



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 04:07 AM EDT

PDB ID : 3GH1  
Title : Crystal structure of predicted nucleotide-binding protein from *Vibrio cholerae*  
Authors : Malashkevich, V.N.; Toro, R.; Wasserman, S.; Sauder, J.M.; Burley, S.K.;  
Almo, S.C.; New York SGX Research Center for Structural Genomics (NYS-  
GXRC)  
Deposited on : 2009-03-02  
Resolution : 1.90 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

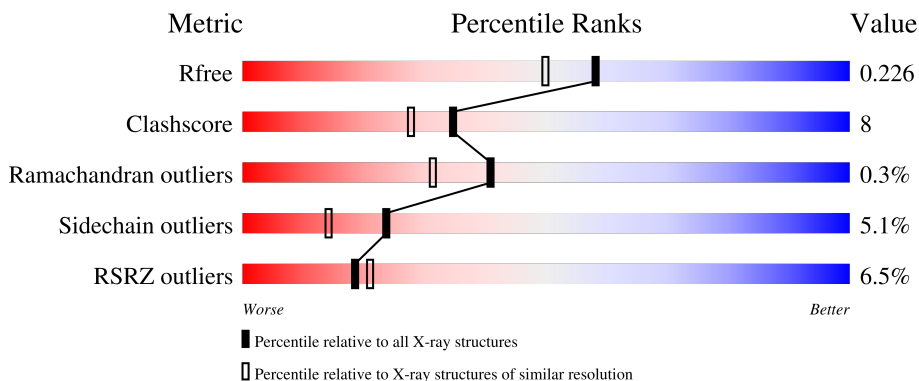
# 1 Overall quality at a glance

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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	462	 6% 81% 14% . .
1	B	462	 6% 79% 15% . .
1	C	462	 8% 76% 17% . 5%
1	D	462	 5% 79% 13% . .

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 15320 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 Predicted nucleotide-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	448	Total 3520	C 2227	N 620	O 651	S 5	Se 17	0	0	0
1	B	446	Total 3510	C 2222	N 619	O 647	S 5	Se 17	0	1	0
1	C	441	Total 3464	C 2196	N 608	O 638	S 5	Se 17	0	2	0
1	D	444	Total 3477	C 2203	N 610	O 642	S 5	Se 17	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

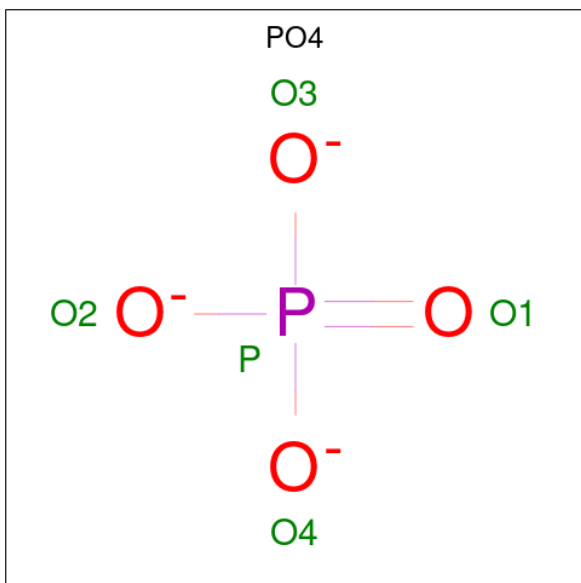
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q9KTK3
A	2	SER	-	expression tag	UNP Q9KTK3
A	3	LEU	-	expression tag	UNP Q9KTK3
A	455	GLU	-	expression tag	UNP Q9KTK3
A	456	GLY	-	expression tag	UNP Q9KTK3
A	457	HIS	-	expression tag	UNP Q9KTK3
A	458	HIS	-	expression tag	UNP Q9KTK3
A	459	HIS	-	expression tag	UNP Q9KTK3
A	460	HIS	-	expression tag	UNP Q9KTK3
A	461	HIS	-	expression tag	UNP Q9KTK3
A	462	HIS	-	expression tag	UNP Q9KTK3
B	1	MSE	-	expression tag	UNP Q9KTK3
B	2	SER	-	expression tag	UNP Q9KTK3
B	3	LEU	-	expression tag	UNP Q9KTK3
B	455	GLU	-	expression tag	UNP Q9KTK3
B	456	GLY	-	expression tag	UNP Q9KTK3
B	457	HIS	-	expression tag	UNP Q9KTK3
B	458	HIS	-	expression tag	UNP Q9KTK3
B	459	HIS	-	expression tag	UNP Q9KTK3
B	460	HIS	-	expression tag	UNP Q9KTK3
B	461	HIS	-	expression tag	UNP Q9KTK3

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	462	HIS	-	expression tag	UNP Q9KTK3
C	1	MSE	-	expression tag	UNP Q9KTK3
C	2	SER	-	expression tag	UNP Q9KTK3
C	3	LEU	-	expression tag	UNP Q9KTK3
C	455	GLU	-	expression tag	UNP Q9KTK3
C	456	GLY	-	expression tag	UNP Q9KTK3
C	457	HIS	-	expression tag	UNP Q9KTK3
C	458	HIS	-	expression tag	UNP Q9KTK3
C	459	HIS	-	expression tag	UNP Q9KTK3
C	460	HIS	-	expression tag	UNP Q9KTK3
C	461	HIS	-	expression tag	UNP Q9KTK3
C	462	HIS	-	expression tag	UNP Q9KTK3
D	1	MSE	-	expression tag	UNP Q9KTK3
D	2	SER	-	expression tag	UNP Q9KTK3
D	3	LEU	-	expression tag	UNP Q9KTK3
D	455	GLU	-	expression tag	UNP Q9KTK3
D	456	GLY	-	expression tag	UNP Q9KTK3
D	457	HIS	-	expression tag	UNP Q9KTK3
D	458	HIS	-	expression tag	UNP Q9KTK3
D	459	HIS	-	expression tag	UNP Q9KTK3
D	460	HIS	-	expression tag	UNP Q9KTK3
D	461	HIS	-	expression tag	UNP Q9KTK3
D	462	HIS	-	expression tag	UNP Q9KTK3

