



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:43 pm BST

PDB ID : 2JBM  
Title : QPRTASE STRUCTURE FROM HUMAN  
Authors : Liu, H.; Naismith, J.H.  
Deposited on : 2006-12-08  
Resolution : 2.00 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

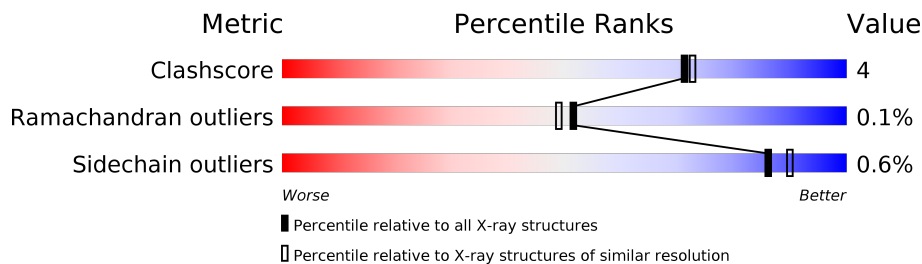
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	299	87% 9% .
1	B	299	89% 7% .
1	C	299	88% 7% . .
1	D	299	89% 6% 5%
1	E	299	91% 5% .
1	F	299	88% 7% 5%
1	G	299	89% 6% 5%
1	H	299	89% 6% 5%
1	I	299	89% 7% . .

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Mol	Chain	Length	Quality of chain
1	J	299	 88% 7% 5%
1	K	299	 89% 6% 5%
1	L	299	 90% 5% 5%

## 2 Entry composition [i](#)

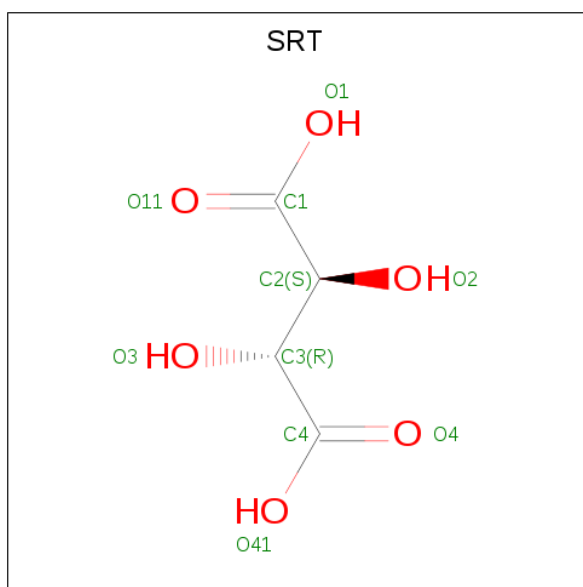
There are 3 unique types of molecules in this entry. The entry contains 28196 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	Total 2109	C 1343	N 366	O 390	S 10	0	0	1
1	B	289	Total 2101	C 1338	N 365	O 389	S 9	0	0	1
1	C	286	Total 2085	C 1329	N 361	O 385	S 10	0	0	0
1	D	285	Total 2077	C 1324	N 360	O 384	S 9	0	0	0
1	E	289	Total 2101	C 1338	N 365	O 389	S 9	0	0	1
1	F	285	Total 2077	C 1324	N 360	O 384	S 9	0	0	0
1	G	285	Total 2077	C 1324	N 360	O 384	S 9	0	0	0
1	H	285	Total 2077	C 1324	N 360	O 384	S 9	0	0	0
1	I	289	Total 2101	C 1338	N 365	O 389	S 9	0	0	1
1	J	285	Total 2077	C 1324	N 360	O 384	S 9	0	0	0
1	K	285	Total 2077	C 1324	N 360	O 384	S 9	0	0	0
1	L	285	Total 2077	C 1324	N 360	O 384	S 9	0	0	0

- Molecule 2 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0
2	C	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0
2	E	1	Total C O 10 4 6	0	0
2	F	1	Total C O 10 4 6	0	0
2	G	1	Total C O 10 4 6	0	0
2	H	1	Total C O 10 4 6	0	0
2	I	1	Total C O 10 4 6	0	0
2	J	1	Total C O 10 4 6	0	0
2	K	1	Total C O 10 4 6	0	0
2	L	1	Total C O 10 4 6	0	0

- Molecule 3 is water.

