	Total O 20 20	0	0

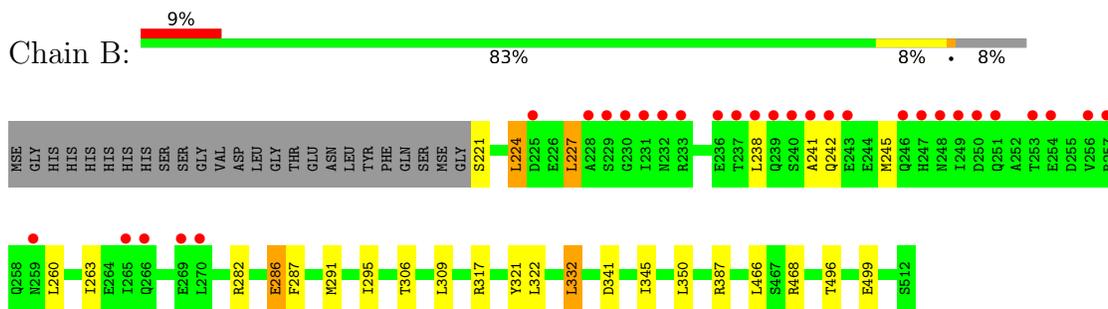
### 3 Residue-property plots [i](#)

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.

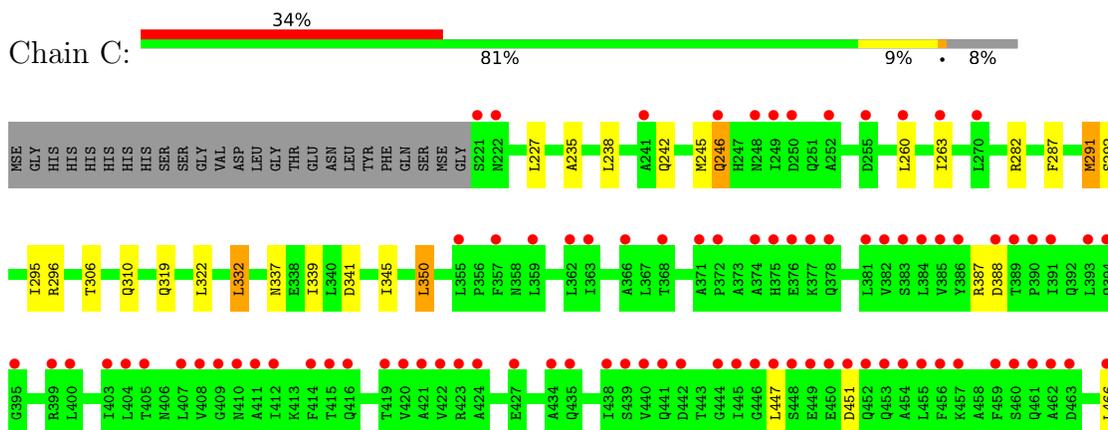
- Molecule 1: Histidine kinase

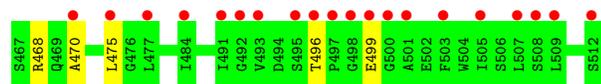


- Molecule 1: Histidine kinase

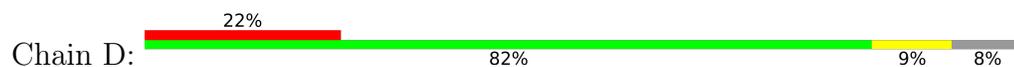


- Molecule 1: Histidine kinase





- Molecule 1: Histidine kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.71Å 76.85Å 178.65Å 90.00° 97.30° 90.00°	Depositor
Resolution (Å)	48.81 – 2.64 48.81 – 2.64	Depositor EDS
% Data completeness (in resolution range)	89.0 (48.81-2.64) 89.0 (48.81-2.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.65Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (3-FEB-2022)	Depositor
R, $R_{free}$	0.259 , 0.264 0.256 , 0.263	Depositor DCC
$R_{free}$ test set	2266 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.8	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.006 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	131.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4744e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.35	0/2291	0.50	0/3081
1	B	0.38	0/2329	0.50	0/3133
1	C	0.31	0/2291	0.47	0/3082
1	D	0.32	0/2282	0.48	0/3070
All	All	0.34	0/9193	0.49	0/12366