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

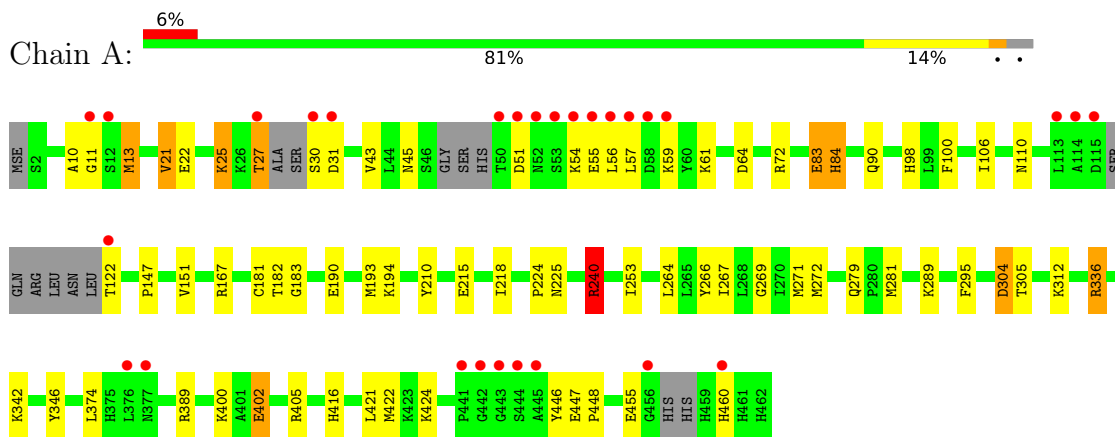
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	116	Total O 116 116	0	0
3	B	80	Total O 80 80	0	0
3	C	99	Total O 99 99	0	0
3	D	1034	Total O 1034 1034	0	0

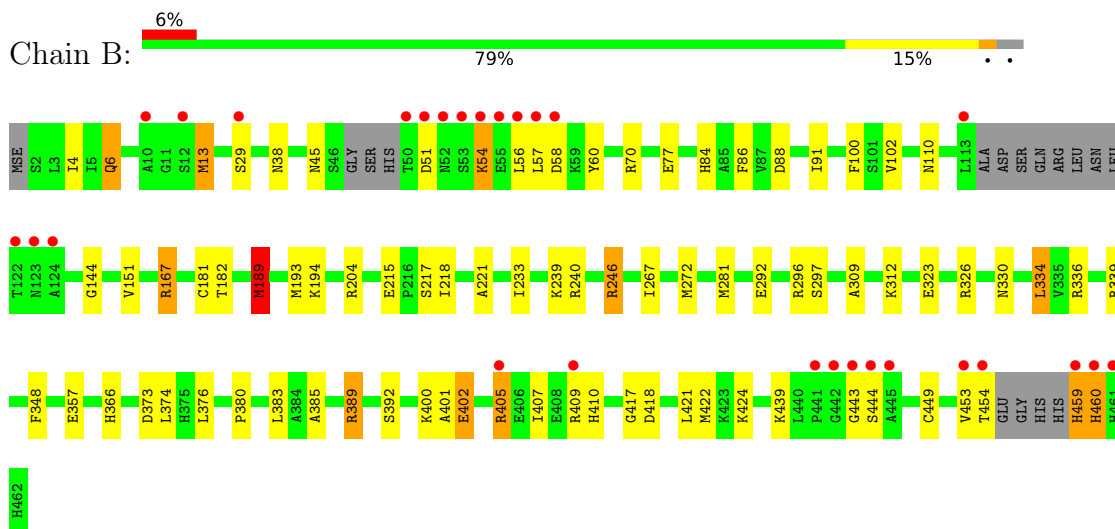
### 3 Residue-property plots [i](#)

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.

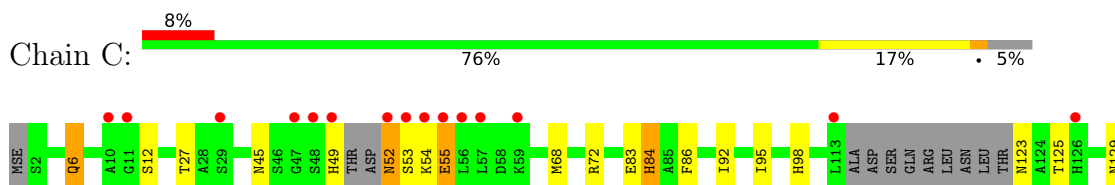
- Molecule 1: Predicted nucleotide-binding protein

