



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:26 am GMT

PDB ID : 3OPV  
Title : Crystal structure of E. Coli purine nucleoside phosphorylase Arg24Ala mutant  
Authors : Mikleusevic, G.; Stefanic, Z.; Narzyk, M.; Wielgus-Kutrowska, B.; Bzowska, A.; Luic, M.  
Deposited on : 2010-09-02  
Resolution : 2.40 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

<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 : trunk28620  
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) : recalc28949

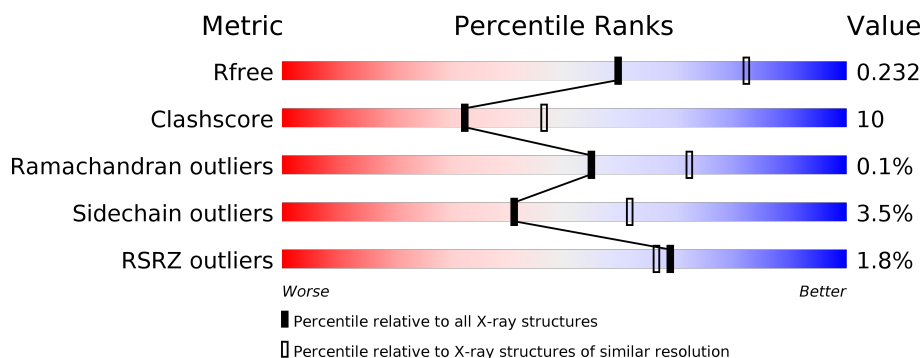
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.




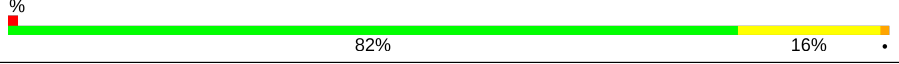

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	237	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	B	237	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	C	237	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
1	D	237	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>24%</div> <div>.</div> </div> </div>
1	E	237	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>.</div> </div> </div>
1	F	237	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	237	
1	H	237	
1	I	237	
1	J	237	
1	K	237	
1	L	237	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	L	239	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22982 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 Purine nucleoside phosphorylase deoD-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1788	1130	304	339	15			
1	B	237	Total	C	N	O	S	0	0	0
			1791	1132	305	339	15			
1	C	237	Total	C	N	O	S	0	1	0
			1796	1135	307	339	15			
1	D	237	Total	C	N	O	S	0	2	0
			1806	1142	310	339	15			
1	E	232	Total	C	N	O	S	0	0	0
			1749	1108	297	329	15			
1	F	237	Total	C	N	O	S	0	0	0
			1788	1130	304	339	15			
1	G	237	Total	C	N	O	S	0	0	0
			1788	1130	304	339	15			
1	H	237	Total	C	N	O	S	0	0	0
			1791	1132	305	339	15			
1	I	237	Total	C	N	O	S	0	0	0
			1791	1132	305	339	15			
1	J	233	Total	C	N	O	S	0	1	0
			1760	1115	299	331	15			
1	K	237	Total	C	N	O	S	0	0	0
			1787	1130	304	338	15			
1	L	237	Total	C	N	O	S	0	0	0
			1784	1127	303	339	15			

There are 12 discrepancies between the modelled and reference sequences:

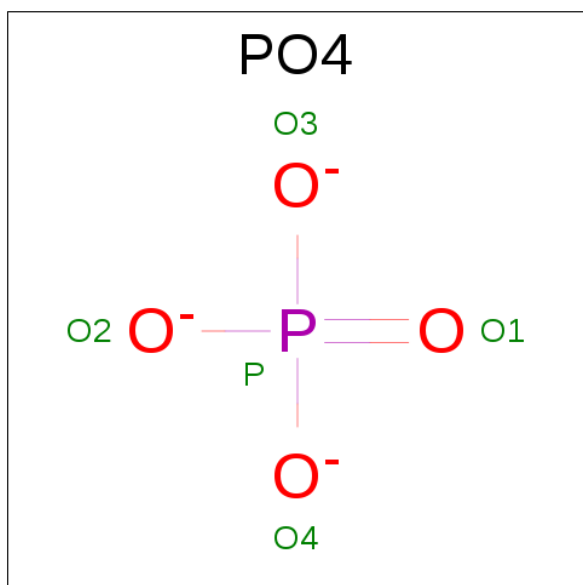
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6
B	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6
C	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6
D	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6
E	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6
G	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6
H	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6
I	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6
J	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6
K	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6
L	24	ALA	ARG	ENGINEERED MUTATION	UNP C9QST6

- 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	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		

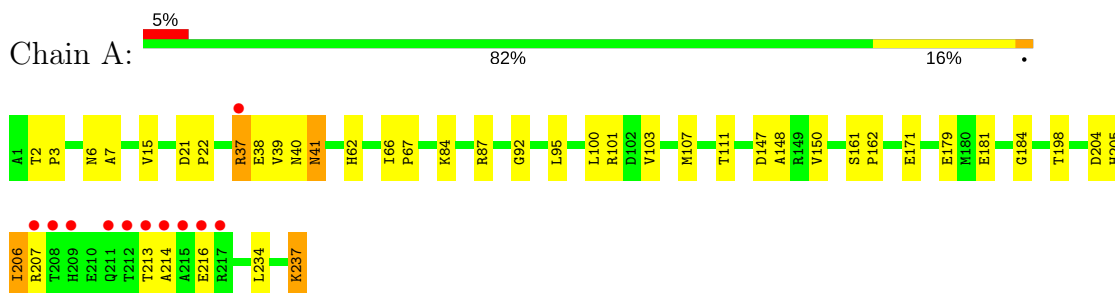
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total	O	0	0
			99	99		
3	B	136	Total	O	0	0
			136	136		
3	C	109	Total	O	0	0
			109	109		
3	D	151	Total	O	0	0
			151	151		
3	E	93	Total	O	0	0
			93	93		
3	F	104	Total	O	0	0
			104	104		
3	G	81	Total	O	0	0
			81	81		
3	H	155	Total	O	0	0
			155	155		
3	I	159	Total	O	0	0
			159	159		
3	J	131	Total	O	0	0
			131	131		
3	K	114	Total	O	0	0
			114	114		
3	L	161	Total	O	0	0
			161	161		

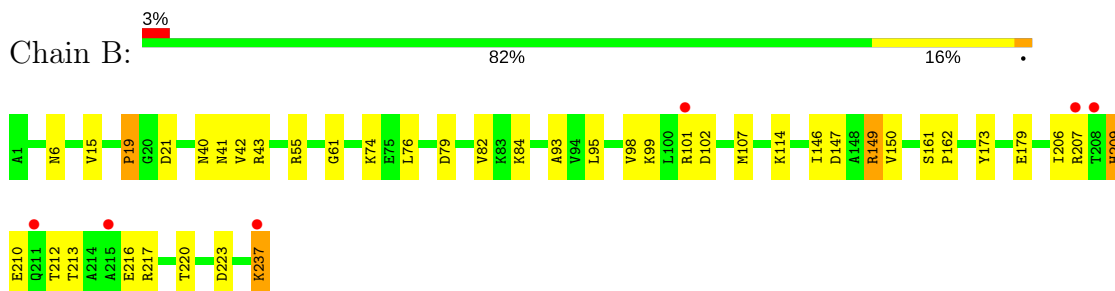
### 3 Residue-property plots [i](#)

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

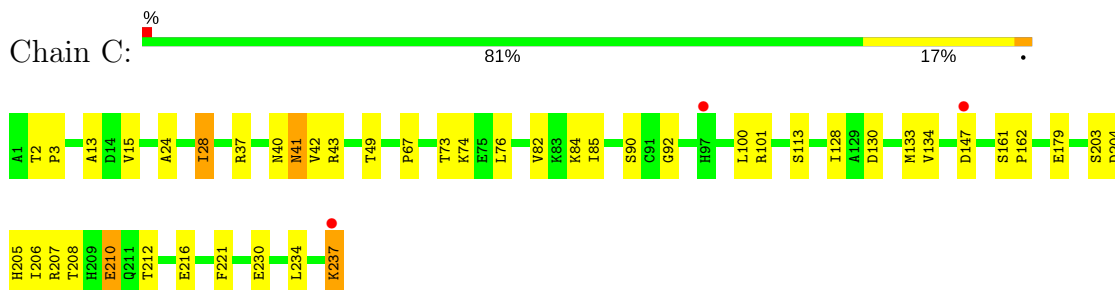
- Molecule 1: Purine nucleoside phosphorylase deoD-type