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 [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	2269	0	2286	26	0
1	B	2299	0	2306	22	0
1	C	2269	0	2283	23	0
1	D	2263	0	2275	20	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	B	15	0	24	0	0
4	A	35	0	0	0	0
4	B	105	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	18	0	0	0	0
4	D	20	0	0	0	0
All	All	9296	0	9174	64	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 4.

All (64) 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:B:286:GLU:HB3	1:C:470:ALA:HB1	1.50	0.92
1:C:242:GLN:HA	1:C:245:MSE:HG2	1.59	0.82
1:C:238:LEU:HD21	1:D:238:LEU:HD21	1.63	0.80
1:C:260:LEU:HA	1:C:263:ILE:HG12	1.65	0.78
1:A:260:LEU:HA	1:A:263:ILE:HG12	1.66	0.77
1:B:260:LEU:HA	1:B:263:ILE:HG12	1.66	0.76
1:D:260:LEU:HA	1:D:263:ILE:HG12	1.67	0.75
1:A:238:LEU:HD21	1:B:238:LEU:HD21	1.73	0.70
1:C:310:GLN:HE21	1:C:319[B]:GLN:HE22	1.41	0.68
1:B:287:PHE:HE2	1:C:475:LEU:HD13	1.58	0.68
1:B:287:PHE:CE2	1:C:475:LEU:HD13	2.28	0.68
1:B:221:SER:HB3	1:D:256:VAL:HG11	1.77	0.66
1:A:291[B]:MSE:SE	1:D:475:LEU:HD22	2.48	0.64
1:A:291[A]:MSE:HE2	1:D:339:ILE:HG12	1.82	0.62
1:A:234:MSE:HE3	1:B:241:ALA:HB3	1.81	0.62
1:A:291[A]:MSE:SE	1:D:291:MSE:SE	3.19	0.60
1:A:384:LEU:HD23	1:A:423:ARG:HD2	1.86	0.58
1:A:242:GLN:HE22	1:C:235:ALA:HB2	1.70	0.56
1:B:295:ILE:HG23	1:C:332:LEU:HD21	1.87	0.55
1:B:282:ARG:HH12	1:C:468:ARG:HG3	1.72	0.54
1:A:350:LEU:HD11	1:A:399:ARG:HH22	1.73	0.54
1:A:350:LEU:HD21	1:A:399:ARG:NH2	2.24	0.53
1:A:353:GLU:HG2	1:A:396:ASP:CG	2.28	0.53
1:B:224:LEU:HD11	1:D:252:ALA:HB3	1.91	0.52
1:A:295:ILE:HG23	1:D:332:LEU:HD21	1.92	0.51
1:B:282:ARG:NH2	1:B:286:GLU:OE2	2.44	0.51
1:C:238:LEU:HD22	1:D:234:MSE:HE3	1.93	0.49
1:A:496:THR:HB	1:A:499:GLU:HB3	1.94	0.49
1:C:496:THR:HB	1:C:499:GLU:HB3	1.95	0.49
1:D:496:THR:HB	1:D:499:GLU:HB3	1.95	0.49
1:A:332:LEU:HD21	1:D:295:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:THR:HG23	1:D:322:LEU:HD22	1.93	0.49
1:A:306:THR:HG23	1:A:322:LEU:HD22	1.94	0.48
1:B:496:THR:HB	1:B:499:GLU:HB3	1.94	0.48
1:C:306:THR:HG23	1:C:322:LEU:HD22	1.95	0.47
1:A:339:ILE:HD11	1:D:291:MSE:HG3	1.96	0.47
1:B:306:THR:HG23	1:B:322:LEU:HD22	1.97	0.47
1:B:468:ARG:HH12	1:C:282:ARG:NE	2.13	0.46
1:B:332:LEU:HD21	1:C:295:ILE:HG23	1.99	0.45
1:A:345:ILE:HG21	1:A:482:ARG:HB3	1.99	0.45
1:A:470:ALA:HB2	1:D:283:ILE:HG12	1.97	0.45
1:B:291:MSE:HG3	1:C:339:ILE:HD11	1.98	0.45
1:B:309:LEU:HB3	1:B:322:LEU:HD11	1.99	0.44
1:A:296:ARG:NH2	1:A:337:ASN:OD1	2.51	0.44
1:A:309:LEU:HB3	1:A:322:LEU:HD11	2.00	0.44
1:A:345:ILE:HG13	1:A:350:LEU:HD13	1.99	0.44
1:A:231:ILE:HD11	1:C:245:MSE:SE	2.68	0.43
1:D:317:ARG:NH1	1:D:321:TYR:OH	2.50	0.43
1:B:227:LEU:HD22	1:D:249:ILE:HD11	2.00	0.42
1:C:246:GLN:HE21	1:C:246:GLN:HB3	1.66	0.42
1:A:447:LEU:HD22	1:A:451:ASP:HB3	2.02	0.41
1:C:296:ARG:NH2	1:C:337:ASN:OD1	2.52	0.41
1:A:350:LEU:HD21	1:A:399:ARG:HH22	1.85	0.41
1:B:317:ARG:NH1	1:B:321:TYR:OH	2.52	0.41
1:B:345:ILE:HG13	1:B:350:LEU:HD13	2.02	0.41
1:A:288:LEU:HD22	1:D:291:MSE:HE1	2.02	0.41
1:D:345:ILE:HG13	1:D:350:LEU:HD13	2.02	0.41
1:D:309:LEU:HB3	1:D:322:LEU:HD11	2.03	0.41
1:B:291:MSE:HE3	1:C:339:ILE:HD13	2.02	0.41
1:C:287:PHE:CE1	1:C:291:MSE:HE3	2.55	0.41
1:C:447:LEU:HD22	1:C:451:ASP:HB3	2.02	0.41
1:D:447:LEU:HD22	1:D:451:ASP:HB3	2.03	0.41
1:A:234:MSE:HE2	1:B:238:LEU:HD22	2.03	0.41
1:C:345:ILE:HG13	1:C:350:LEU:HD13	2.02	0.40

