



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 06:43 am BST

PDB ID : 4WMJ  
Title : Colias eurytheme Phosphoglucose isomerase. Homodimer from 4-5(18) genotype.  
Authors : Hill, J.A.; Watt, W.B.  
Deposited on : 2014-10-09  
Resolution : 1.50 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
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

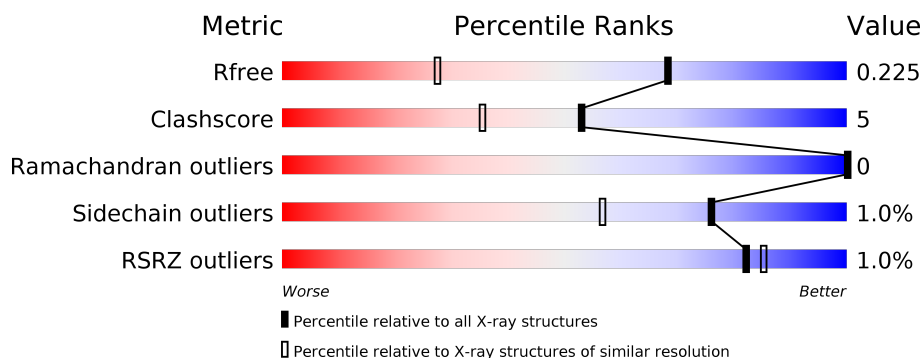
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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  $\leq 5\%$ . 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	556	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 88%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>88%</span> <span>11%</span> <span>•</span> </div> </div>
1	B	556	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 86%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>14%</span> </div> </div>
1	C	556	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 87%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>87%</span> <span>13%</span> </div> </div>
1	D	556	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 87%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>87%</span> <span>12%</span> <span>•</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18508 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 Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4348	2791	740	805	12			
1	B	555	Total	C	N	O	S	0	0	0
			4364	2801	742	809	12			
1	C	554	Total	C	N	O	S	0	0	0
			4355	2796	741	806	12			
1	D	553	Total	C	N	O	S	0	0	0
			4348	2791	740	805	12			

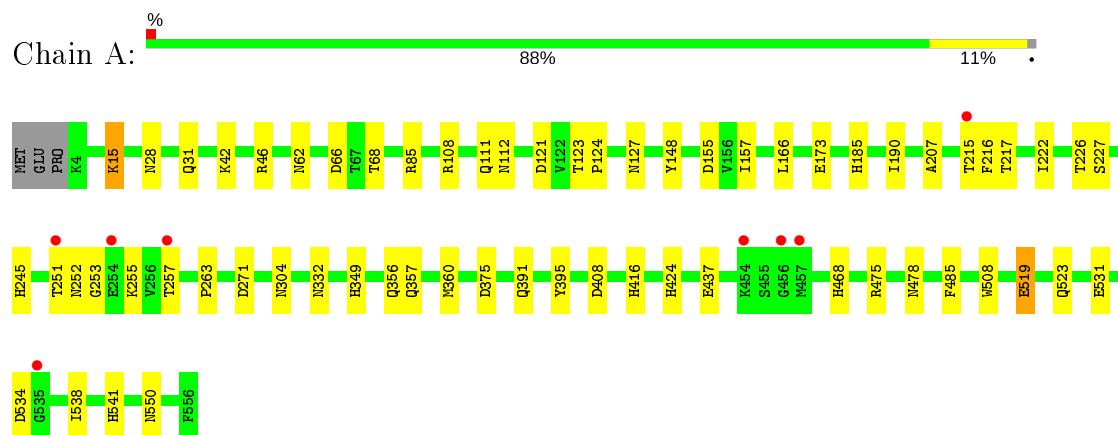
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	264	Total	O	0	0
			264	264		
2	B	251	Total	O	0	0
			251	251		
2	C	289	Total	O	0	0
			289	289		
2	D	289	Total	O	0	0
			289	289		