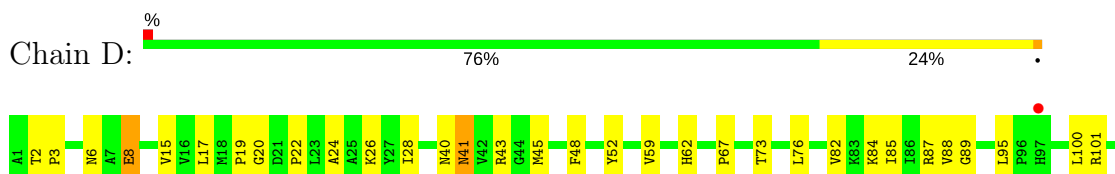
- Molecule 1: Purine nucleoside phosphorylase deoD-type



- Molecule 1: Purine nucleoside phosphorylase deoD-type

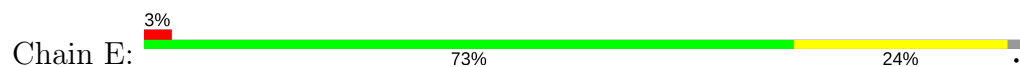


- Molecule 1: Purine nucleoside phosphorylase deoD-type

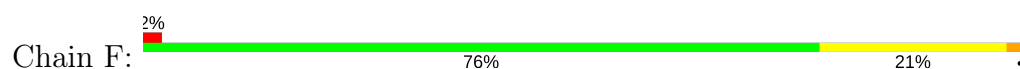




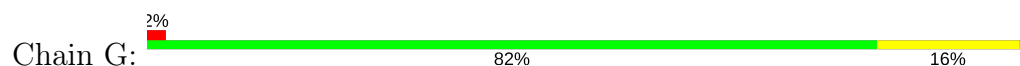
- Molecule 1: Purine nucleoside phosphorylase deoD-type



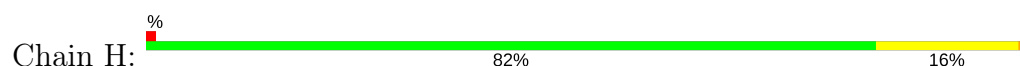
- Molecule 1: Purine nucleoside phosphorylase deoD-type



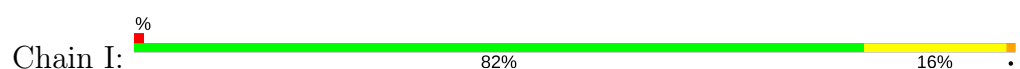
- Molecule 1: Purine nucleoside phosphorylase deoD-type



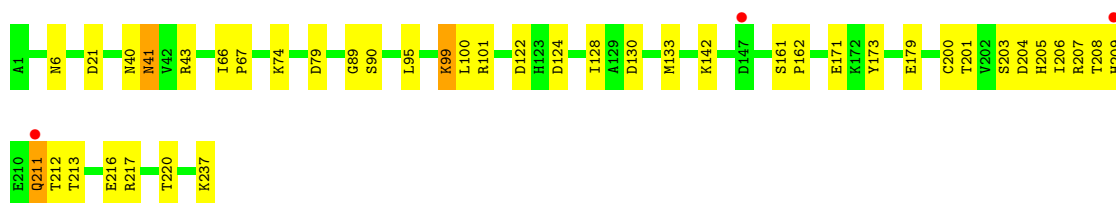
- Molecule 1: Purine nucleoside phosphorylase deoD-type



- Molecule 1: Purine nucleoside phosphorylase deoD-type

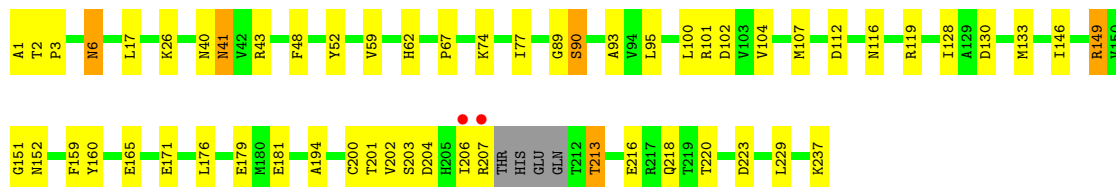






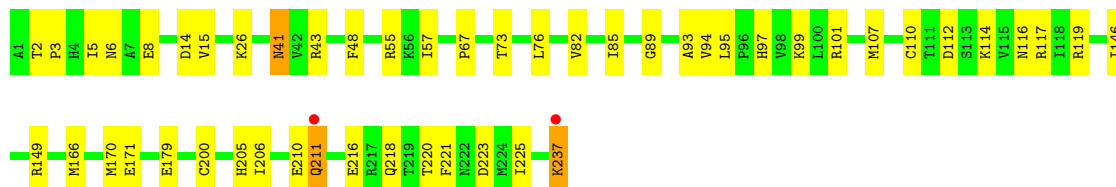
- Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain J: 74% 22%



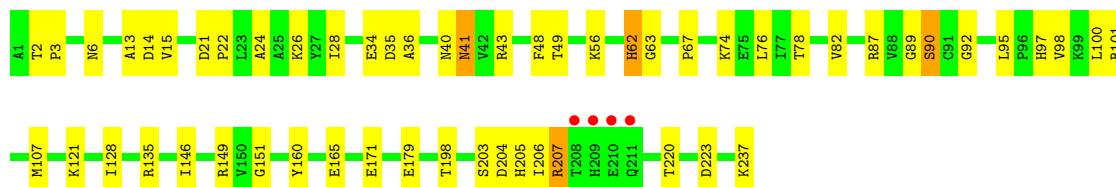
- Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain K: 79% 20%



- Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain L: 76% 22%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.21Å 158.78Å 122.24Å 90.00° 93.80° 90.00°	Depositor
Resolution (Å)	19.10 – 2.40 19.12 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.10-2.40) 100.0 (19.12-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.181 , 0.238 0.173 , 0.232	Depositor DCC
$R_{free}$ test set	1767 reflections (1.58%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.56 % 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 3.6178e-04. 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/1817	0.44	0/2451
1	B	0.27	0/1820	0.44	0/2454
1	C	0.25	0/1828	0.44	0/2465
1	D	0.28	0/1842	0.44	0/2483
1	E	0.25	0/1776	0.43	0/2392
1	F	0.28	0/1817	0.47	0/2451
1	G	0.25	0/1817	0.44	0/2451
1	H	0.27	0/1820	0.44	0/2454
1	I	0.27	0/1820	0.45	0/2454
1	J	0.26	0/1791	0.44	0/2414
1	K	0.26	0/1816	0.44	0/2449
1	L	0.28	0/1813	0.45	0/2447
All	All	0.27	0/21777	0.44	0/29365

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

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	1788	0	1785	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1791	0	1794	35	0
1	C	1796	0	1798	38	0
1	D	1806	0	1814	40	0
1	E	1749	0	1758	35	0
1	F	1788	0	1785	47	0
1	G	1788	0	1785	37	0
1	H	1791	0	1794	45	0
1	I	1791	0	1794	36	0
1	J	1760	0	1763	46	0
1	K	1787	0	1782	35	0
1	L	1784	0	1774	40	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
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	15	0	0	0	0
3	A	99	0	0	1	0
3	B	136	0	0	5	0
3	C	109	0	0	6	0
3	D	151	0	0	5	0
3	E	93	0	0	2	0
3	F	104	0	0	1	0
3	G	81	0	0	1	0
3	H	155	0	0	0	0
3	I	159	0	0	3	0
3	J	131	0	0	2	0
3	K	114	0	0	2	0
3	L	161	0	0	3	0
All	All	22982	0	21426	427	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 10.