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	292/317 (92%)	290 (99%)	2 (1%)	0	100	100
1	B	296/317 (93%)	294 (99%)	2 (1%)	0	100	100
1	C	292/317 (92%)	290 (99%)	2 (1%)	0	100	100
1	D	291/317 (92%)	289 (99%)	2 (1%)	0	100	100
All	All	1171/1268 (92%)	1163 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	251/262 (96%)	241 (96%)	10 (4%)	31	47
1	B	255/262 (97%)	246 (96%)	9 (4%)	36	53
1	C	251/262 (96%)	241 (96%)	10 (4%)	31	47
1	D	250/262 (95%)	242 (97%)	8 (3%)	39	56
All	All	1007/1048 (96%)	970 (96%)	37 (4%)	34	51

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	ASP
1	A	227	LEU

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Mol	Chain	Res	Type
1	A	286	GLU
1	A	292	SER
1	A	320	ASP
1	A	332	LEU
1	A	369	MSE
1	A	375	HIS
1	A	387	ARG
1	A	466	LEU
1	B	224	LEU
1	B	227	LEU
1	B	242	GLN
1	B	245	MSE
1	B	286	GLU
1	B	332	LEU
1	B	341	ASP
1	B	387	ARG
1	B	466	LEU
1	C	227	LEU
1	C	246	GLN
1	C	291	MSE
1	C	292	SER
1	C	332	LEU
1	C	341	ASP
1	C	350	LEU
1	C	387	ARG
1	C	388	ASP
1	C	466	LEU
1	D	227	LEU
1	D	242	GLN
1	D	246	GLN
1	D	292	SER
1	D	332	LEU
1	D	369	MSE
1	D	387	ARG
1	D	466	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	A	461	GLN
1	B	246	GLN