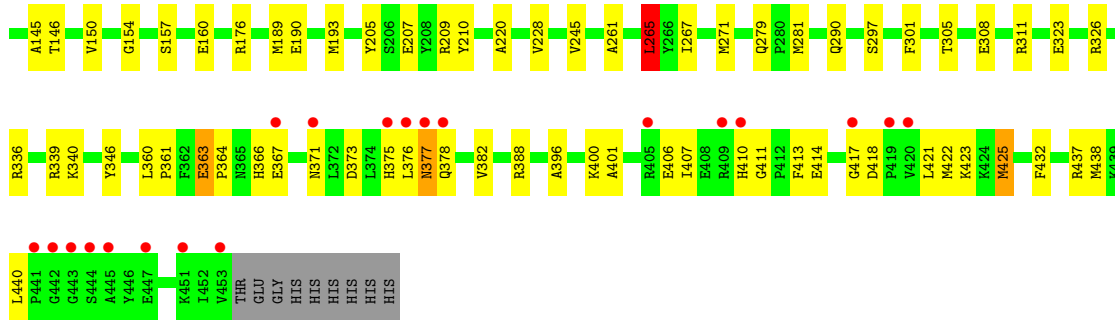


- Molecule 1: Predicted nucleotide-binding protein

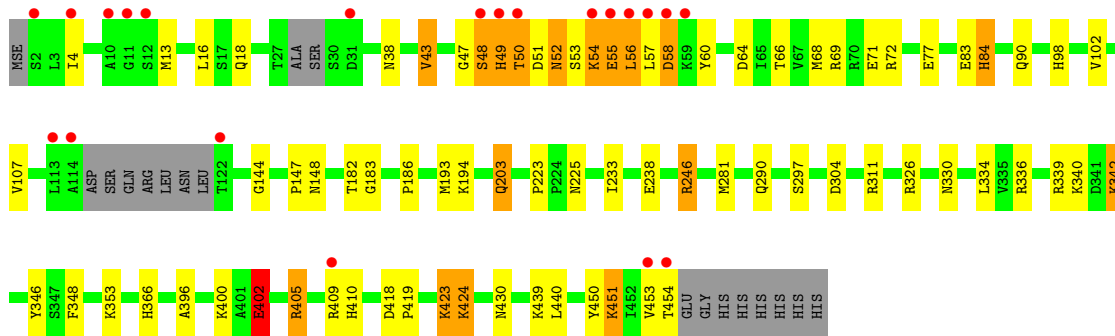
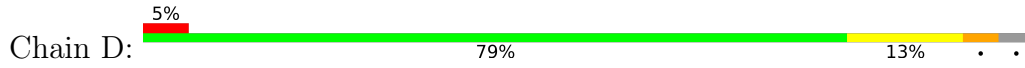


- Molecule 1: Predicted nucleotide-binding protein





● Molecule 1: Predicted nucleotide-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.03Å 181.55Å 95.77Å 90.00° 103.32° 90.00°	Depositor
Resolution (Å)	19.92 – 1.90 19.92 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.2 (19.92-1.90) 90.2 (19.92-1.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 1.90Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.169 , 0.226 0.170 , 0.226	Depositor DCC
$R_{free}$ test set	6921 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtrriage
Anisotropy	0.035	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15320	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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 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	1.08	8/3578 (0.2%)	1.00	9/4810 (0.2%)
1	B	1.04	1/3572 (0.0%)	0.98	16/4804 (0.3%)
1	C	1.05	6/3527 (0.2%)	0.92	7/4745 (0.1%)
1	D	1.11	4/3534 (0.1%)	0.94	9/4755 (0.2%)
All	All	1.07	19/14211 (0.1%)	0.96	41/19114 (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	B	0	1
1	D	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	402	GLU	CG-CD	6.28	1.61	1.51
1	C	207	GLU	CG-CD	5.80	1.60	1.51
1	A	336	ARG	CD-NE	-5.75	1.36	1.46
1	C	150	VAL	CB-CG2	5.74	1.64	1.52
1	A	336	ARG	CG-CD	5.66	1.66	1.51
1	D	238	GLU	CG-CD	5.53	1.60	1.51
1	A	295	PHE	CD2-CE2	5.52	1.50	1.39
1	C	346	TYR	CD1-CE1	5.41	1.47	1.39
1	D	402	GLU	CB-CG	5.33	1.62	1.52
1	C	205	TYR	CD2-CE2	5.33	1.47	1.39
1	B	239	LYS	CD-CE	5.30	1.64	1.51
1	A	402	GLU	CB-CG	5.25	1.62	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	GLU	CG-CD	5.24	1.59	1.51
1	A	21	VAL	CB-CG1	-5.21	1.41	1.52
1	A	402	GLU	CG-CD	5.15	1.59	1.51
1	D	107	VAL	CB-CG1	5.14	1.63	1.52
1	C	145	ALA	CA-CB	5.13	1.63	1.52
1	A	266	TYR	CG-CD2	5.11	1.45	1.39
1	C	339	ARG	CG-CD	5.04	1.64	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ARG	NE-CZ-NH1	-14.70	112.95	120.30
1	A	336	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	A	240	ARG	NE-CZ-NH2	10.98	125.79	120.30
1	A	336	ARG	NE-CZ-NH1	9.87	125.24	120.30
1	B	336	ARG	NE-CZ-NH2	9.06	124.83	120.30
1	B	167	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	D	246	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	D	336	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	194	LYS	CD-CE-NZ	-7.05	95.48	111.70
1	D	43	VAL	CG1-CB-CG2	6.99	122.09	110.90
1	B	70	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	B	167	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	B	240	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	C	336	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	C	340	LYS	CD-CE-NZ	-6.66	96.39	111.70
1	B	194	LYS	CD-CE-NZ	-6.64	96.44	111.70
1	A	167	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	246	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	D	49	HIS	N-CA-C	-6.28	94.05	111.00
1	B	336	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	D	69	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	70	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	C	176	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	240	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	265	LEU	CA-CB-CG	-5.84	101.87	115.30
1	A	64	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	246	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	304	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	69	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	339	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	204	ARG	NE-CZ-NH2	-5.66	117.47	120.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	425	MSE	CB-CG-SE	-5.60	95.90	112.70
1	A	240	ARG	CD-NE-CZ	5.54	131.36	123.60
1	C	209	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	D	64	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	64	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	189	MSE	CG-SE-CE	5.40	110.79	98.90
1	B	389	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	B	334	LEU	CB-CG-CD1	5.33	120.06	111.00
1	C	437	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	339	ARG	CG-CD-NE	-5.03	101.24	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	460	HIS	Peptide
1	D	48	SER	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	3520	0	3498	59	0
1	B	3510	0	3497	57	0
1	C	3464	0	3467	48	0
1	D	3477	0	3471	70	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	116	0	0	15	0
3	B	80	0	0	4	0
3	C	99	0	0	1	0
3	D	1034	0	0	41	0
All	All	15320	0	13933	231	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 8.