All (427) 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:G:207:ARG:HH11	1:G:207:ARG:HG2	1.22	0.99
1:C:128:ILE:HD12	1:E:107:MET:HE3	1.53	0.89
1:F:207:ARG:HG2	1:F:208:THR:N	1.86	0.87
1:J:213:THR:HG22	1:J:216:GLU:H	1.39	0.87
1:G:107:MET:HE3	1:L:128:ILE:HD12	1.56	0.86
1:F:9:MET:SD	1:I:211:GLN:HB3	2.15	0.86
1:H:205:HIS:HD2	1:H:207:ARG:NH2	1.75	0.85
1:F:96:PRO:HG3	1:F:207:ARG:HH22	1.44	0.80
1:E:6:ASN:H	1:E:40:ASN:HD22	1.34	0.76
1:K:101:ARG:HB3	1:K:220:THR:HG21	1.67	0.76
1:A:234:LEU:O	1:A:237:LYS:HD2	1.86	0.76
1:B:101:ARG:HD3	1:B:216:GLU:HB2	1.68	0.75
1:F:15:VAL:HG22	1:F:84:LYS:HB2	1.69	0.74
1:E:15:VAL:HG22	1:E:84:LYS:HB2	1.70	0.74
1:I:211:GLN:HE21	1:I:211:GLN:H	1.34	0.73
1:F:212:THR:HG21	1:F:217:ARG:HG3	1.70	0.73
1:G:97:HIS:CD2	1:G:97:HIS:H	2.05	0.73
1:B:107:MET:SD	3:D:1020:HOH:O	2.47	0.72
1:C:90:SER:HB2	1:C:203:SER:HB3	1.70	0.72
1:I:100:LEU:HD11	1:I:204:ASP:HA	1.71	0.72
1:B:210:GLU:HG2	1:J:1:ALA:HB3	1.72	0.72
1:F:100:LEU:HD11	1:F:204:ASP:HA	1.71	0.71
1:K:73:THR:HG22	1:K:85:ILE:HD13	1.73	0.71
1:A:107:MET:HE2	1:A:150:VAL:HG12	1.71	0.71
1:G:15:VAL:HG22	1:G:84:LYS:HB2	1.72	0.71
1:F:213:THR:HB	1:F:216:GLU:HG2	1.73	0.70
1:H:205:HIS:CD2	1:H:207:ARG:NH2	2.59	0.70
1:H:128:ILE:HD12	1:J:107:MET:HE3	1.74	0.69
3:B:304:HOH:O	1:D:107:MET:SD	2.50	0.69
1:J:100:LEU:HD11	1:J:204:ASP:HA	1.75	0.69
1:H:101:ARG:HB3	1:H:220:THR:HG21	1.76	0.68
1:B:107:MET:HE1	1:D:131:PHE:HB2	1.76	0.68
1:H:15:VAL:HG22	1:H:84:LYS:HB2	1.76	0.68
1:A:6:ASN:H	1:A:40:ASN:ND2	1.92	0.67
1:H:101:ARG:HD2	1:H:220:THR:HG21	1.76	0.67
1:J:107:MET:HE2	1:J:151:GLY:HA2	1.77	0.67
1:L:171:GLU:OE1	1:L:207:ARG:NH2	2.28	0.66
1:F:217:ARG:HD2	3:F:1187:HOH:O	1.94	0.66
1:L:101:ARG:HD2	1:L:220:THR:OG1	1.96	0.66
1:B:107:MET:HE2	1:B:150:VAL:HG12	1.77	0.66
1:C:100:LEU:HD11	1:C:204:ASP:HA	1.78	0.66
1:F:96:PRO:HA	1:F:207:ARG:NH1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:HG22	1:B:216:GLU:HG2	1.78	0.65
1:C:76:LEU:HB3	1:C:82:VAL:HG21	1.78	0.65
1:G:135:ARG:NH1	1:L:135:ARG:HD2	2.11	0.65
1:H:205:HIS:CD2	1:H:207:ARG:HH22	2.14	0.65
1:F:212:THR:CG2	1:F:217:ARG:HG3	2.26	0.65
1:C:73:THR:HG22	1:C:85:ILE:HD13	1.78	0.65
1:G:207:ARG:HH11	1:G:207:ARG:CG	2.03	0.64
1:G:237:LYS:HE3	3:G:340:HOH:O	1.96	0.64
1:A:95:LEU:HD23	1:A:171:GLU:HG3	1.78	0.64
1:H:207:ARG:HD2	1:H:208:THR:H	1.62	0.64
1:A:100:LEU:HD11	1:A:204:ASP:HA	1.81	0.63
1:K:210:GLU:N	1:K:210:GLU:OE1	2.31	0.63
1:A:6:ASN:H	1:A:40:ASN:HD22	1.46	0.63
1:G:6:ASN:H	1:G:40:ASN:ND2	1.97	0.63
1:F:76:LEU:HB3	1:F:82:VAL:HG21	1.81	0.63
1:J:6:ASN:H	1:J:40:ASN:ND2	1.96	0.62
1:J:95:LEU:HD23	1:J:171:GLU:HG3	1.81	0.62
1:B:101:ARG:HG2	1:B:220:THR:HB	1.82	0.62
1:L:100:LEU:HD13	1:L:204:ASP:HA	1.80	0.62
1:E:6:ASN:H	1:E:40:ASN:ND2	1.97	0.62
1:E:95:LEU:HB2	1:E:98:VAL:HG23	1.82	0.62
1:H:41:ASN:N	1:H:41:ASN:HD22	1.98	0.62
1:I:90:SER:HB2	1:I:203:SER:HB3	1.81	0.61
1:G:52:TYR:HB3	1:G:57:ILE:HD12	1.83	0.61
1:G:221:PHE:O	1:G:225:ILE:HG12	2.01	0.61
1:C:208:THR:OG1	1:C:210:GLU:HG3	2.00	0.60
1:C:43:ARG:HA	1:F:21:ASP:OD1	2.01	0.60
1:A:67:PRO:HD2	1:D:67:PRO:HG2	1.82	0.60
1:B:76:LEU:HB3	1:B:82:VAL:HG21	1.84	0.60
1:G:62:HIS:CE1	1:G:181:GLU:HG2	2.35	0.60
1:J:26:LYS:HA	1:J:48:PHE:CE1	2.36	0.60
1:L:6:ASN:H	1:L:40:ASN:ND2	2.00	0.59
1:G:13:ALA:HB2	1:G:56:LYS:HG2	1.83	0.59
1:G:100:LEU:HD12	1:G:202:VAL:HG12	1.85	0.59
1:E:13:ALA:HB2	1:E:56:LYS:HG2	1.85	0.59
1:L:107:MET:HE2	1:L:151:GLY:HA2	1.84	0.59
1:D:233:LEU:N	3:D:1276:HOH:O	2.36	0.59
1:A:37:ARG:NE	1:A:37:ARG:HA	2.17	0.58
1:A:15:VAL:HG22	1:A:84:LYS:HB2	1.86	0.58
1:G:207:ARG:HG2	1:G:207:ARG:NH1	2.02	0.58
1:J:62:HIS:CE1	1:J:181:GLU:HG2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:HG	1:C:212:THR:HG23	1.86	0.58
1:F:205:HIS:HB3	1:F:208:THR:H	1.68	0.58
1:B:206:ILE:O	1:B:209:HIS:CE1	2.57	0.58
1:C:49:THR:HG23	3:C:276:HOH:O	2.02	0.58
1:I:128:ILE:HD12	1:K:107:MET:HE3	1.86	0.58
1:F:2:THR:HG22	1:F:79:ASP:OD2	2.04	0.58
1:A:41:ASN:HD22	1:A:41:ASN:H	1.52	0.57
1:G:205:HIS:ND1	1:G:207:ARG:HB3	2.19	0.57
1:C:205:HIS:CE1	1:C:207:ARG:HB2	2.38	0.57
1:F:237:LYS:HD3	1:F:237:LYS:O	2.03	0.57
1:F:90:SER:HB2	1:F:203:SER:HB3	1.86	0.57
1:I:67:PRO:HD2	1:L:67:PRO:HG2	1.86	0.57
1:J:41:ASN:HD22	1:J:41:ASN:H	1.52	0.57
1:H:41:ASN:H	1:H:41:ASN:HD22	1.52	0.57
1:A:41:ASN:HD22	1:A:41:ASN:N	2.01	0.57
1:D:230:GLU:O	3:D:1276:HOH:O	2.17	0.57
1:J:149:ARG:HG3	1:J:176:LEU:HD13	1.87	0.57
1:D:15:VAL:HG22	1:D:84:LYS:HB2	1.85	0.57
1:F:2:THR:HB	1:F:3:PRO:HD2	1.86	0.57
1:E:100:LEU:HD11	1:E:204:ASP:HA	1.87	0.57
1:C:101:ARG:HD3	1:C:216:GLU:OE1	2.04	0.56
1:I:204:ASP:HB2	3:I:1329:HOH:O	2.05	0.56
1:D:230:GLU:C	3:D:1276:HOH:O	2.43	0.56
1:G:234:LEU:O	1:G:237:LYS:HD2	2.04	0.56
1:H:73:THR:HG22	1:H:85:ILE:HD13	1.87	0.56
1:D:147:ASP:HA	3:D:775:HOH:O	2.04	0.56
1:G:67:PRO:HD2	1:J:67:PRO:HG2	1.86	0.56
1:C:230:GLU:HB3	3:C:262:HOH:O	2.05	0.56
1:C:37:ARG:NE	1:C:37:ARG:HA	2.21	0.56
1:J:107:MET:HB2	3:J:534:HOH:O	2.06	0.56
1:L:97:HIS:CD2	1:L:149:ARG:HH12	2.24	0.56
1:E:101:ARG:NH1	1:E:216:GLU:HB3	2.21	0.55
1:H:130:ASP:OD2	1:H:133:MET:HG3	2.07	0.55
1:G:95:LEU:HD23	1:G:171:GLU:HG3	1.88	0.55
1:E:205:HIS:ND1	1:E:207:ARG:HG2	2.22	0.55
1:G:205:HIS:HB3	1:G:210:GLU:OE1	2.07	0.55
1:H:6:ASN:H	1:H:40:ASN:ND2	2.04	0.55
1:J:146:ILE:HD13	1:J:223:ASP:HB3	1.88	0.55
1:D:8:GLU:HA	1:D:8:GLU:OE2	2.07	0.55
1:I:201:THR:HG21	1:I:220:THR:HG22	1.89	0.55
1:B:237:LYS:HD2	3:B:1016:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ALA:O	1:D:28:ILE:HG13	2.07	0.55
1:C:40:ASN:HD21	1:C:42:VAL:HG23	1.72	0.55
1:L:76:LEU:HB3	1:L:82:VAL:HG21	1.88	0.55
1:A:87:ARG:HG2	1:A:198:THR:HG23	1.89	0.54
1:C:15:VAL:HG22	1:C:84:LYS:HB2	1.89	0.54
1:B:19:PRO:O	1:B:61:GLY:HA2	2.06	0.54
1:E:66:ILE:HB	1:E:67:PRO:HD3	1.89	0.54
1:F:41:ASN:N	1:F:41:ASN:HD22	2.04	0.54
1:K:237:LYS:HD3	1:K:237:LYS:O	2.08	0.54
1:F:96:PRO:CA	1:F:207:ARG:HH12	2.21	0.54
1:B:99:LYS:O	1:B:102:ASP:HB2	2.07	0.54
1:F:96:PRO:HA	1:F:207:ARG:HH12	1.71	0.54
1:H:207:ARG:HD2	1:H:207:ARG:H	1.73	0.54
1:G:66:ILE:HB	1:G:67:PRO:HD3	1.90	0.54
1:E:74:LYS:C	1:E:74:LYS:HD3	2.28	0.54
1:A:107:MET:HE1	1:F:131:PHE:HB2	1.90	0.53