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Mol	Chain	Res	Type
1	B	364	GLN
1	B	392	GLN
1	B	461	GLN
1	C	246	GLN
1	C	310	GLN
1	C	364	GLN
1	C	461	GLN
1	D	246	GLN
1	D	461	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	PGR	B	602	-	3,4,4	0.11	0	1,4,4	0.07	0
3	PGR	B	603	-	3,4,4	0.16	0	1,4,4	0.06	0
3	PGR	B	601	-	3,4,4	0.11	0	1,4,4	0.05	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	PGR	B	602	-	-	0/2/2/2	-
3	PGR	B	603	-	-	2/2/2/2	-
3	PGR	B	601	-	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	PGR	O1-C1-C2-O2
3	B	603	PGR	O1-C1-C2-C3
3	B	603	PGR	O1-C1-C2-O2
3	B	601	PGR	O1-C1-C2-C3

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

### 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	286/317 (90%)	1.26	62 (21%) 0 0	51, 131, 219, 230	0
1	B	286/317 (90%)	0.79	30 (10%) 6 4	45, 62, 215, 223	0
1	C	286/317 (90%)	2.38	107 (37%) 0 0	51, 208, 240, 245	0
1	D	286/317 (90%)	1.29	71 (24%) 0 0	47, 150, 229, 236	0
All	All	1144/1268 (90%)	1.43	270 (23%) 0 0	45, 130, 231, 245	0