All (231) 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:334:LEU:HG	3:B:1308:HOH:O	1.31	1.26
1:B:6:GLN:HG2	3:B:1458:HOH:O	1.58	1.02
1:B:424:LYS:HD2	3:D:773:HOH:O	1.62	0.98
1:A:45:ASN:OD1	1:A:84:HIS:HE1	1.45	0.98
1:A:271:MSE:HE3	3:D:675:HOH:O	1.64	0.98
1:D:405:ARG:HD2	1:D:409:ARG:HH21	1.29	0.97
1:D:203:GLN:CD	3:D:989:HOH:O	2.06	0.93
1:D:72:ARG:NH1	3:D:1390:HOH:O	2.01	0.93
1:A:304:ASP:OD2	1:A:424:LYS:HE2	1.72	0.90
1:A:421:LEU:HG	1:A:422:MSE:HE2	1.55	0.89
1:B:407:ILE:HD13	1:B:449:CYS:HB2	1.53	0.89
1:A:45:ASN:OD1	1:A:84:HIS:CE1	2.26	0.87
1:A:240:ARG:CD	3:A:1262:HOH:O	2.23	0.86
1:A:240:ARG:HD3	3:A:1262:HOH:O	1.77	0.82
1:A:455:GLU:HG2	3:A:1453:HOH:O	1.80	0.82
1:D:402:GLU:CG	3:D:882:HOH:O	2.30	0.78
1:C:366:HIS:CE1	1:C:410:HIS:HB2	2.19	0.78
1:C:6:GLN:HE21	1:C:6:GLN:HA	1.47	0.77
1:A:10:ALA:HB3	1:A:13:MSE:HB2	1.67	0.76
1:C:54:LYS:HZ2	1:C:401:ALA:H	1.33	0.74
1:A:10:ALA:HB1	3:A:1140:HOH:O	1.88	0.73
1:C:190:GLU:OE1	3:D:696:HOH:O	2.06	0.73
1:D:334:LEU:HD12	3:D:1452:HOH:O	1.87	0.73
1:B:309:ALA:O	1:B:312:LYS:HE3	1.89	0.72
1:A:281:MSE:HB2	3:D:801:HOH:O	1.91	0.71
1:C:367:GLU:CG	1:C:371:ASN:HD21	2.04	0.70
1:C:6:GLN:HE22	1:C:68:MSE:HE1	1.57	0.70
1:C:311:ARG:HH11	1:C:311:ARG:HG3	1.57	0.70
1:B:374:LEU:HB3	1:B:422:MSE:HE1	1.73	0.69
1:A:72:ARG:NH1	1:D:144:GLY:O	2.26	0.69
1:D:49:HIS:HE1	1:D:223:PRO:HG3	1.58	0.68
1:C:281:MSE:HB2	3:D:790:HOH:O	1.93	0.68
1:D:54:LYS:HD2	3:D:993:HOH:O	1.94	0.67
1:D:68:MSE:HE2	1:D:77:GLU:HB2	1.74	0.67
1:C:323:GLU:OE2	3:C:1007:HOH:O	2.11	0.66
1:C:146[A]:THR:HG22	3:D:1374:HOH:O	1.95	0.66
1:B:402:GLU:H	1:B:402:GLU:CD	1.99	0.65
1:D:402:GLU:H	1:D:402:GLU:CD	2.00	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASN:N	3:D:818:HOH:O	2.30	0.65
1:A:240:ARG:HD2	3:A:1262:HOH:O	1.89	0.65
1:B:182:THR:HG22	1:B:193:MSE:HE3	1.78	0.64
1:D:334:LEU:HG	3:D:1452:HOH:O	1.98	0.63
1:A:182:THR:HG22	1:A:193:MSE:HE3	1.81	0.63
1:D:203:GLN:CG	3:D:989:HOH:O	2.43	0.63
1:A:194:LYS:HE2	3:A:1320:HOH:O	1.99	0.62
1:B:88:ASP:OD2	3:D:683:HOH:O	2.15	0.62
1:D:203:GLN:HG3	3:D:989:HOH:O	1.99	0.62
1:D:402:GLU:HG3	3:D:882:HOH:O	1.97	0.62
1:C:261:ALA:O	1:C:265:LEU:HD12	1.99	0.61
1:C:367:GLU:HG3	1:C:371:ASN:HD21	1.64	0.61
1:A:10:ALA:HB2	1:A:100:PHE:CG	2.36	0.61
1:D:334:LEU:CD1	3:D:1452:HOH:O	2.45	0.61
1:D:54:LYS:HD3	3:D:1282:HOH:O	2.01	0.60
1:D:281:MSE:HB2	3:D:845:HOH:O	2.02	0.60
1:B:357:GLU:HG3	1:B:385:ALA:HB1	1.83	0.60
1:C:84:HIS:H	1:C:84:HIS:CD2	2.18	0.60
1:B:4:ILE:HG23	1:B:77:GLU:HG3	1.84	0.60
1:B:459:HIS:ND1	1:B:459:HIS:O	2.34	0.60
1:D:182:THR:HG22	1:D:193:MSE:HE3	1.84	0.60
1:D:453:VAL:HG12	1:D:454:THR:H	1.67	0.59
1:A:56:LEU:HD23	1:A:59:LYS:HD3	1.83	0.59
1:A:271:MSE:CE	3:D:675:HOH:O	2.37	0.58
1:C:367:GLU:HG2	1:C:371:ASN:HD21	1.68	0.58
1:A:11:GLY:N	3:A:1433:HOH:O	2.37	0.58
1:C:421:LEU:HG	1:C:422:MSE:HE2	1.84	0.58
1:B:45:ASN:OD1	1:B:84:HIS:NE2	2.34	0.58
1:B:357:GLU:OE2	1:B:389:ARG:NH2	2.35	0.58
1:A:43:VAL:HG22	1:A:224:PRO:HG2	1.86	0.57
1:D:203:GLN:OE1	3:D:989:HOH:O	2.13	0.57
1:D:58:ASP:N	1:D:58:ASP:OD1	2.38	0.57
1:C:92:ILE:HB	1:C:95:ILE:HD12	1.87	0.56
1:D:304:ASP:HB2	1:D:424:LYS:HE2	1.87	0.56
1:A:84:HIS:H	1:A:84:HIS:CD2	2.23	0.56
1:D:400:LYS:HB3	1:D:402:GLU:OE2	2.05	0.56
1:C:311:ARG:HG3	1:C:311:ARG:NH1	2.21	0.55
1:A:11:GLY:CA	3:A:1433:HOH:O	2.54	0.55
1:D:334:LEU:CG	3:D:1452:HOH:O	2.54	0.55
1:B:13:MSE:HG3	1:B:100:PHE:HB3	1.88	0.54
1:B:401:ALA:O	1:B:405:ARG:HD3	2.06	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:HIS:C	1:C:377:ASN:H	2.10	0.54