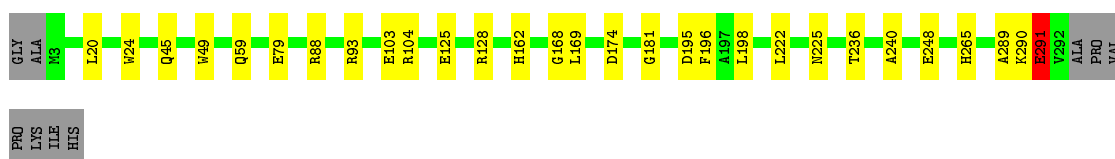
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	375	Total 375	O 375	0	0
3	B	324	Total 324	O 324	0	0
3	C	280	Total 280	O 280	0	0
3	D	292	Total 292	O 292	0	0
3	E	267	Total 267	O 267	0	0
3	F	315	Total 315	O 315	0	0
3	G	181	Total 181	O 181	0	0
3	H	127	Total 127	O 127	0	0
3	I	269	Total 269	O 269	0	0
3	J	256	Total 256	O 256	0	0
3	K	206	Total 206	O 206	0	0
3	L	148	Total 148	O 148	0	0

### 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. 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. 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: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain A: 




- Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain B: 



- Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain C: 



- Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain D: 




- Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain E: 



- Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain F: 



- Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain G: 89% 6% 5%



- Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain H: 89% 6% 5%



- Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain I: 89% 7% . .



- Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain J: 88% 7% 5%



- Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain K: 89% 6% 5%



- Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain L: 90% 5% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.92Å 179.29Å 194.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.97 – 2.00 60.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.4 (60.97-2.00) 86.1 (60.98-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.208 0.247 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtrriage
Anisotropy	0.286	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 34.3	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	0.92	EDS
Total number of atoms	28196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	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 22.48 % 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 5.6514e-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: SRT

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	0.65	0/2152	0.67	2/2933 (0.1%)
1	B	0.57	0/2144	0.64	1/2923 (0.0%)
1	C	0.54	0/2128	0.61	2/2901 (0.1%)
1	D	0.51	0/2120	0.60	1/2891 (0.0%)
1	E	0.54	0/2144	0.63	1/2923 (0.0%)
1	F	0.54	0/2120	0.62	1/2891 (0.0%)
1	G	0.43	0/2120	0.55	1/2891 (0.0%)
1	H	0.40	0/2120	0.52	0/2891
1	I	0.52	0/2144	0.60	1/2923 (0.0%)
1	J	0.50	0/2120	0.62	2/2891 (0.1%)
1	K	0.44	0/2120	0.53	0/2891
1	L	0.42	0/2120	0.53	0/2891
All	All	0.51	0/25552	0.60	12/34840 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	45	GLN	CA-CB-CG	8.53	132.16	113.40
1	B	174	ASP	CB-CG-OD1	7.39	124.95	118.30
1	D	174	ASP	CB-CG-OD1	6.92	124.53	118.30
1	I	174	ASP	CB-CG-OD1	6.82	124.43	118.30
1	E	174	ASP	CB-CG-OD1	6.38	124.04	118.30
1	J	45	GLN	CB-CG-CD	6.12	127.51	111.60
1	G	169	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	104	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	F	174	ASP	CB-CG-OD1	5.82	123.53	118.30
1	C	169	LEU	CA-CB-CG	5.76	128.54	115.30
1	C	174	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	104	ARG	NE-CZ-NH1	5.64	123.12	120.30