1:F:6:ASN:H	1:F:40:ASN:ND2	2.06	0.53
1:I:237:LYS:HD2	3:I:1156:HOH:O	2.08	0.53
1:E:100:LEU:O	1:E:101:ARG:HB2	2.08	0.53
1:H:87:ARG:HG2	1:H:198:THR:HG23	1.89	0.53
1:H:116:ASN:ND2	1:H:119:ARG:HH11	2.06	0.53
1:I:43:ARG:HA	1:L:21:ASP:OD1	2.08	0.53
1:F:213:THR:HG22	1:F:215:ALA:H	1.73	0.53
1:K:146:ILE:HD13	1:K:223:ASP:HB3	1.91	0.53
1:A:37:ARG:HA	1:A:37:ARG:HE	1.74	0.52
1:I:101:ARG:HD3	1:I:216:GLU:HB3	1.91	0.52
1:H:98:VAL:HA	1:H:149:ARG:NH1	2.24	0.52
1:C:24:ALA:O	1:C:28:ILE:HD12	2.09	0.52
1:G:21:ASP:OD1	1:J:43:ARG:HA	2.10	0.52
1:H:98:VAL:HG22	1:H:149:ARG:HH11	1.75	0.52
1:K:166:MET:O	1:K:170:MET:HG3	2.10	0.52
1:F:2:THR:HB	1:F:3:PRO:CD	2.40	0.52
1:J:89:GLY:O	1:J:200:CYS:HA	2.10	0.52
1:A:205:HIS:C	1:A:207:ARG:H	2.14	0.51
1:B:213:THR:HG22	1:B:216:GLU:CG	2.40	0.51
1:K:89:GLY:O	1:K:200:CYS:HA	2.10	0.51
1:B:212:THR:CG2	1:B:217:ARG:HG3	2.40	0.51
1:I:89:GLY:O	1:I:200:CYS:HA	2.10	0.51
1:F:237:LYS:C	1:F:237:LYS:HD3	2.31	0.51
1:E:6:ASN:HB2	1:E:42:VAL:HG23	1.92	0.51
1:C:74:LYS:C	1:C:74:LYS:HD3	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:THR:HG22	1:A:214:ALA:H	1.75	0.51
1:A:67:PRO:HG2	1:D:67:PRO:HD2	1.93	0.51
1:D:101:ARG:HB3	1:D:220:THR:HG21	1.93	0.51
1:E:97:HIS:H	1:E:97:HIS:CD2	2.28	0.51
1:D:6:ASN:H	1:D:40:ASN:ND2	2.08	0.51
1:L:74:LYS:C	1:L:74:LYS:HD3	2.31	0.51
1:D:107:MET:CE	1:D:151:GLY:HA2	2.40	0.50
1:B:95:LEU:O	1:B:98:VAL:HG22	2.11	0.50
1:C:101:ARG:HD3	1:C:216:GLU:CD	2.31	0.50
1:I:95:LEU:HD23	1:I:171:GLU:HG3	1.94	0.50
1:I:74:LYS:HD3	1:I:74:LYS:C	2.32	0.50
1:F:41:ASN:H	1:F:41:ASN:HD22	1.60	0.50
1:D:26:LYS:HA	1:D:48:PHE:CE1	2.46	0.50
1:I:237:LYS:O	1:I:237:LYS:HD3	2.12	0.50
1:J:6:ASN:H	1:J:40:ASN:HD22	1.59	0.50
1:K:93:ALA:HB3	1:K:205:HIS:CD2	2.46	0.50
1:E:89:GLY:O	1:E:200:CYS:HA	2.12	0.50
1:C:28:ILE:HD11	1:C:221:PHE:CZ	2.47	0.50
1:E:95:LEU:HD23	1:E:171:GLU:HG3	1.93	0.49
1:G:107:MET:HE3	1:L:128:ILE:CD1	2.38	0.49
1:C:237:LYS:HE3	3:C:1349:HOH:O	2.12	0.49
1:D:73:THR:HG22	1:D:85:ILE:HD13	1.93	0.49
1:H:76:LEU:HB3	1:H:82:VAL:HG21	1.93	0.49
1:B:98:VAL:HA	1:B:149:ARG:NH1	2.27	0.49
1:E:90:SER:HB2	1:E:203:SER:HB3	1.94	0.49
1:A:147:ASP:HA	3:A:849:HOH:O	2.12	0.49
1:F:74:LYS:HD3	1:F:74:LYS:C	2.32	0.49
1:G:207:ARG:CG	1:G:207:ARG:NH1	2.68	0.49
1:C:234:LEU:O	1:C:237:LYS:HD2	2.13	0.49
1:G:74:LYS:C	1:G:74:LYS:HD3	2.33	0.49
1:L:41:ASN:HD22	1:L:41:ASN:C	2.15	0.49
1:G:114:LYS:HE2	1:J:112:ASP:O	2.13	0.49
1:L:2:THR:HB	1:L:3:PRO:HD2	1.94	0.49
1:H:98:VAL:O	1:H:205:HIS:HE1	1.96	0.49
1:K:95:LEU:HD23	1:K:171:GLU:HG3	1.95	0.49
1:L:13:ALA:HB2	1:L:56:LYS:HG2	1.94	0.49
1:K:221:PHE:O	1:K:225:ILE:HG12	2.13	0.48
1:L:146:ILE:HD13	1:L:223:ASP:HB3	1.95	0.48
1:E:6:ASN:HB2	1:E:42:VAL:CG2	2.43	0.48
1:H:52:TYR:HB3	1:H:57:ILE:HD12	1.96	0.48
1:B:146:ILE:HD13	1:B:223:ASP:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:212:THR:HG22	1:I:217:ARG:HG3	1.95	0.48
1:J:101:ARG:HD2	1:J:220:THR:OG1	2.12	0.48
1:F:221:PHE:O	1:F:225:ILE:HG12	2.13	0.48
1:D:107:MET:HE3	1:D:151:GLY:HA2	1.96	0.48
1:G:24:ALA:O	1:G:28:ILE:HG13	2.13	0.48
1:C:37:ARG:HE	1:C:37:ARG:HA	1.79	0.48
1:G:6:ASN:H	1:G:40:ASN:HD22	1.62	0.48
1:H:101:ARG:HD2	1:H:220:THR:CG2	2.44	0.48
1:C:13:ALA:HB2	3:C:276:HOH:O	2.14	0.48
1:H:67:PRO:HD2	1:K:67:PRO:HG2	1.96	0.48
1:K:26:LYS:HA	1:K:48:PHE:CE1	2.49	0.48
1:F:21:ASP:OD1	1:F:22:PRO:HD2	2.14	0.47
1:I:74:LYS:HD2	1:L:160:TYR:CE2	2.49	0.47
1:C:40:ASN:HA	3:C:248:HOH:O	2.14	0.47
1:E:146:ILE:HD13	1:E:223:ASP:HB3	1.96	0.47
1:I:173:TYR:CE2	1:K:119:ARG:HD3	2.50	0.47
1:K:76:LEU:HB3	1:K:82:VAL:HG21	1.96	0.47
1:L:87:ARG:HG2	1:L:198:THR:HG23	1.96	0.47
1:E:87:ARG:HG2	1:E:198:THR:HG23	1.95	0.47
1:F:212:THR:HG21	1:F:217:ARG:CG	2.40	0.47
1:B:93:ALA:HB1	1:B:98:VAL:CG2	2.43	0.47
1:H:207:ARG:CD	1:H:207:ARG:H	2.26	0.47
1:J:100:LEU:HD12	1:J:202:VAL:HG12	1.97	0.47
1:K:93:ALA:O	1:K:206:ILE:HG23	2.15	0.47
1:L:24:ALA:O	1:L:28:ILE:HG13	2.15	0.47
3:B:304:HOH:O	1:D:107:MET:HB2	2.15	0.47
1:I:100:LEU:CD1	1:I:204:ASP:HA	2.41	0.47
1:B:6:ASN:H	1:B:40:ASN:ND2	2.13	0.47
1:J:100:LEU:HD11	1:J:204:ASP:CA	2.44	0.47
1:L:74:LYS:HE2	1:L:78:THR:HG21	1.96	0.47
1:E:130:ASP:O	1:E:134:VAL:HG23	2.15	0.47
1:F:29:ALA:O	1:F:33:LEU:HB2	2.15	0.47
1:F:96:PRO:N	1:F:207:ARG:HH12	2.13	0.47
1:H:207:ARG:HD2	1:H:207:ARG:N	2.30	0.47
1:C:2:THR:HB	1:C:3:PRO:HD2	1.97	0.47
1:D:22:PRO:HG3	1:D:45:MET:SD	2.54	0.47
1:D:100:LEU:CD1	1:D:204:ASP:HA	2.45	0.46
1:F:95:LEU:HD23	1:F:171:GLU:HG3	1.96	0.46
1:K:97:HIS:HD2	1:K:149:ARG:NH2	2.13	0.46
1:B:213:THR:HG23	1:B:216:GLU:H	1.81	0.46
1:D:2:THR:HB	1:D:3:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:98:VAL:O	1:H:205:HIS:CE1	2.68	0.46
1:F:13:ALA:HB2	1:F:56:LYS:HG2	1.98	0.46
1:F:140:ALA:HB2	1:F:234:LEU:HD12	1.98	0.46
1:I:211:GLN:HE21	1:I:211:GLN:N	2.07	0.46
1:B:40:ASN:HA	3:B:276:HOH:O	2.15	0.46
1:I:205:HIS:ND1	1:I:207:ARG:HB2	2.30	0.46
1:B:43:ARG:HD3	3:E:281:HOH:O	2.15	0.46
1:H:128:ILE:HD13	1:J:152:ASN:OD1	2.16	0.46
1:I:99:LYS:HA	1:I:99:LYS:NZ	2.31	0.46
1:A:7:ALA:HB2	1:A:39:VAL:O	2.15	0.46
1:J:41:ASN:ND2	1:J:41:ASN:N	2.61	0.46
1:D:146:ILE:HD13	1:D:223:ASP:HB3	1.98	0.46
1:F:113:SER:OG	1:F:115:VAL:HG22	2.16	0.46
1:H:62:HIS:CE1	1:H:181:GLU:HG2	2.50	0.46
1:H:121:LYS:HD2	1:J:165:GLU:OE2	2.16	0.46
1:K:14:ASP:OD1	1:K:15:VAL:HG23	2.16	0.46
1:A:213:THR:HG22	1:A:214:ALA:N	2.31	0.45
1:E:73:THR:HG22	1:E:85:ILE:HD13	1.98	0.45
1:D:2:THR:HB	1:D:3:PRO:CD	2.46	0.45
1:E:166:MET:O	1:E:170:MET:HG3	2.17	0.45
1:B:210:GLU:CG	1:J:1:ALA:HB3	2.43	0.45
1:A:161:SER:HA	1:A:162:PRO:HD3	1.79	0.45
1:G:135:ARG:CZ	1:L:135:ARG:HD2	2.45	0.45
1:J:41:ASN:HD22	1:J:41:ASN:N	2.08	0.45
1:D:87:ARG:HG2	1:D:198:THR:HG23	1.97	0.45
1:D:41:ASN:H	1:D:41:ASN:HD22	1.63	0.45
1:I:124:ASP:O	1:K:110:CYS:HB3	2.17	0.45
1:B:74:LYS:HD3	1:B:74:LYS:C	2.37	0.45
1:C:13:ALA:CB	3:C:276:HOH:O	2.65	0.45
1:G:66:ILE:HG23	1:G:184:GLY:HA3	1.97	0.45
1:G:205:HIS:CB	1:G:210:GLU:OE1	2.64	0.45
1:E:214:ALA:HA	1:E:217:ARG:HH11	1.80	0.45
1:G:228:ALA:O	1:G:232:VAL:HG23	2.15	0.45
1:I:6:ASN:H	1:I:40:ASN:ND2	2.14	0.45
1:A:2:THR:HB	1:A:3:PRO:HD2	1.99	0.45
1:A:37:ARG:CZ	1:A:38:GLU:H	2.29	0.45
1:I:209:HIS:HA	3:I:1329:HOH:O	2.16	0.45