1:B:407:ILE:CD1	1:B:449:CYS:HB2	2.31	0.54
1:B:417:GLY:HA3	1:B:422:MSE:HE3	1.88	0.54
1:A:446:TYR:CE1	1:A:448:PRO:HA	2.43	0.54
1:A:22:GLU:O	1:A:25:LYS:HG3	2.08	0.54
1:B:144:GLY:O	1:C:72:ARG:NH1	2.42	0.53
1:A:10:ALA:CB	3:A:1140:HOH:O	2.52	0.53
1:D:419:PRO:HB3	3:D:1183:HOH:O	2.09	0.53
1:B:439:LYS:HE2	1:B:444:SER:O	2.08	0.53
1:B:38[B]:ASN:OD1	1:B:57:LEU:HD21	2.10	0.52
1:B:443:GLY:O	3:D:1238:HOH:O	2.19	0.52
1:D:49:HIS:CD2	1:D:56:LEU:HD11	2.45	0.51
1:D:60:TYR:OH	1:D:84:HIS:HE1	1.93	0.51
1:D:83:GLU:HG2	3:D:1174:HOH:O	2.11	0.51
1:D:54:LYS:C	1:D:56:LEU:H	2.12	0.51
1:D:55:GLU:HA	1:D:55:GLU:OE1	2.10	0.51
1:D:203:GLN:OE1	1:D:203:GLN:HA	2.10	0.51
1:C:432:PHE:HB2	1:C:438:MSE:HE2	1.93	0.50
1:C:366:HIS:HE1	1:C:406:GLU:O	1.94	0.50
1:D:451:LYS:HD3	1:D:453:VAL:HG22	1.93	0.50
1:A:271:MSE:HE1	1:A:279:GLN:HB2	1.94	0.50
1:C:271:MSE:HE1	1:C:279:GLN:HB2	1.92	0.50
1:A:402:GLU:H	1:A:402:GLU:CD	2.15	0.50
1:A:374:LEU:HB3	1:A:422:MSE:HE1	1.93	0.50
1:D:430:ASN:OD1	3:D:1039:HOH:O	2.20	0.50
1:A:421:LEU:HG	1:A:422:MSE:CE	2.35	0.49
1:B:326:ARG:HG2	1:B:330:ASN:ND2	2.26	0.49
1:A:45:ASN:HD21	1:A:56:LEU:HD22	1.76	0.49
1:B:374:LEU:CB	1:B:422:MSE:HE1	2.41	0.49
1:B:357:GLU:HG3	1:B:385:ALA:CB	2.43	0.49
1:A:98:HIS:HE1	1:A:225:ASN:O	1.96	0.49
1:A:151:VAL:HA	1:A:181:CYS:O	2.13	0.49
1:B:86:PHE:CE1	1:B:91:ILE:CG1	2.96	0.49
1:D:50:THR:O	1:D:440:LEU:HD12	2.13	0.48
1:C:49:HIS:HB2	1:C:52:ASN:N	2.27	0.48
1:A:267:ILE:HD11	1:A:281:MSE:HE1	1.93	0.48
1:D:49:HIS:CE1	1:D:223:PRO:HG3	2.45	0.48
1:D:453:VAL:HG12	1:D:454:THR:N	2.29	0.48
1:C:407:ILE:HD11	1:C:413:PHE:CE1	2.48	0.48
1:C:301:PHE:O	1:C:305:THR:HG23	2.13	0.48
1:A:10:ALA:HB2	1:A:100:PHE:CD2	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ARG:O	1:B:409:ARG:HG2	2.13	0.47
1:C:54:LYS:NZ	1:C:401:ALA:H	2.08	0.47
1:C:86:PHE:N	1:C:86:PHE:CD2	2.81	0.47
1:A:218:ILE:HG13	1:A:218:ILE:O	2.13	0.47
1:B:54:LYS:HE3	1:B:221:ALA:HB2	1.96	0.47
1:B:84:HIS:HB2	3:B:1325:HOH:O	2.15	0.47
1:D:4:ILE:HG23	1:D:77:GLU:HG3	1.96	0.47
1:D:18:GLN:HG2	3:D:1086:HOH:O	2.13	0.47
1:D:340:LYS:HE3	1:D:346:TYR:OH	2.14	0.47
1:D:246:ARG:HD2	1:D:348:PHE:CZ	2.50	0.47
1:B:272:MSE:HE1	1:B:380:PRO:HB2	1.96	0.47
1:B:439:LYS:CE	1:B:444:SER:O	2.63	0.47
1:A:312:LYS:HB3	1:A:312:LYS:HE3	1.74	0.46
1:D:423:LYS:HA	1:D:423:LYS:HD2	1.54	0.46
1:C:421:LEU:HG	1:C:422:MSE:CE	2.46	0.46
1:A:122:THR:N	3:A:1010:HOH:O	2.48	0.46
1:B:102:VAL:HA	1:B:233:ILE:HD13	1.97	0.46
1:B:281:MSE:HE2	1:B:281:MSE:HB3	1.86	0.46
1:D:52:ASN:ND2	1:D:52:ASN:H	2.12	0.46
1:D:84:HIS:HB2	3:D:1200:HOH:O	2.15	0.46
1:B:215:GLU:OE2	1:B:217:SER:OG	2.32	0.46
1:C:55:GLU:OE2	1:C:55:GLU:HA	2.15	0.46
1:D:182:THR:HG23	1:D:183:GLY:O	2.16	0.46
1:A:269:GLY:HA2	1:A:272:MSE:HE2	1.98	0.45
1:A:54:LYS:O	1:A:55:GLU:HG3	2.16	0.45
1:B:86:PHE:CZ	1:B:91:ILE:HD11	2.51	0.45
1:D:55:GLU:OE1	1:D:55:GLU:CA	2.64	0.45
1:A:10:ALA:CA	3:A:1140:HOH:O	2.65	0.45
1:A:51:ASP:N	1:A:51:ASP:OD1	2.50	0.45
1:A:90:GLN:OE1	3:D:928:HOH:O	2.20	0.45
1:B:357:GLU:HB2	3:B:1337:HOH:O	2.16	0.45
1:B:459:HIS:O	1:B:459:HIS:CG	2.69	0.45
1:C:366:HIS:NE2	1:C:411:GLY:O	2.36	0.45
1:C:367:GLU:HG2	1:C:371:ASN:ND2	2.31	0.45
1:B:453:VAL:HG12	1:B:454:THR:N	2.31	0.45
1:C:378:GLN:OE1	1:C:382:VAL:HG12	2.16	0.45
1:D:366:HIS:CE1	1:D:410:HIS:HB2	2.52	0.45
1:B:421:LEU:HG	1:B:422:MSE:HE2	1.99	0.45
1:B:296:ARG:NE	3:D:885:HOH:O	2.22	0.45
1:B:233:ILE:HD12	1:B:233:ILE:N	2.32	0.45