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	2109	0	2128	20	3
1	B	2101	0	2119	18	0
1	C	2085	0	2104	18	0
1	D	2077	0	2095	11	0
1	E	2101	0	2119	17	0
1	F	2077	0	2095	18	0
1	G	2077	0	2095	11	0
1	H	2077	0	2095	13	0
1	I	2101	0	2119	23	3
1	J	2077	0	2095	15	0
1	K	2077	0	2095	12	0
1	L	2077	0	2095	10	0
2	A	10	0	4	1	0
2	B	10	0	4	0	0
2	C	10	0	4	2	0
2	D	10	0	4	2	0
2	E	10	0	4	0	0
2	F	10	0	4	2	0
2	G	10	0	4	1	0
2	H	10	0	4	1	0
2	I	10	0	4	0	0
2	J	10	0	4	2	0
2	K	10	0	4	0	0
2	L	10	0	4	1	0
3	A	375	0	0	11	0
3	B	324	0	0	6	0
3	C	280	0	0	7	0
3	D	292	0	0	2	0
3	E	267	0	0	10	0
3	F	315	0	0	6	0
3	G	181	0	0	2	0
3	H	127	0	0	1	0
3	I	269	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	256	0	0	7	0
3	K	206	0	0	2	0
3	L	148	0	0	5	0
All	All	28196	0	25302	178	3