1:H:114:LYS:HE2	1:K:112:ASP:O	2.17	0.45
1:K:43:ARG:HD3	3:K:562:HOH:O	2.17	0.45
1:C:40:ASN:ND2	1:C:42:VAL:HG23	2.30	0.45
1:A:21:ASP:OD1	1:D:43:ARG:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:ARG:CZ	1:H:216:GLU:HB3	2.47	0.44
1:F:24:ALA:O	1:F:28:ILE:HG13	2.16	0.44
1:I:205:HIS:HB3	1:I:208:THR:H	1.82	0.44
1:L:14:ASP:OD1	1:L:15:VAL:HG23	2.17	0.44
1:E:122:ASP:HB2	3:E:272:HOH:O	2.16	0.44
1:H:205:HIS:HD2	1:H:207:ARG:CZ	2.27	0.44
1:K:211:GLN:H	1:K:211:GLN:HG2	1.39	0.44
1:K:55:ARG:HG3	1:K:57:ILE:HD11	2.00	0.44
1:I:206:ILE:H	1:I:206:ILE:HG12	1.63	0.44
1:K:116:ASN:ND2	1:K:119:ARG:HH11	2.16	0.44
1:K:94:VAL:HG12	1:K:206:ILE:HG21	1.99	0.44
1:D:20:GLY:HA2	1:D:62:HIS:CE1	2.52	0.44
1:B:43:ARG:HA	1:E:21:ASP:OD1	2.18	0.44
1:I:66:ILE:HB	1:I:67:PRO:HD3	1.99	0.44
1:L:26:LYS:HA	1:L:48:PHE:CE1	2.51	0.44
1:B:161:SER:HA	1:B:162:PRO:HD3	1.82	0.44
1:C:67:PRO:HG2	1:F:67:PRO:HD2	2.00	0.44
1:I:130:ASP:OD2	1:I:133:MET:HG3	2.18	0.44
1:G:62:HIS:ND1	1:G:63:GLY:O	2.49	0.44
1:B:237:LYS:HD3	1:B:237:LYS:O	2.18	0.44
1:J:104:VAL:HG12	1:J:149:ARG:CG	2.47	0.44
1:L:62:HIS:ND1	1:L:63:GLY:O	2.50	0.44
1:H:107:MET:HE3	1:J:128:ILE:HD12	2.00	0.43
1:K:2:THR:HB	1:K:3:PRO:CD	2.48	0.43
1:A:66:ILE:HB	1:A:67:PRO:HD3	2.00	0.43
1:H:205:HIS:CD2	1:H:207:ARG:CZ	3.01	0.43
1:H:74:LYS:C	1:H:74:LYS:HD3	2.39	0.43
1:A:103:VAL:O	1:A:148:ALA:HA	2.18	0.43
1:D:76:LEU:HB3	1:D:82:VAL:HG21	1.99	0.43
1:E:26:LYS:HA	1:E:48:PHE:CE1	2.53	0.43
1:G:73:THR:HG22	1:G:85:ILE:HD13	1.99	0.43
1:D:221:PHE:O	1:D:225:ILE:HG12	2.19	0.43
1:A:111:THR:HG22	1:F:124:ASP:HB2	2.00	0.43
1:H:227:ILE:O	1:H:231:SER:HB3	2.19	0.43
1:J:2:THR:HB	1:J:3:PRO:CD	2.48	0.43
1:B:15:VAL:HG22	1:B:84:LYS:HB2	2.01	0.43
1:E:62:HIS:CE1	1:E:181:GLU:HG2	2.53	0.43
1:E:99:LYS:HB2	1:E:102:ASP:OD1	2.18	0.43
1:L:92:GLY:HA3	1:L:206:ILE:HD11	2.01	0.43
1:C:130:ASP:O	1:C:134:VAL:HG23	2.18	0.43
1:C:237:LYS:HD3	1:C:237:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:SER:HA	1:D:162:PRO:HD3	1.86	0.43
1:L:2:THR:HB	1:L:3:PRO:CD	2.49	0.43
1:D:41:ASN:N	1:D:41:ASN:HD22	2.15	0.43
1:H:207:ARG:HD2	1:H:208:THR:N	2.33	0.43
1:A:100:LEU:O	1:A:101:ARG:HB2	2.19	0.43
1:A:101:ARG:NH1	1:A:216:GLU:HB2	2.34	0.43
3:J:533:HOH:O	1:K:114:LYS:HE3	2.18	0.43
1:J:116:ASN:ND2	1:J:119:ARG:HH11	2.16	0.43
1:K:41:ASN:HD22	1:K:41:ASN:C	2.21	0.43
1:B:114:LYS:HE2	1:E:112:ASP:O	2.18	0.43
1:I:212:THR:CG2	1:I:217:ARG:HG3	2.48	0.43
1:J:41:ASN:ND2	1:J:41:ASN:H	2.17	0.43
1:K:2:THR:OG1	1:K:5:ILE:HB	2.19	0.42
1:A:62:HIS:CE1	1:A:181:GLU:HG2	2.53	0.42
1:B:212:THR:HG22	1:B:217:ARG:HG3	2.00	0.42
1:C:161:SER:HA	1:C:162:PRO:HD3	1.87	0.42
1:H:6:ASN:H	1:H:40:ASN:HD22	1.67	0.42
1:K:101:ARG:NH1	1:K:216:GLU:HB3	2.34	0.42
1:K:2:THR:HB	1:K:3:PRO:HD2	2.00	0.42
1:L:90:SER:HB3	1:L:203:SER:HB3	2.01	0.42
1:J:93:ALA:O	1:J:206:ILE:HG13	2.19	0.42
1:J:52:TYR:CD1	1:J:229:LEU:HD13	2.54	0.42
1:B:147:ASP:HA	3:B:1253:HOH:O	2.19	0.42
1:D:19:PRO:HA	1:D:88:VAL:O	2.19	0.42
1:D:89:GLY:O	1:D:200:CYS:HA	2.19	0.42
1:E:18:MET:CE	1:E:62:HIS:HB3	2.50	0.42
1:G:41:ASN:N	1:G:41:ASN:HD22	2.17	0.42
1:H:73:THR:HG22	1:H:85:ILE:CD1	2.49	0.42
1:L:34:GLU:O	1:L:35:ASP:HB2	2.20	0.42
1:A:21:ASP:HA	1:A:22:PRO:HD2	1.91	0.42
1:F:146:ILE:HD13	1:F:223:ASP:HB3	2.01	0.42
1:F:96:PRO:HG3	1:F:207:ARG:NH2	2.22	0.42
1:E:213:THR:HG23	1:E:215:ALA:H	1.85	0.42
1:E:5:ILE:HA	1:E:40:ASN:ND2	2.35	0.42
1:F:210:GLU:O	1:F:211:GLN:NE2	2.46	0.42
1:L:6:ASN:HB3	3:L:628:HOH:O	2.19	0.42
1:H:38:GLU:OE2	1:H:41:ASN:HB3	2.20	0.42
1:L:36:ALA:HA	1:L:49:THR:O	2.19	0.42
1:H:67:PRO:HG2	1:K:67:PRO:HD2	2.02	0.42
1:C:2:THR:HB	1:C:3:PRO:CD	2.50	0.42
1:J:6:ASN:HD22	1:J:6:ASN:C	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:165:GLU:HG2	3:L:622:HOH:O	2.20	0.42
1:I:21:ASP:OD1	1:L:43:ARG:HA	2.19	0.42
1:B:149:ARG:H	1:B:149:ARG:HG2	1.77	0.41
1:H:98:VAL:HA	1:H:149:ARG:HH11	1.85	0.41
1:H:128:ILE:CD1	1:J:107:MET:HE3	2.46	0.41
1:J:207:ARG:HD3	1:J:207:ARG:HA	1.83	0.41
1:C:133:MET:HE2	1:C:133:MET:HB3	1.73	0.41
1:D:17:LEU:O	1:D:59:VAL:HA	2.19	0.41
1:J:159:PHE:HD1	1:J:160:TYR:CE2	2.38	0.41
1:C:130:ASP:OD2	1:C:133:MET:HG3	2.20	0.41
1:C:24:ALA:O	1:C:28:ILE:CD1	2.68	0.41
1:I:74:LYS:HE3	1:L:160:TYR:CE1	2.55	0.41
1:L:95:LEU:O	1:L:205:HIS:HE1	2.03	0.41
1:C:92:GLY:HA3	1:C:206:ILE:HD11	2.02	0.41
1:D:95:LEU:HD23	1:D:171:GLU:HG3	2.01	0.41
1:G:2:THR:HB	1:G:3:PRO:HD2	2.01	0.41
1:I:41:ASN:HD22	1:I:41:ASN:C	2.24	0.41
1:J:206:ILE:O	1:J:206:ILE:HG22	2.20	0.41
1:K:8:GLU:HG2	3:K:563:HOH:O	2.21	0.41
1:A:92:GLY:HA3	1:A:206:ILE:HD11	2.02	0.41
1:D:52:TYR:CE2	1:D:233:LEU:HD11	2.56	0.41
1:K:99:LYS:HD3	1:K:99:LYS:HA	1.92	0.41
1:L:21:ASP:HA	1:L:22:PRO:HD2	1.94	0.41
1:B:21:ASP:OD1	1:E:43:ARG:HA	2.20	0.41
1:E:88:VAL:O	1:E:88:VAL:HG23	2.21	0.41
1:G:95:LEU:HA	1:G:96:PRO:HD3	1.92	0.41
1:I:213:THR:OG1	1:I:216:GLU:HG3	2.20	0.41
1:J:104:VAL:HG12	1:J:149:ARG:HG2	2.01	0.41
1:L:98:VAL:O	1:L:205:HIS:NE2	2.54	0.41
1:J:74:LYS:HD3	1:J:74:LYS:C	2.41	0.41
1:F:100:LEU:HA	1:F:100:LEU:HD12	1.89	0.41
1:F:165:GLU:O	1:F:165:GLU:HG2	2.20	0.41
1:H:13:ALA:HB2	1:H:56:LYS:HG2	2.01	0.41
1:H:18:MET:HA	1:H:60:MET:O	2.20	0.41
1:J:102:ASP:O	1:J:201:THR:HA	2.21	0.41
1:D:165:GLU:O	1:D:165:GLU:HG2	2.19	0.41
1:F:116:ASN:ND2	1:F:119:ARG:HH11	2.19	0.41
1:I:122:ASP:O	1:K:117:ARG:NH2	2.52	0.41
1:C:100:LEU:O	1:C:101:ARG:HB2	2.21	0.41
1:D:130:ASP:O	1:D:134:VAL:HG23	2.21	0.41
1:D:213:THR:O	1:D:217:ARG:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2:THR:HB	1:J:3:PRO:HD2	2.03	0.41
1:B:173:TYR:CZ	1:D:119:ARG:HB3	2.56	0.40
1:I:161:SER:HA	1:I:162:PRO:HD3	1.88	0.40
1:L:87:ARG:CG	1:L:198:THR:HG23	2.50	0.40
1:L:89:GLY:HA2	3:L:807:HOH:O	2.20	0.40
1:G:100:LEU:HD22	1:G:210:GLU:HG3	2.03	0.40
1:J:90:SER:HB2	1:J:203:SER:HB3	2.03	0.40
1:A:66:ILE:HG23	1:A:184:GLY:HA3	2.03	0.40
1:C:41:ASN:HD22	1:C:41:ASN:N	2.18	0.40
1:J:17:LEU:O	1:J:59:VAL:HA	2.21	0.40
1:J:77:ILE:HD13	1:J:194:ALA:HB3	2.03	0.40
1:B:40:ASN:HD21	1:B:42:VAL:HG23	1.87	0.40
1:F:51:THR:HA	1:F:55:ARG:O	2.22	0.40
1:F:95:LEU:HA	1:F:96:PRO:HD3	1.84	0.40
1:J:130:ASP:OD2	1:J:133:MET:HG3	2.22	0.40
1:L:121:LYS:HE2	1:L:121:LYS:HB3	1.90	0.40