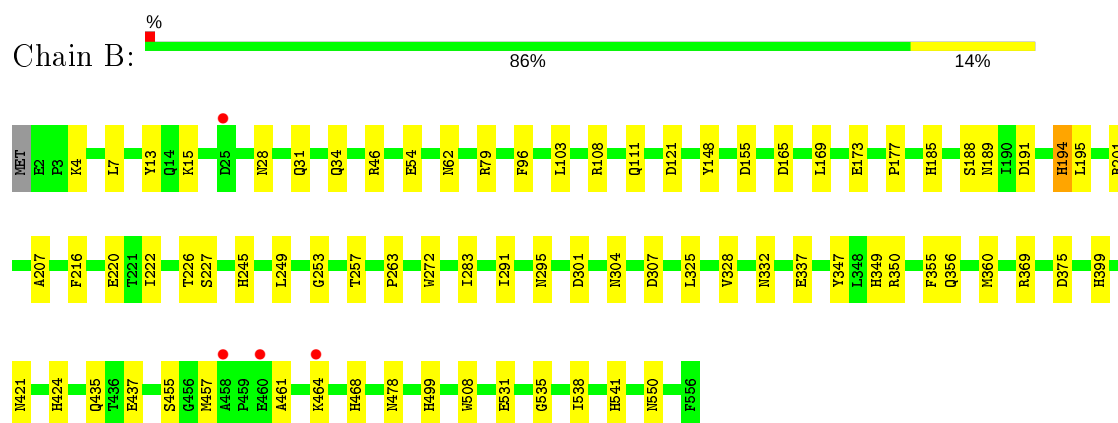
### 3 Residue-property plots [i](#)

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.

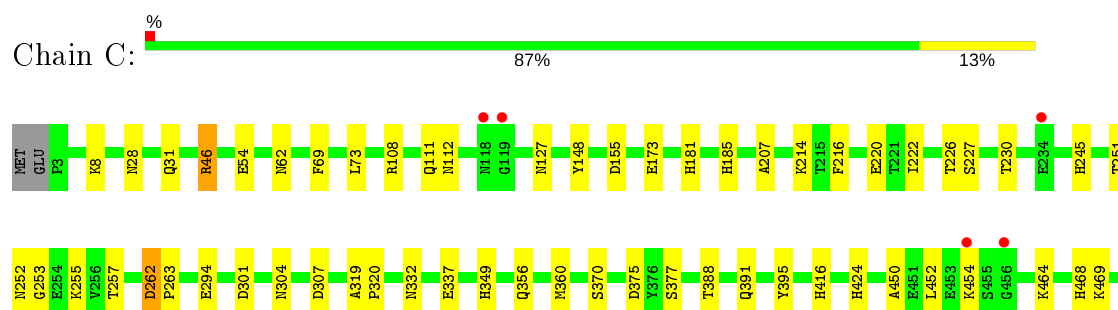
#### • Molecule 1: Glucose-6-phosphate isomerase



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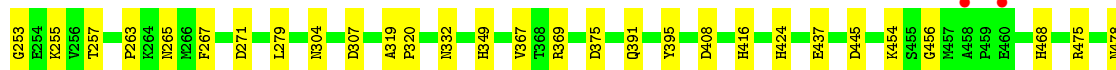
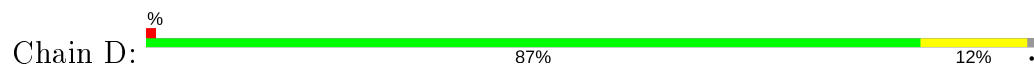