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	459	PHE	18.0
1	C	415	THR	15.6
1	C	445	ILE	13.9
1	C	411	ALA	12.7
1	C	456	PHE	12.1
1	C	498	GLY	11.6
1	C	448	SER	10.2
1	C	453	GLN	10.1
1	C	408	VAL	9.7
1	C	372	PRO	9.7
1	D	386	TYR	9.6
1	C	454	ALA	9.4
1	C	452	GLN	9.3
1	C	390	PRO	9.1
1	C	460	SER	9.0
1	A	240	SER	8.8
1	C	455	LEU	8.5
1	C	446	GLY	8.2
1	C	447	LEU	8.0
1	D	388	ASP	8.0
1	A	434	ALA	8.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	375	HIS	7.9
1	C	503	PHE	7.7
1	C	493	VAL	7.4
1	C	422	VAL	7.3
1	C	497	PRO	7.1
1	C	500	GLY	7.1
1	A	222	ASN	7.0
1	C	450	GLU	6.9
1	C	249	ILE	6.8
1	C	362	LEU	6.6
1	C	420	VAL	6.2
1	C	438	ILE	6.1
1	D	389	THR	6.1
1	D	387	ARG	6.0
1	B	238	LEU	6.0
1	D	265	ILE	6.0
1	D	500	GLY	5.9
1	C	412	ILE	5.9
1	D	391	ILE	5.8
1	A	239	GLN	5.7
1	C	466	LEU	5.7
1	C	424	ALA	5.7
1	C	440	VAL	5.6
1	A	509	LEU	5.6
1	C	366	ALA	5.6
1	D	263	ILE	5.6
1	C	499	GLU	5.5
1	C	404	LEU	5.5
1	C	414	PHE	5.4
1	C	252	ALA	5.4
1	C	359	LEU	5.3
1	C	409	GLY	5.3
1	D	225	ASP	5.3
1	A	400	LEU	5.3
1	C	376	GLU	5.2
1	A	449	GLU	5.1
1	C	378	GLN	5.1
1	C	368	THR	5.1
1	C	509	LEU	5.0
1	C	388	ASP	5.0
1	A	229	SER	4.9
1	A	236	GLU	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	248	ASN	4.8
1	B	236	GLU	4.8
1	C	496	THR	4.8
1	B	228	ALA	4.7
1	B	225	ASP	4.7
1	D	499	GLU	4.7
1	C	371	ALA	4.6
1	D	447	LEU	4.6
1	D	450	GLU	4.6
1	B	233	ARG	4.6
1	D	385	VAL	4.6
1	C	449	GLU	4.6
1	D	236	GLU	4.6
1	D	446	GLY	4.5
1	A	512	SER	4.5
1	C	501	ALA	4.5
1	C	421	ALA	4.5
1	C	475	LEU	4.5
1	D	384	LEU	4.5
1	A	507	LEU	4.5
1	A	432	ASP	4.4
1	B	249	ILE	4.4
1	D	501	ALA	4.4
1	D	424	ALA	4.4
1	A	233	ARG	4.4
1	D	390	PRO	4.4
1	B	237	THR	4.3
1	C	462	ALA	4.3
1	C	250	ASP	4.3
1	C	441	GLN	4.3
1	A	228	ALA	4.3
1	D	249	ILE	4.3
1	B	266	GLN	4.3
1	C	416	GLN	4.3
1	C	505	ILE	4.2
1	C	355	LEU	4.2
1	D	455	LEU	4.1
1	D	453	GLN	4.1
1	D	221	SER	4.1
1	C	451	ASP	4.0
1	A	243	GLU	4.0
1	A	484	ILE	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	255	ASP	3.9
1	D	454	ALA	3.9
1	A	270	LEU	3.8
1	D	366	ALA	3.8
1	D	254	GLU	3.8
1	D	456	PHE	3.8
1	A	433	ARG	3.7
1	C	491	ILE	3.7
1	B	259	ASN	3.7
1	C	419	THR	3.7
1	D	243	GLU	3.7
1	C	512	SER	3.7
1	C	407	LEU	3.7
1	A	241	ALA	3.7
1	C	495	SER	3.7
1	B	242	GLN	3.7
1	C	484	ILE	3.6
1	A	386	TYR	3.6
1	D	232	ASN	3.6
1	A	451	ASP	3.6
1	B	239	GLN	3.6
1	D	452	GLN	3.6
1	D	362	LEU	3.6
1	C	470	ALA	3.6
1	C	400	LEU	3.6
1	B	240	SER	3.6
1	D	359	LEU	3.5
1	A	249	ILE	3.5
1	D	445	ILE	3.5
1	A	259	ASN	3.5
1	C	263	ILE	3.5
1	A	447	LEU	3.5
1	A	390	PRO	3.5
1	B	270	LEU	3.5
1	A	252	ALA	3.4
1	C	383	SER	3.4
1	A	237	THR	3.4
1	D	498	GLY	3.4
1	A	342	PHE	3.4
1	C	270	LEU	3.4
1	C	434	ALA	3.3