There are no symmetry-related clashes.

## 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	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
1	B	235/237 (99%)	225 (96%)	9 (4%)	1 (0%)	38	54
1	C	236/237 (100%)	221 (94%)	15 (6%)	0	100	100
1	D	237/237 (100%)	228 (96%)	9 (4%)	0	100	100
1	E	228/237 (96%)	218 (96%)	10 (4%)	0	100	100
1	F	235/237 (99%)	220 (94%)	14 (6%)	1 (0%)	38	54
1	G	235/237 (99%)	226 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	235/237 (99%)	228 (97%)	7 (3%)	0	100	100
1	I	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
1	J	230/237 (97%)	223 (97%)	7 (3%)	0	100	100
1	K	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
1	L	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
All	All	2811/2844 (99%)	2686 (96%)	123 (4%)	2 (0%)	55	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	210	GLU
1	B	209	HIS

### 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	186/187 (100%)	181 (97%)	5 (3%)	50	71
1	B	187/187 (100%)	179 (96%)	8 (4%)	33	52
1	C	187/187 (100%)	180 (96%)	7 (4%)	39	59
1	D	189/187 (101%)	184 (97%)	5 (3%)	51	72
1	E	182/187 (97%)	174 (96%)	8 (4%)	33	51
1	F	186/187 (100%)	179 (96%)	7 (4%)	38	58
1	G	186/187 (100%)	179 (96%)	7 (4%)	38	58
1	H	187/187 (100%)	182 (97%)	5 (3%)	50	71
1	I	187/187 (100%)	181 (97%)	6 (3%)	44	65
1	J	183/187 (98%)	175 (96%)	8 (4%)	33	51
1	K	185/187 (99%)	179 (97%)	6 (3%)	44	65
1	L	185/187 (99%)	179 (97%)	6 (3%)	44	65
All	All	2230/2244 (99%)	2152 (96%)	78 (4%)	41	61