1:B:357:GLU:OE2	1:B:389:ARG:NH1	2.49	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:HZ1	1:B:221:ALA:H	1.65	0.45
1:A:305:THR:HG22	1:A:421:LEU:HD13	1.99	0.44
1:B:60:TYR:OH	1:B:84:HIS:HE1	2.00	0.44
1:A:416:HIS:CD2	1:A:455:GLU:HB3	2.52	0.44
1:A:336:ARG:HD3	3:D:1164:HOH:O	2.17	0.44
1:B:189:MSE:HA	1:B:189:MSE:HE2	1.99	0.44
1:A:194:LYS:CE	3:A:1320:HOH:O	2.64	0.44
1:A:193:MSE:SE	1:A:210:TYR:HB3	2.68	0.44
1:A:31:ASP:HA	3:A:1406:HOH:O	2.18	0.43
1:C:98:HIS:HE1	1:C:228:VAL:O	2.01	0.43
1:D:102:VAL:HA	1:D:233:ILE:HD13	2.00	0.43
1:D:342:LYS:HZ2	1:D:342:LYS:HA	1.83	0.43
1:C:360:LEU:HD12	1:C:361:PRO:HD2	2.01	0.43
1:A:193:MSE:HG3	3:D:652:HOH:O	2.18	0.43
1:A:336:ARG:HD2	3:A:1279:HOH:O	2.19	0.43
1:C:154:GLY:O	1:C:189:MSE:HE3	2.19	0.43
1:C:326:ARG:NH1	3:D:591:HOH:O	2.51	0.43
1:D:47:GLY:O	1:D:49:HIS:N	2.51	0.43
1:D:182:THR:CG2	1:D:193:MSE:HE3	2.48	0.43
1:A:182:THR:HG23	1:A:183:GLY:O	2.18	0.43
1:C:157:SER:HB2	1:C:440:LEU:HD23	2.00	0.43
1:D:182:THR:HG22	1:D:193:MSE:CE	2.48	0.43
1:B:267:ILE:HD11	1:B:281:MSE:HE1	2.00	0.43
1:D:60:TYR:OH	1:D:84:HIS:CE1	2.72	0.43
1:C:396:ALA:HA	1:C:400:LYS:HD3	2.01	0.43
1:B:182:THR:CG2	1:B:193:MSE:HE3	2.45	0.42
1:B:86:PHE:CE1	1:B:91:ILE:HG12	2.54	0.42
1:B:376:LEU:HD23	1:B:383:LEU:CD2	2.49	0.42
1:C:54:LYS:HG2	1:C:220:ALA:HB3	2.01	0.42
1:C:376:LEU:HD13	1:C:421:LEU:HB2	2.01	0.42
1:D:13:MSE:HE2	1:D:16:LEU:HD11	2.00	0.42
1:D:49:HIS:HD2	1:D:51:ASP:O	2.01	0.42
1:D:423:LYS:HD3	3:D:1002:HOH:O	2.19	0.42
1:D:4:ILE:HG23	1:D:77:GLU:CG	2.49	0.42
1:A:389:ARG:NH2	3:D:1431:HOH:O	2.46	0.42
1:B:323:GLU:OE1	1:B:326:ARG:NH1	2.48	0.42
1:B:272:MSE:HE2	1:B:272:MSE:HB2	1.88	0.42
1:D:49:HIS:CD2	1:D:51:ASP:O	2.72	0.42
1:D:450:TYR:OH	3:D:1039:HOH:O	2.10	0.42
1:A:83:GLU:HB3	3:A:1344:HOH:O	2.19	0.42
1:D:53:SER:O	1:D:56:LEU:HD22	2.20	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:GLU:HA	1:C:364:PRO:HD3	1.77	0.42
1:C:417:GLY:O	1:C:418:ASP:C	2.58	0.42
1:A:346:TYR:CE1	1:D:71:GLU:HB2	2.55	0.41
1:B:217:SER:OG	1:B:400:LYS:HE3	2.19	0.41
1:D:326:ARG:HG2	1:D:330:ASN:ND2	2.35	0.41
1:D:396:ALA:HA	1:D:400:LYS:HD3	2.02	0.41
1:C:125:THR:HG22	1:C:129:ASN:ND2	2.35	0.41
1:B:281:MSE:HB2	3:D:1188:HOH:O	2.20	0.41
1:D:38:ASN:OD1	1:D:57:LEU:HD22	2.19	0.41
1:D:98:HIS:HE1	1:D:225:ASN:O	2.04	0.41
1:A:342:LYS:HB3	1:A:342:LYS:HE2	1.86	0.41
1:B:189:MSE:H	1:B:189:MSE:HG2	1.63	0.41
1:C:45:ASN:OD1	1:C:84:HIS:HE1	2.04	0.41
1:C:193:MSE:SE	1:C:210:TYR:HB3	2.70	0.41
1:A:106:ILE:HD13	1:A:106:ILE:HA	1.83	0.41
1:B:246:ARG:HD2	1:B:348:PHE:CZ	2.56	0.41
1:B:366:HIS:CE1	1:B:410:HIS:HB2	2.56	0.41
1:D:290:GLN:HG3	3:D:760:HOH:O	2.21	0.41
1:A:25:LYS:O	1:A:27:THR:HG22	2.20	0.41
1:C:245:VAL:HG11	1:C:267:ILE:HD13	2.03	0.41
1:D:281:MSE:HE2	1:D:281:MSE:HB3	1.88	0.41
1:D:430:ASN:ND2	3:D:1095:HOH:O	2.54	0.41
1:D:66:THR:HB	1:D:77:GLU:HB3	2.02	0.41
1:B:151:VAL:HA	1:B:181:CYS:O	2.21	0.40
1:D:51:ASP:HB3	1:D:56:LEU:HD11	2.03	0.40
1:A:253:ILE:HD12	1:A:264:LEU:HD13	2.04	0.40
1:C:146[B]:THR:HG23	3:D:672:HOH:O	2.21	0.40
1:A:147:PRO:HD2	1:A:336:ARG:CG	2.52	0.40
1:D:52:ASN:H	1:D:52:ASN:HD22	1.70	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	438/462 (95%)	427 (98%)	11 (2%)	0	100	100
1	B	439/462 (95%)	426 (97%)	12 (3%)	1 (0%)	47	38
1	C	437/462 (95%)	419 (96%)	18 (4%)	0	100	100
1	D	438/462 (95%)	422 (96%)	12 (3%)	4 (1%)	17	7
All	All	1752/1848 (95%)	1694 (97%)	53 (3%)	5 (0%)	41	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	460	HIS
1	D	48	SER
1	D	54	LYS
1	D	148	ASN
1	D	186	PRO