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 (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:HB2	3:A:2248:HOH:O	1.40	1.22
1:A:196:PHE:HB2	3:C:2187:HOH:O	1.55	1.06
1:K:128:ARG:NH1	3:K:2111:HOH:O	1.83	1.05
1:A:225:ASN:HB3	3:A:2295:HOH:O	1.58	1.01
1:C:162:HIS:CE1	3:C:2187:HOH:O	2.13	0.99
1:C:162:HIS:HE1	3:C:2187:HOH:O	1.51	0.87
1:J:229:GLU:HG3	3:J:2208:HOH:O	1.76	0.84
3:A:2249:HOH:O	1:B:286:LYS:HD2	1.77	0.83
1:L:162:HIS:HE1	3:L:2092:HOH:O	1.62	0.82
1:L:162:HIS:CE1	3:L:2092:HOH:O	2.34	0.79
1:L:180:ALA:O	1:L:185:LYS:HD3	1.83	0.79
1:E:291:GLU:HA	3:E:2265:HOH:O	1.82	0.78
1:F:230:GLU:HG3	3:F:2135:HOH:O	1.86	0.74
1:C:211:VAL:O	1:C:215:GLU:HG3	1.87	0.74
1:H:196:PHE:HB2	3:L:2092:HOH:O	1.88	0.74
1:E:291:GLU:CA	3:E:2265:HOH:O	2.37	0.73
1:I:173:LYS:HE2	3:J:2118:HOH:O	1.88	0.73
1:A:196:PHE:CB	3:C:2187:HOH:O	2.24	0.71
1:I:39:SER:O	1:I:290:LYS:NZ	2.24	0.70
1:D:195:ASP:OD1	1:E:135:HIS:ND1	2.24	0.70
1:J:46:ALA:HB2	1:J:287:LEU:HD12	1.75	0.68
1:A:181:GLY:HA2	3:A:2251:HOH:O	1.96	0.66
1:A:49:TRP:CZ3	1:A:88:ARG:HB2	2.31	0.65
1:J:77:LEU:HD12	1:J:89:VAL:HG12	1.78	0.65
1:B:4:ASP:N	3:B:2002:HOH:O	2.30	0.64
1:E:93:ARG:HD2	3:E:2127:HOH:O	1.99	0.62
1:H:196:PHE:CB	3:L:2092:HOH:O	2.45	0.62
1:D:4:ASP:N	3:D:2002:HOH:O	2.33	0.60
1:E:291:GLU:CB	3:E:2265:HOH:O	2.49	0.60
1:F:171:MET:HE3	1:F:172:VAL:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ALA:HB2	1:B:290:LYS:HD2	1.85	0.59
1:F:26:ARG:CZ	3:F:2041:HOH:O	2.51	0.58
1:J:230:GLU:HG3	3:J:2209:HOH:O	2.03	0.58
1:E:4:ASP:N	3:E:2003:HOH:O	2.36	0.58
3:A:2236:HOH:O	1:C:196:PHE:HB2	2.03	0.58
1:D:135:HIS:ND1	1:E:195:ASP:OD1	2.37	0.57
1:E:291:GLU:HG3	3:E:2265:HOH:O	2.04	0.57
1:B:195:ASP:OD1	1:F:135:HIS:ND1	2.36	0.57
1:G:210:ALA:HB1	1:G:238:LEU:HD11	1.86	0.57
1:B:20:LEU:HG	1:B:24:TRP:CZ2	2.41	0.55
1:D:20:LEU:HG	1:D:24:TRP:CZ2	2.42	0.55
1:E:20:LEU:HG	1:E:24:TRP:CZ2	2.42	0.55
1:F:26:ARG:NH1	3:F:2046:HOH:O	2.38	0.55
3:B:2053:HOH:O	1:D:26:ARG:CZ	2.54	0.54
1:E:59:GLN:HG3	1:E:79:GLU:OE1	2.06	0.54
1:A:290:LYS:O	1:A:291:GLU:HB3	2.08	0.54
1:A:103:GLU:OE2	1:B:173:LYS:NZ	2.34	0.54
1:C:104:ARG:HD3	2:D:401:SRT:O2	2.08	0.54
1:C:59:GLN:HG3	1:C:79:GLU:OE1	2.07	0.54
1:A:59:GLN:HG3	1:A:79:GLU:OE1	2.08	0.53
1:A:93:ARG:HD3	3:A:2173:HOH:O	2.08	0.53
2:D:401:SRT:H2	3:D:2172:HOH:O	2.08	0.53
1:G:103:GLU:OE2	1:H:173:LYS:NZ	2.42	0.53
1:H:215:GLU:HG2	3:H:2106:HOH:O	2.09	0.53
1:F:20:LEU:HG	1:F:24:TRP:CZ2	2.44	0.52
1:B:15:VAL:HB	3:B:2031:HOH:O	2.08	0.52
1:K:91:GLU:OE2	1:K:93:ARG:HD3	2.09	0.52
1:G:20:LEU:HG	1:G:24:TRP:CZ2	2.44	0.52
1:I:20:LEU:HG	1:I:24:TRP:CZ2	2.45	0.52
1:I:125:GLU:OE2	3:I:2147:HOH:O	2.18	0.52
1:D:59:GLN:HG3	1:D:79:GLU:OE1	2.09	0.52
1:H:26:ARG:CZ	3:J:2033:HOH:O	2.59	0.51
1:C:173:LYS:HE3	2:C:401:SRT:C1	2.40	0.51
1:K:20:LEU:HG	1:K:24:TRP:CZ2	2.45	0.51
1:C:173:LYS:HE3	2:C:401:SRT:O11	2.10	0.51
1:I:128:ARG:CZ	3:I:2147:HOH:O	2.59	0.51
1:J:20:LEU:HG	1:J:24:TRP:CZ2	2.46	0.51
2:A:401:SRT:H2	3:A:2216:HOH:O	2.09	0.51
1:H:20:LEU:HG	1:H:24:TRP:CZ2	2.45	0.51
1:A:20:LEU:HG	1:A:24:TRP:CZ2	2.46	0.51
1:H:77:LEU:HD12	1:H:89:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:GLU:HG2	3:A:2371:HOH:O	2.11	0.50
1:L:20:LEU:HG	1:L:24:TRP:CZ2	2.46	0.50
1:G:241:GLN:HG2	1:G:242:PHE:CE1	2.46	0.50
1:I:125:GLU:OE1	1:I:128:ARG:NH2	2.44	0.50
1:F:59:GLN:HG3	1:F:79:GLU:OE1	2.12	0.49
1:I:104:ARG:HD3	2:J:401:SRT:O2	2.12	0.49
1:F:77:LEU:HD12	1:F:89:VAL:HG12	1.93	0.49
1:J:59:GLN:HG3	1:J:79:GLU:OE1	2.11	0.49
1:B:59:GLN:HG3	1:B:79:GLU:OE1	2.12	0.49
1:I:128:ARG:NH2	3:I:2147:HOH:O	2.45	0.49
1:D:92:VAL:HG12	1:D:99:LEU:CD2	2.42	0.49
1:J:26:ARG:CZ	3:J:2033:HOH:O	2.59	0.49
1:J:135:HIS:ND1	1:K:195:ASP:OD1	2.46	0.49
1:K:59:GLN:HG3	1:K:79:GLU:OE1	2.13	0.49
1:C:20:LEU:HG	1:C:24:TRP:CZ2	2.47	0.48
1:B:135:HIS:HD1	1:F:195:ASP:CG	2.16	0.48
1:B:286:LYS:HE2	3:B:2314:HOH:O	2.13	0.48
1:E:42:GLY:HA3	3:E:2265:HOH:O	2.14	0.48
1:I:104:ARG:HD2	2:J:401:SRT:O4	2.14	0.48
1:I:265:HIS:HD2	3:I:2239:HOH:O	1.95	0.47