#### • Molecule 1: Glucose-6-phosphate isomerase





• Molecule 1: Glucose-6-phosphate isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.29Å 115.50Å 135.08Å 90.00° 101.70° 90.00°	Depositor
Resolution (Å)	41.19 – 1.50 41.19 – 1.50	Depositor EDS
% Data completeness (in resolution range)	77.7 (41.19-1.50) 77.7 (41.19-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.183 , 0.218 0.192 , 0.225	Depositor DCC
$R_{free}$ test set	14357 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18508	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.98	1/4455 (0.0%)	0.95	10/6045 (0.2%)
1	B	0.99	2/4472 (0.0%)	1.02	11/6069 (0.2%)
1	C	0.99	6/4463 (0.1%)	0.97	8/6056 (0.1%)
1	D	1.04	3/4455 (0.1%)	0.96	8/6045 (0.1%)
All	All	1.00	12/17845 (0.1%)	0.98	37/24215 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	GLU	CD-OE1	9.73	1.36	1.25
1	B	337	GLU	CD-OE2	-8.09	1.16	1.25
1	D	220	GLU	CD-OE1	7.02	1.33	1.25
1	A	519	GLU	CD-OE2	6.44	1.32	1.25
1	C	294	GLU	CG-CD	6.14	1.61	1.51
1	D	54	GLU	CD-OE1	-5.82	1.19	1.25
1	C	473	GLY	N-CA	-5.71	1.37	1.46
1	C	337	GLU	CD-OE2	-5.67	1.19	1.25
1	C	377	SER	CB-OG	-5.26	1.35	1.42
1	C	220	GLU	CD-OE1	5.17	1.31	1.25
1	C	370	SER	CB-OG	5.14	1.49	1.42
1	D	19	TYR	CB-CG	-5.01	1.44	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ARG	NE-CZ-NH1	15.57	128.08	120.30
1	B	201	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	C	8	LYS	CD-CE-NZ	7.77	129.57	111.70
1	A	46	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	D	271	ASP	CB-CG-OD1	7.48	125.03	118.30
1	D	65	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	375	ASP	CB-CG-OD1	6.73	124.36	118.30
1	C	46	ARG	NE-CZ-NH1	6.73	123.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	375	ASP	CB-CG-OD1	6.53	124.18	118.30
1	A	42	LYS	CD-CE-NZ	6.18	125.91	111.70
1	A	271	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	220	GLU	CG-CD-OE2	-6.05	106.19	118.30
1	C	475	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	D	475	ARG	CG-CD-NE	6.03	124.47	111.80
1	B	350	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	85	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	85	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	375	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	165	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	408	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	262	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	D	65	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	301	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	191	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	534	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	66	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	D	408	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	294	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	D	513	PHE	CB-CG-CD1	-5.34	117.06	120.80
1	B	121	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	301	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	355	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	D	85	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	534	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	C	554	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	B	195	LEU	CB-CG-CD1	5.03	119.54	111.00
1	A	475	ARG	NE-CZ-NH1	5.02	122.81	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	4348	0	4301	45	0
1	B	4364	0	4314	55	0
1	C	4355	0	4309	48	0
1	D	4348	0	4301	51	0
2	A	264	0	0	7	0
2	B	251	0	0	6	0
2	C	289	0	0	5	0
2	D	289	0	0	6	0
All	All	18508	0	17225	186	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 5.