1	C	423	ARG	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	492	GLY	3.3
1	D	240	SER	3.3
1	D	357	PHE	3.3
1	B	231	ILE	3.3
1	A	242	GLN	3.2
1	A	472	GLY	3.2
1	C	382	VAL	3.2
1	D	420	VAL	3.2
1	C	384	LEU	3.2
1	C	389	THR	3.1
1	C	381	LEU	3.1
1	B	265	ILE	3.1
1	D	253	THR	3.1
1	C	374	ALA	3.1
1	A	453	GLN	3.1
1	A	404	LEU	3.1
1	A	391	ILE	3.0
1	A	431	ASP	3.0
1	A	345	ILE	3.0
1	B	248	ASN	3.0
1	C	457	LYS	3.0
1	B	250	ASP	3.0
1	D	404	LEU	3.0
1	A	235	ALA	3.0
1	D	222	ASN	2.9
1	A	260	LEU	2.9
1	C	395	GLY	2.9
1	B	232	ASN	2.9
1	A	430	SER	2.9
1	D	360	ARG	2.9
1	C	222	ASN	2.9
1	A	444	GLY	2.9
1	B	254	GLU	2.9
1	C	461	GLN	2.8
1	C	221	SER	2.8
1	D	436	LEU	2.8
1	A	420	VAL	2.8
1	C	477	LEU	2.8
1	C	439	SER	2.8
1	C	427	GLU	2.8
1	D	246	GLN	2.8
1	C	394	GLN	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	357	PHE	2.8
1	C	386	TYR	2.7
1	B	246	GLN	2.7
1	C	391	ILE	2.7
1	C	508	SER	2.7
1	C	248	ASN	2.7
1	C	393	LEU	2.7
1	C	255	ASP	2.7
1	B	243	GLU	2.6
1	D	233	ARG	2.6
1	A	223	GLU	2.6
1	D	375	HIS	2.6
1	A	384	LEU	2.6
1	D	507	LEU	2.6
1	D	416	GLN	2.6
1	A	224	LEU	2.6
1	C	442	ASP	2.6
1	A	445	ILE	2.5
1	B	253	THR	2.5
1	C	435	GLN	2.5
1	D	367	LEU	2.5
1	B	257	ARG	2.5
1	A	438	ILE	2.5
1	A	256	VAL	2.5
1	D	242	GLN	2.5
1	D	363	ILE	2.5
1	C	377	LYS	2.5
1	B	256	VAL	2.5
1	D	379	LEU	2.5
1	D	237	THR	2.5
1	D	241	ALA	2.5
1	D	260	LEU	2.5
1	C	463	ASP	2.5
1	A	416	GLN	2.5
1	A	360	ARG	2.5
1	C	444	GLY	2.4
1	A	247	HIS	2.4
1	A	253	THR	2.4
1	A	415	THR	2.4
1	A	503	PHE	2.4
1	C	410	ASN	2.4
1	B	229	SER	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	507	LEU	2.4
1	D	262	THR	2.4
1	A	244	GLU	2.4
1	C	403	ILE	2.4
1	D	256	VAL	2.4
1	D	493	VAL	2.4
1	B	247	HIS	2.3
1	D	284	LYS	2.3
1	B	230	GLY	2.3
1	C	246	GLN	2.3
1	D	239	GLN	2.3
1	C	363	ILE	2.3
1	A	450	GLU	2.3
1	C	405	THR	2.3
1	D	400	LEU	2.3
1	D	496	THR	2.2
1	C	399	ARG	2.2
1	A	497	PRO	2.2
1	D	274	ARG	2.2
1	D	431	ASP	2.2
1	D	259	ASN	2.2
1	A	436	LEU	2.2
1	A	442	ASP	2.2
1	A	274	ARG	2.2
1	A	238	LEU	2.1
1	C	385	VAL	2.1
1	C	260	LEU	2.1
1	D	252	ALA	2.1
1	D	426	LEU	2.1
1	D	258	GLN	2.1
1	B	241	ALA	2.1
1	B	269	GLU	2.0
1	C	241	ALA	2.0
1	D	261	GLU	2.0
1	D	434	ALA	2.0
1	D	449	GLU	2.0
1	B	251	GLN	2.0
1	D	288	LEU	2.0
1	A	250	ASP	2.0

## 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 monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	B	604	1/1	0.57	0.25	117,117,117,117	0
3	PGR	B	601	5/5	0.76	0.28	101,101,101,101	0
3	PGR	B	603	5/5	0.79	0.19	87,87,87,87	0
2	CA	B	605	1/1	0.91	0.15	119,119,119,119	0
2	CA	A	601	1/1	0.92	0.11	112,112,112,112	0
3	PGR	B	602	5/5	0.93	0.26	69,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.