1:I:173:LYS:NZ	1:J:103:GLU:OE2	2.45	0.47
1:A:45:GLN:CD	1:A:289:ALA:HB3	2.35	0.47
1:I:59:GLN:HG3	1:I:79:GLU:OE1	2.15	0.47
2:G:401:SRT:H2	3:G:2106:HOH:O	2.15	0.47
1:L:59:GLN:HG3	1:L:79:GLU:OE1	2.15	0.47
1:A:125:GLU:OE1	1:A:128:ARG:NH2	2.46	0.47
1:C:3:MET:HB3	3:C:2002:HOH:O	2.15	0.47
1:I:125:GLU:CD	3:I:2147:HOH:O	2.52	0.47
1:I:183:VAL:O	1:I:187:VAL:HG23	2.14	0.46
1:G:195:ASP:HB3	3:G:2139:HOH:O	2.16	0.46
1:G:188:ARG:O	1:G:192:GLN:HG3	2.15	0.46
1:G:59:GLN:HG3	1:G:79:GLU:OE1	2.15	0.46
1:E:6:GLU:HG3	3:E:2001:HOH:O	2.14	0.46
1:C:192:GLN:HG3	3:C:2209:HOH:O	2.15	0.46
1:A:195:ASP:OD1	1:C:135:HIS:ND1	2.49	0.46
1:K:4:ASP:N	3:K:2002:HOH:O	2.48	0.46
1:A:265:HIS:HE1	3:A:2340:HOH:O	1.98	0.45
1:C:46:ALA:HB2	1:C:287:LEU:HD12	1.97	0.45
1:L:4:ASP:HA	3:L:2001:HOH:O	2.17	0.45
1:G:125:GLU:OE1	1:G:128:ARG:NH2	2.49	0.45
1:B:222:LEU:HD13	1:B:248:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:401:SRT:H2	3:F:2173:HOH:O	2.15	0.45
1:A:168:GLY:O	1:A:198:LEU:HD22	2.16	0.45
1:E:291:GLU:CG	3:E:2265:HOH:O	2.60	0.45
1:J:192:GLN:HG3	3:J:2176:HOH:O	2.16	0.45
1:K:111:ALA:HB1	1:K:280:ALA:HB1	1.99	0.45
1:B:173:LYS:HB3	1:B:173:LYS:HE3	1.82	0.44
1:I:173:LYS:HE3	1:I:173:LYS:HB3	1.67	0.44
1:F:220:LEU:HG	1:F:246:ALA:HB3	1.97	0.44
1:G:173:LYS:HA	1:G:203:GLU:HB3	1.99	0.44
1:H:59:GLN:HG3	1:H:79:GLU:OE1	2.17	0.44
1:I:92:VAL:HG12	1:I:99:LEU:CD2	2.47	0.44
1:A:225:ASN:CB	3:A:2295:HOH:O	2.35	0.44
1:G:104:ARG:HH11	2:H:401:SRT:C1	2.31	0.44
1:C:141:LYS:HE2	3:C:2170:HOH:O	2.17	0.44
1:F:171:MET:HE3	1:F:172:VAL:H	1.83	0.44
1:B:135:HIS:ND1	1:F:195:ASP:OD1	2.51	0.44
1:J:15:VAL:HB	3:J:2020:HOH:O	2.18	0.44
1:H:111:ALA:HB1	1:H:280:ALA:HB1	1.99	0.43
1:J:187:VAL:HG22	1:J:202:VAL:HG21	2.00	0.43
1:A:222:LEU:HD13	1:A:248:GLU:HG2	1.99	0.43
1:B:292:VAL:N	3:B:2320:HOH:O	2.51	0.43
1:F:125:GLU:OE1	1:F:128:ARG:NH2	2.51	0.43
1:K:44:SER:HB3	1:K:287:LEU:HD21	2.00	0.43
1:H:135:HIS:ND1	1:L:195:ASP:OD1	2.51	0.43
1:L:173:LYS:HA	1:L:203:GLU:HB3	2.01	0.43
1:C:169:LEU:O	1:C:169:LEU:HD12	2.19	0.43
1:F:84:VAL:HB	1:I:93:ARG:NH1	2.33	0.43
1:B:92:VAL:HG12	1:B:99:LEU:CD2	2.48	0.43
1:K:77:LEU:HD12	1:K:89:VAL:HG22	2.00	0.43
1:I:128:ARG:HH11	1:I:128:ARG:HG2	1.83	0.43
1:B:26:ARG:CZ	3:B:2053:HOH:O	2.66	0.43
1:H:222:LEU:HD13	1:H:248:GLU:HG2	2.01	0.43
1:E:104:ARG:HD3	2:F:401:SRT:O2	2.19	0.43
1:H:215:GLU:HG3	1:H:242:PHE:HZ	1.83	0.43
1:D:125:GLU:OE1	1:D:128:ARG:NH2	2.51	0.43
1:J:173:LYS:HA	1:J:203:GLU:HB3	2.01	0.42
1:K:125:GLU:OE1	1:K:128:ARG:NH2	2.52	0.42
1:C:239:LYS:HE2	1:C:245:VAL:O	2.19	0.42
1:H:125:GLU:OE1	1:H:128:ARG:NH2	2.53	0.42
1:I:174:ASP:HB2	3:I:2182:HOH:O	2.19	0.42
1:I:290:LYS:O	1:I:291:GLU:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:VAL:HG22	1:D:202:VAL:HG21	2.03	0.41
1:F:173:LYS:HA	1:F:203:GLU:HB3	2.02	0.41
1:L:163:ARG:HE	2:L:401:SRT:C4	2.34	0.41
1:A:162:HIS:CE1	3:A:2236:HOH:O	2.73	0.41
1:E:93:ARG:NH2	3:E:2126:HOH:O	2.53	0.41
1:F:77:LEU:HG	3:I:2117:HOH:O	2.19	0.41
1:D:168:GLY:O	1:D:198:LEU:HD22	2.20	0.41
1:E:92:VAL:HG12	1:E:99:LEU:CD2	2.50	0.41
1:I:239:LYS:HE3	1:I:247:VAL:HG23	2.03	0.41
1:K:75:TRP:CE3	1:K:90:ALA:HB2	2.56	0.41
1:C:125:GLU:OE1	1:C:128:ARG:NH2	2.53	0.41
1:G:239:LYS:HE2	1:G:245:VAL:O	2.20	0.41
1:F:195:ASP:HB3	3:F:2232:HOH:O	2.21	0.41
1:I:222:LEU:HD13	1:I:248:GLU:HG2	2.02	0.41
1:D:222:LEU:HD13	1:D:248:GLU:HG2	2.03	0.41
1:C:220:LEU:HG	1:C:246:ALA:HB3	2.03	0.41
1:J:173:LYS:HE3	1:J:173:LYS:HB2	1.94	0.41
1:J:48:LEU:HD23	1:J:89:VAL:HG23	2.03	0.41
1:E:125:GLU:OE1	1:E:128:ARG:NH2	2.52	0.40
1:L:132:TRP:HB2	1:L:262:CYS:HB3	2.03	0.40
1:F:188:ARG:NH2	3:F:2219:HOH:O	2.52	0.40
1:B:125:GLU:OE1	1:B:128:ARG:NH2	2.55	0.40
1:B:290:LYS:O	1:B:291:GLU:HB2	2.21	0.40
1:I:290:LYS:NZ	3:I:2263:HOH:O	2.43	0.40
1:K:21:VAL:HG22	1:K:65:ILE:HG13	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ALA:CB	1:I:128:ARG:NH1[4_466]	1.25	0.95
1:A:236:THR:CG2	1:I:125:GLU:OE2[4_466]	1.67	0.53
1:A:240:ALA:CA	1:I:128:ARG:NH1[4_466]	1.84	0.36