### 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	379/373 (102%)	362 (96%)	17 (4%)	27	18
1	B	379/373 (102%)	360 (95%)	19 (5%)	24	15
1	C	374/373 (100%)	354 (95%)	20 (5%)	22	13
1	D	374/373 (100%)	353 (94%)	21 (6%)	21	11
All	All	1506/1492 (101%)	1429 (95%)	77 (5%)	24	14

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MSE
1	A	21	VAL
1	A	25	LYS
1	A	27	THR
1	A	30	SER
1	A	57	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	61	LYS
1	A	83	GLU
1	A	84	HIS
1	A	110	ASN
1	A	190	GLU
1	A	240	ARG
1	A	289	LYS
1	A	400	LYS
1	A	405	ARG
1	A	447	GLU
1	A	460	HIS
1	B	6	GLN
1	B	13	MSE
1	B	29	SER
1	B	51	ASP
1	B	54	LYS
1	B	56	LEU
1	B	58	ASP
1	B	110	ASN
1	B	167	ARG
1	B	189	MSE
1	B	218	ILE
1	B	292	GLU
1	B	297	SER
1	B	373	ASP
1	B	392	SER
1	B	402	GLU
1	B	405	ARG
1	B	418	ASP
1	B	459	HIS
1	C	6	GLN
1	C	12	SER
1	C	27	THR
1	C	52	ASN
1	C	53	SER
1	C	55	GLU
1	C	83	GLU
1	C	84	HIS
1	C	160	GLU
1	C	265	LEU
1	C	290	GLN
1	C	297	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	308	GLU
1	C	363	GLU
1	C	373	ASP
1	C	377	ASN
1	C	388	ARG
1	C	414	GLU
1	C	423	LYS
1	C	425	MSE
1	D	43	VAL
1	D	50	THR
1	D	52	ASN
1	D	55	GLU
1	D	56	LEU
1	D	58	ASP
1	D	84	HIS
1	D	90	GLN
1	D	147	PRO
1	D	203	GLN
1	D	297	SER
1	D	311	ARG
1	D	342	LYS
1	D	353	LYS
1	D	402	GLU
1	D	405	ARG
1	D	418	ASP
1	D	423	LYS
1	D	424	LYS
1	D	439	LYS
1	D	451	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	330	ASN
1	B	112	HIS
1	B	430	ASN
1	B	462	HIS
1	C	6	GLN
1	C	84	HIS
1	C	98	HIS
1	C	112	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	371	ASN
1	C	377	ASN
1	C	430	ASN
1	D	49	HIS
1	D	330	ASN