All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	41	ASN
1	A	179	GLU
1	A	206	ILE
1	A	237	LYS
1	B	19	PRO
1	B	41	ASN
1	B	55	ARG
1	B	79	ASP
1	B	149	ARG
1	B	179	GLU
1	B	207	ARG
1	B	237	LYS
1	C	28	ILE
1	C	41	ASN
1	C	113	SER
1	C	147	ASP
1	C	179	GLU
1	C	210	GLU
1	C	237	LYS
1	D	8	GLU
1	D	41	ASN
1	D	157	ASP
1	D	179	GLU
1	D	237	LYS
1	E	6	ASN
1	E	41	ASN
1	E	55	ARG
1	E	79	ASP
1	E	120	PHE
1	E	179	GLU
1	E	218	GLN
1	E	237	LYS
1	F	6	ASN
1	F	41	ASN
1	F	179	GLU
1	F	207	ARG
1	F	208	THR
1	F	209	HIS
1	F	212	THR
1	G	6	ASN
1	G	41	ASN

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Mol	Chain	Res	Type
1	G	97	HIS
1	G	179	GLU
1	G	207	ARG
1	G	211	GLN
1	G	237	LYS
1	H	41	ASN
1	H	149	ARG
1	H	175	ILE
1	H	179	GLU
1	H	207	ARG
1	I	41	ASN
1	I	79	ASP
1	I	99	LYS
1	I	142	LYS
1	I	179	GLU
1	I	211	GLN
1	J	6	ASN
1	J	41	ASN
1	J	90	SER
1	J	149	ARG
1	J	179	GLU
1	J	213	THR
1	J	218	GLN
1	J	237	LYS
1	K	6	ASN
1	K	41	ASN
1	K	179	GLU
1	K	211	GLN
1	K	218	GLN
1	K	237	LYS
1	L	41	ASN
1	L	62	HIS
1	L	90	SER
1	L	179	GLU
1	L	207	ARG
1	L	237	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	40	ASN