## 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	288/299 (96%)	284 (99%)	3 (1%)	1 (0%)	41	37
1	B	287/299 (96%)	281 (98%)	5 (2%)	1 (0%)	41	37
1	C	284/299 (95%)	281 (99%)	3 (1%)	0	100	100
1	D	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
1	E	287/299 (96%)	281 (98%)	5 (2%)	1 (0%)	41	37
1	F	283/299 (95%)	281 (99%)	2 (1%)	0	100	100
1	G	283/299 (95%)	279 (99%)	4 (1%)	0	100	100
1	H	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
1	I	287/299 (96%)	282 (98%)	4 (1%)	1 (0%)	41	37
1	J	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
1	K	283/299 (95%)	279 (99%)	4 (1%)	0	100	100
1	L	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
All	All	3414/3588 (95%)	3368 (99%)	42 (1%)	4 (0%)	51	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	GLU
1	B	291	GLU
1	E	291	GLU
1	I	291	GLU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/219 (97%)	210 (99%)	2 (1%)	78	83
1	B	211/219 (96%)	209 (99%)	2 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	210/219 (96%)	207 (99%)	3 (1%)	67	72
1	D	209/219 (95%)	209 (100%)	0	100	100
1	E	211/219 (96%)	211 (100%)	0	100	100
1	F	209/219 (95%)	209 (100%)	0	100	100
1	G	209/219 (95%)	208 (100%)	1 (0%)	88	92
1	H	209/219 (95%)	208 (100%)	1 (0%)	88	92
1	I	211/219 (96%)	209 (99%)	2 (1%)	78	83
1	J	209/219 (95%)	207 (99%)	2 (1%)	76	81
1	K	209/219 (95%)	208 (100%)	1 (0%)	88	92
1	L	209/219 (95%)	207 (99%)	2 (1%)	76	81
All	All	2518/2628 (96%)	2502 (99%)	16 (1%)	86	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	A	291	GLU
1	B	206	SER
1	B	291	GLU
1	C	169	LEU
1	C	173	LYS
1	C	287	LEU
1	G	169	LEU
1	H	195	ASP
1	I	184	GLU
1	I	244	SER
1	J	45	GLN
1	J	241	GLN
1	K	287	LEU
1	L	188	ARG
1	L	287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	HIS
1	C	162	HIS