### 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](#)

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	$\# Z  > 2$
2	PO4	D	501	-	4,4,4	1.00	0	6,6,6	0.73	0
2	PO4	A	501	-	4,4,4	1.14	1 (25%)	6,6,6	1.50	1 (16%)
2	PO4	B	501	-	4,4,4	0.83	0	6,6,6	1.29	1 (16%)
2	PO4	C	501	-	4,4,4	0.95	0	6,6,6	1.13	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PO4	P-O4	-2.19	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PO4	O4-P-O3	2.56	116.19	107.97
2	B	501	PO4	O4-P-O2	2.28	115.28	107.97

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

### 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	431/462 (93%)	0.05	28 (6%) 18 21	9, 17, 45, 90	2 (0%)
1	B	429/462 (92%)	0.11	28 (6%) 18 21	9, 18, 44, 95	0
1	C	424/462 (91%)	0.11	35 (8%) 11 13	7, 17, 47, 77	0
1	D	427/462 (92%)	-0.02	21 (4%) 29 33	7, 16, 40, 74	0
All	All	1711/1848 (92%)	0.06	112 (6%) 18 21	7, 17, 45, 95	2 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	56	LEU	11.8
1	A	56	LEU	11.0
1	B	50	THR	9.8
1	D	50	THR	8.5
1	A	57	LEU	8.2
1	D	57	LEU	8.0
1	B	442	GLY	7.9
1	B	454	THR	6.7
1	B	51	ASP	6.3
1	A	442	GLY	6.2
1	B	443	GLY	6.1
1	B	460	HIS	5.8
1	A	50	THR	5.7
1	D	454	THR	5.7
1	A	115	ASP	5.6
1	B	57	LEU	5.3
1	C	443	GLY	5.3
1	B	54	LYS	5.2
1	A	114	ALA	5.1
1	A	11	GLY	5.1
1	D	48	SER	5.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	113	LEU	5.1
1	C	56	LEU	4.9
1	C	10	ALA	4.8
1	A	27	THR	4.8
1	D	54	LYS	4.8
1	A	113	LEU	4.8
1	B	459	HIS	4.7
1	C	441	PRO	4.7
1	C	453	VAL	4.6
1	A	441	PRO	4.5
1	A	30	SER	4.5
1	C	444	SER	4.5
1	C	113	LEU	4.4
1	B	29	SER	4.2
1	B	441	PRO	4.2
1	C	29	SER	4.2
1	B	445	ALA	4.1
1	C	445	ALA	4.1
1	A	55	GLU	4.0
1	D	56	LEU	4.0
1	C	376	LEU	4.0
1	B	124	ALA	4.0
1	A	51	ASP	4.0
1	A	444	SER	4.0
1	C	53	SER	3.9
1	B	444	SER	3.9
1	C	409	ARG	3.9
1	C	57	LEU	3.9
1	A	52	ASN	3.8
1	D	453	VAL	3.8
1	C	377	ASN	3.7
1	D	114	ALA	3.7
1	C	375	HIS	3.7
1	A	377	ASN	3.7
1	A	443	GLY	3.7
1	A	54	LYS	3.6
1	C	48	SER	3.6
1	A	445	ALA	3.6
1	B	453	VAL	3.5
1	C	378	GLN	3.5
1	A	59	LYS	3.5
1	C	49	HIS	3.4

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	31	ASP	3.4
1	B	52	ASN	3.3
1	C	11	GLY	3.3
1	B	122	THR	3.3
1	C	451	LYS	3.2
1	D	122	THR	3.1
1	D	11	GLY	3.1
1	D	58	ASP	3.1
1	C	410	HIS	3.0
1	B	55	GLU	2.9
1	C	420	VAL	2.9
1	A	122	THR	2.9
1	A	53	SER	2.9
1	B	461	HIS	2.9
1	C	367	GLU	2.9
1	D	12	SER	2.8
1	B	58	ASP	2.8
1	C	47	GLY	2.8
1	B	53	SER	2.8
1	A	456	GLY	2.8
1	B	409	ARG	2.8
1	A	12	SER	2.8
1	D	59	LYS	2.8
1	B	113	LEU	2.7
1	C	447	GLU	2.7
1	D	10	ALA	2.7
1	C	52	ASN	2.7
1	C	442	GLY	2.7
1	D	2	SER	2.7
1	C	55	GLU	2.6
1	D	49	HIS	2.6
1	D	409	ARG	2.6
1	C	419	PRO	2.5
1	C	417	GLY	2.5
1	C	54	LYS	2.5
1	A	376	LEU	2.5
1	C	371	ASN	2.5
1	B	10	ALA	2.4
1	D	31	ASP	2.3
1	A	460	HIS	2.3
1	B	123	ASN	2.2
1	B	12	SER	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	59	LYS	2.2
1	C	126	HIS	2.2
1	C	405	ARG	2.2
1	D	55	GLU	2.1
1	B	405	ARG	2.1
1	A	58	ASP	2.1
1	D	4	ILE	2.1

## 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(Å <sup>2</sup> )	Q<0.9
2	PO4	A	501	5/5	0.99	0.04	15,16,18,18	0
2	PO4	B	501	5/5	0.99	0.04	15,16,18,18	0
2	PO4	C	501	5/5	0.99	0.06	17,17,17,17	0
2	PO4	D	501	5/5	0.99	0.03	14,15,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.