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Mol	Chain	Res	Type
1	A	41	ASN
1	A	116	ASN
1	A	136	ASN
1	A	211	GLN
1	A	222	ASN
1	B	6	ASN
1	B	40	ASN
1	B	41	ASN
1	B	116	ASN
1	B	209	HIS
1	B	222	ASN
1	C	6	ASN
1	C	40	ASN
1	C	41	ASN
1	C	116	ASN
1	C	222	ASN
1	D	6	ASN
1	D	40	ASN
1	D	41	ASN
1	D	116	ASN
1	D	222	ASN
1	E	6	ASN
1	E	40	ASN
1	E	41	ASN
1	E	97	HIS
1	E	116	ASN
1	E	218	GLN
1	E	222	ASN
1	F	6	ASN
1	F	40	ASN
1	F	41	ASN
1	F	116	ASN
1	G	6	ASN
1	G	40	ASN
1	G	41	ASN
1	G	97	HIS
1	G	116	ASN
1	G	222	ASN
1	H	6	ASN
1	H	40	ASN
1	H	41	ASN
1	H	116	ASN

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Mol	Chain	Res	Type
1	H	205	HIS
1	H	209	HIS
1	H	218	GLN
1	H	222	ASN
1	I	6	ASN
1	I	40	ASN
1	I	41	ASN
1	I	116	ASN
1	I	211	GLN
1	I	218	GLN
1	I	222	ASN
1	J	6	ASN
1	J	40	ASN
1	J	41	ASN
1	J	116	ASN
1	J	218	GLN
1	J	222	ASN
1	K	6	ASN
1	K	40	ASN
1	K	41	ASN
1	K	97	HIS
1	K	116	ASN
1	K	222	ASN
1	L	6	ASN
1	L	40	ASN
1	L	41	ASN
1	L	116	ASN
1	L	222	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

14 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	A	238	-	4,4,4	0.75	0	6,6,6	0.47	0
2	PO4	B	238	-	4,4,4	0.80	0	6,6,6	0.50	0
2	PO4	C	238	-	4,4,4	0.76	0	6,6,6	0.38	0
2	PO4	D	238	-	4,4,4	0.75	0	6,6,6	0.44	0
2	PO4	E	238	-	4,4,4	0.77	0	6,6,6	0.50	0
2	PO4	F	238	-	4,4,4	0.73	0	6,6,6	0.45	0
2	PO4	G	238	-	4,4,4	0.77	0	6,6,6	0.41	0
2	PO4	H	238	-	4,4,4	0.71	0	6,6,6	0.51	0
2	PO4	I	238	-	4,4,4	0.78	0	6,6,6	0.42	0
2	PO4	J	238	-	4,4,4	0.72	0	6,6,6	0.40	0
2	PO4	K	238	-	4,4,4	0.74	0	6,6,6	0.36	0
2	PO4	L	238	-	4,4,4	0.83	0	6,6,6	0.36	0
2	PO4	L	239	-	4,4,4	0.72	0	6,6,6	0.38	0
2	PO4	L	240	-	4,4,4	0.74	0	6,6,6	0.45	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
2	PO4	A	238	-	-	0/0/0/0	0/0/0/0
2	PO4	B	238	-	-	0/0/0/0	0/0/0/0
2	PO4	C	238	-	-	0/0/0/0	0/0/0/0
2	PO4	D	238	-	-	0/0/0/0	0/0/0/0
2	PO4	E	238	-	-	0/0/0/0	0/0/0/0
2	PO4	F	238	-	-	0/0/0/0	0/0/0/0
2	PO4	G	238	-	-	0/0/0/0	0/0/0/0
2	PO4	H	238	-	-	0/0/0/0	0/0/0/0
2	PO4	I	238	-	-	0/0/0/0	0/0/0/0
2	PO4	J	238	-	-	0/0/0/0	0/0/0/0
2	PO4	K	238	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	L	238	-	-	0/0/0/0	0/0/0/0
2	PO4	L	239	-	-	0/0/0/0	0/0/0/0
2	PO4	L	240	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	237/237 (100%)	-0.40	11 (4%) 33 31	19, 33, 70, 109	0
1	B	237/237 (100%)	-0.66	6 (2%) 58 55	15, 26, 57, 90	0
1	C	237/237 (100%)	-0.47	3 (1%) 77 75	20, 35, 55, 69	0
1	D	237/237 (100%)	-0.70	2 (0%) 86 84	15, 27, 46, 64	0
1	E	232/237 (97%)	-0.44	6 (2%) 56 54	17, 36, 70, 108	0
1	F	237/237 (100%)	-0.50	5 (2%) 64 61	18, 32, 60, 101	0
1	G	237/237 (100%)	-0.34	5 (2%) 64 61	21, 39, 72, 95	0
1	H	237/237 (100%)	-0.65	2 (0%) 86 84	17, 30, 47, 68	0
1	I	237/237 (100%)	-0.68	3 (1%) 77 75	17, 27, 46, 72	0
1	J	233/237 (98%)	-0.63	2 (0%) 84 82	18, 32, 48, 72	0
1	K	237/237 (100%)	-0.65	2 (0%) 86 84	18, 31, 52, 77	0
1	L	237/237 (100%)	-0.69	4 (1%) 70 68	17, 29, 45, 78	0
All	All	2835/2844 (99%)	-0.57	51 (1%) 69 66	15, 31, 58, 109	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	215	ALA	6.4
1	A	211	GLN	5.0
1	E	213	THR	4.9
1	F	208	THR	4.5
1	F	209	HIS	4.5
1	I	209	HIS	4.4
1	J	206	ILE	4.3
1	A	208	THR	4.2
1	B	101	ARG	4.2
1	J	207	ARG	4.0
1	B	211	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	213	THR	3.9
1	I	211	GLN	3.9
1	A	207	ARG	3.8
1	A	215	ALA	3.7
1	A	214	ALA	3.7
1	G	214	ALA	3.5
1	E	99	LYS	3.5
1	A	212	THR	3.5
1	A	213	THR	3.3
1	A	209	HIS	3.3
1	F	211	GLN	3.2
1	C	237	LYS	3.1
1	E	218	GLN	3.0
1	G	215	ALA	2.9
1	L	209	HIS	2.9
1	I	147	ASP	2.9
1	A	217	ARG	2.9
1	C	147	ASP	2.8
1	E	237	LYS	2.8
1	H	209	HIS	2.8
1	B	237	LYS	2.8
1	B	208	THR	2.8
1	L	208	THR	2.8
1	A	37	ARG	2.8
1	K	237	LYS	2.7
1	K	211	GLN	2.7
1	F	210	GLU	2.7
1	B	207	ARG	2.7
1	B	215	ALA	2.7
1	E	214	ALA	2.7
1	F	146	ILE	2.6
1	L	211	GLN	2.6
1	G	207	ARG	2.4
1	D	97[A]	HIS	2.3
1	G	237	LYS	2.3
1	C	97	HIS	2.2
1	A	216	GLU	2.2
1	D	237	LYS	2.1
1	H	1	ALA	2.1
1	L	210	GLU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	L	239	5/5	0.92	0.32	3.76	49,56,58,67	0
2	PO4	L	240	5/5	0.97	0.13	0.62	45,52,56,66	0
2	PO4	G	238	5/5	0.99	0.10	0.35	35,37,37,38	0
2	PO4	A	238	5/5	0.99	0.08	-0.22	27,33,34,37	0
2	PO4	E	238	5/5	0.99	0.08	-0.80	30,30,34,35	0
2	PO4	B	238	5/5	0.99	0.08	-0.81	21,22,27,32	0
2	PO4	H	238	5/5	0.98	0.07	-1.11	27,30,31,36	0
2	PO4	K	238	5/5	0.99	0.06	-1.30	27,32,36,37	0
2	PO4	J	238	5/5	0.99	0.06	-1.46	27,30,35,40	0
2	PO4	L	238	5/5	0.99	0.06	-1.60	24,28,29,29	0
2	PO4	I	238	5/5	0.99	0.06	-1.62	24,25,29,31	0
2	PO4	F	238	5/5	0.99	0.06	-1.81	23,31,33,33	0
2	PO4	C	238	5/5	0.98	0.06	-1.91	31,39,41,44	0
2	PO4	D	238	5/5	0.99	0.05	-2.28	26,28,31,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.