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Mol	Chain	Res	Type
1	D	192	GLN
1	E	265	HIS
1	I	265	HIS
1	I	276	GLN
1	J	265	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

12 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	SRT	J	401	-	3,9,9	0.43	0	6,12,12	2.67	2 (33%)
2	SRT	H	401	-	3,9,9	0.24	0	6,12,12	1.11	0
2	SRT	D	401	-	3,9,9	0.40	0	6,12,12	1.89	1 (16%)
2	SRT	B	401	-	3,9,9	0.15	0	6,12,12	1.15	1 (16%)
2	SRT	K	401	-	3,9,9	0.42	0	6,12,12	1.38	0
2	SRT	F	401	-	3,9,9	0.21	0	6,12,12	2.59	3 (50%)
2	SRT	I	401	-	3,9,9	0.26	0	6,12,12	1.33	1 (16%)
2	SRT	G	401	-	3,9,9	0.20	0	6,12,12	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SRT	E	401	-	3,9,9	0.34	0	6,12,12	1.15	1 (16%)
2	SRT	C	401	-	3,9,9	0.16	0	6,12,12	1.60	1 (16%)
2	SRT	A	401	-	3,9,9	0.22	0	6,12,12	2.10	2 (33%)
2	SRT	L	401	-	3,9,9	0.64	0	6,12,12	0.95	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	SRT	J	401	-	-	4/4/12/12	-
2	SRT	H	401	-	-	4/4/12/12	-
2	SRT	D	401	-	-	4/4/12/12	-
2	SRT	B	401	-	-	4/4/12/12	-
2	SRT	K	401	-	-	4/4/12/12	-
2	SRT	F	401	-	-	4/4/12/12	-
2	SRT	I	401	-	-	4/4/12/12	-
2	SRT	G	401	-	-	4/4/12/12	-
2	SRT	E	401	-	-	0/4/12/12	-
2	SRT	C	401	-	-	4/4/12/12	-
2	SRT	A	401	-	-	4/4/12/12	-
2	SRT	L	401	-	-	4/4/12/12	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	SRT	O3-C3-C2	-5.20	91.52	108.90
2	F	401	SRT	O3-C3-C2	-4.26	94.66	108.90
2	D	401	SRT	O3-C3-C2	-3.91	95.85	108.90
2	A	401	SRT	O3-C3-C2	-3.63	96.77	108.90
2	F	401	SRT	O2-C2-C3	3.20	119.60	108.90
2	F	401	SRT	O2-C2-C1	3.13	118.64	111.10
2	C	401	SRT	O3-C3-C2	-3.06	98.68	108.90
2	J	401	SRT	O2-C2-C1	2.76	117.75	111.10
2	I	401	SRT	O3-C3-C2	-2.58	100.29	108.90
2	A	401	SRT	O2-C2-C3	2.38	116.84	108.90
2	E	401	SRT	C1-C2-C3	-2.10	108.59	113.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SRT	O3-C3-C2	-2.10	101.90	108.90

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	401	SRT	C1-C2-C3-C4
2	J	401	SRT	O2-C2-C3-O3
2	J	401	SRT	O2-C2-C3-C4
2	H	401	SRT	C1-C2-C3-C4
2	H	401	SRT	O2-C2-C3-O3
2	D	401	SRT	C1-C2-C3-C4
2	D	401	SRT	O2-C2-C3-O3
2	D	401	SRT	O2-C2-C3-C4
2	B	401	SRT	C1-C2-C3-O3
2	B	401	SRT	C1-C2-C3-C4
2	B	401	SRT	O2-C2-C3-O3
2	B	401	SRT	O2-C2-C3-C4
2	K	401	SRT	C1-C2-C3-O3
2	K	401	SRT	C1-C2-C3-C4
2	K	401	SRT	O2-C2-C3-O3
2	K	401	SRT	O2-C2-C3-C4
2	F	401	SRT	C1-C2-C3-C4
2	F	401	SRT	O2-C2-C3-O3
2	F	401	SRT	O2-C2-C3-C4
2	I	401	SRT	C1-C2-C3-O3
2	I	401	SRT	C1-C2-C3-C4
2	I	401	SRT	O2-C2-C3-O3
2	I	401	SRT	O2-C2-C3-C4
2	G	401	SRT	C1-C2-C3-C4
2	G	401	SRT	O2-C2-C3-O3
2	C	401	SRT	C1-C2-C3-O3
2	C	401	SRT	C1-C2-C3-C4
2	C	401	SRT	O2-C2-C3-O3
2	C	401	SRT	O2-C2-C3-C4
2	A	401	SRT	C1-C2-C3-C4
2	A	401	SRT	O2-C2-C3-O3
2	A	401	SRT	O2-C2-C3-C4
2	L	401	SRT	C1-C2-C3-O3
2	L	401	SRT	C1-C2-C3-C4
2	L	401	SRT	O2-C2-C3-O3
2	L	401	SRT	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	J	401	SRT	C1-C2-C3-O3
2	D	401	SRT	C1-C2-C3-O3
2	H	401	SRT	O2-C2-C3-C4
2	F	401	SRT	C1-C2-C3-O3
2	G	401	SRT	O2-C2-C3-C4
2	A	401	SRT	C1-C2-C3-O3
2	H	401	SRT	C1-C2-C3-O3
2	G	401	SRT	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	401	SRT	2	0
2	H	401	SRT	1	0
2	D	401	SRT	2	0
2	F	401	SRT	2	0
2	G	401	SRT	1	0
2	C	401	SRT	2	0
2	A	401	SRT	1	0
2	L	401	SRT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.