All (186) 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:7:LEU:HD21	1:B:13:TYR:CD2	1.63	1.33
1:C:468:HIS:CD2	1:D:367:VAL:HG11	1.81	1.16
1:B:7:LEU:HD21	1:B:13:TYR:CE2	1.83	1.11
1:A:111:GLN:HE22	1:A:304:ASN:HD21	1.15	0.94
1:B:7:LEU:CD2	1:B:13:TYR:CD2	2.51	0.94
1:C:468:HIS:CD2	1:D:367:VAL:CG1	2.53	0.92
1:A:538:ILE:H	1:A:550:ASN:HD21	1.19	0.90
1:B:111:GLN:HE22	1:B:304:ASN:HD21	1.21	0.89
1:A:215:THR:HG23	1:A:217:THR:H	1.36	0.89
1:A:15:LYS:CE	2:A:664:HOH:O	2.23	0.87
1:B:7:LEU:HD23	1:B:7:LEU:C	1.95	0.86
1:D:247:VAL:HG13	1:D:265:ASN:O	1.78	0.83
1:A:257:THR:HG22	1:A:263:PRO:HD3	1.62	0.81
1:B:7:LEU:HD23	1:B:7:LEU:O	1.79	0.81
1:C:538:ILE:H	1:C:550:ASN:HD21	1.28	0.81
1:B:538:ILE:H	1:B:550:ASN:HD21	1.27	0.81
1:C:253:GLY:O	1:C:257:THR:HG23	1.78	0.81
1:C:349:HIS:HD2	2:C:771:HOH:O	1.64	0.79
1:B:148:TYR:H	1:B:245:HIS:HE1	1.30	0.79
1:B:7:LEU:CD2	1:B:13:TYR:CE2	2.67	0.78
1:B:253:GLY:O	1:B:257:THR:HG23	1.84	0.77
1:C:531:GLU:OE1	1:C:541:HIS:HE1	1.68	0.77
1:D:257:THR:HG21	2:D:863:HOH:O	1.84	0.76
1:D:247:VAL:HG11	1:D:267:PHE:HE1	1.51	0.75
1:A:148:TYR:H	1:A:245:HIS:HE1	1.31	0.74
1:D:538:ILE:H	1:D:550:ASN:HD21	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:GLU:OE1	1:B:541:HIS:HE1	1.70	0.73
1:D:15:LYS:HE2	2:D:832:HOH:O	1.88	0.72
1:C:111:GLN:HE22	1:C:304:ASN:HD21	1.38	0.71
1:D:121:ASP:OD1	1:D:123:THR:HG23	1.91	0.71
1:A:531:GLU:OE1	1:A:541:HIS:HE1	1.73	0.71
1:B:222:ILE:O	1:B:226:THR:HG23	1.92	0.70
1:A:185:HIS:HD2	2:A:721:HOH:O	1.76	0.69
1:D:252:ASN:ND2	1:D:255:LYS:HG3	2.07	0.69
1:D:307:ASP:OD1	1:D:499:HIS:HE1	1.76	0.68
1:C:46:ARG:NH2	1:C:54:GLU:OE1	2.28	0.67
1:A:222:ILE:O	1:A:226:THR:HG23	1.94	0.66
1:C:252:ASN:ND2	1:C:255:LYS:HG3	2.10	0.66
1:C:227:SER:OG	1:D:424:HIS:HE1	1.77	0.66
1:A:332:ASN:HD21	1:A:508:TRP:HE1	1.44	0.66
1:D:253:GLY:O	1:D:257:THR:HG23	1.96	0.66
1:D:367:VAL:O	1:D:367:VAL:HG13	1.97	0.65
1:C:28:ASN:HD22	1:C:31:GLN:H	1.45	0.64
1:B:188:SER:H	1:B:194:HIS:CD2	2.15	0.64
1:B:189:ASN:H	1:B:194:HIS:HD2	1.45	0.64
1:A:541:HIS:HD2	1:B:437:GLU:OE2	1.82	0.62
1:B:7:LEU:C	1:B:7:LEU:CD2	2.68	0.62
1:D:207:ALA:O	1:D:245:HIS:HD2	1.83	0.62
1:D:247:VAL:HG11	1:D:267:PHE:CE1	2.35	0.62
1:C:424:HIS:HE1	1:D:227:SER:OG	1.83	0.61
1:D:349:HIS:HD2	2:D:783:HOH:O	1.82	0.61
1:A:28:ASN:HD22	1:A:31:GLN:H	1.46	0.61
1:A:349:HIS:HD2	2:A:680:HOH:O	1.82	0.61
1:A:227:SER:OG	1:B:424:HIS:HE1	1.84	0.61
1:D:155:ASP:OD1	1:D:185:HIS:HE1	1.83	0.61
1:C:173:GLU:OE1	1:C:349:HIS:HE1	1.84	0.60
1:B:169:LEU:HD23	1:B:169:LEU:C	2.22	0.60
1:D:222:ILE:O	1:D:226:THR:HG23	2.01	0.60
1:D:62:ASN:HD21	1:D:478:ASN:ND2	2.00	0.60
1:D:332:ASN:HD21	1:D:508:TRP:HE1	1.50	0.60
1:B:155:ASP:OD2	1:B:185:HIS:HE1	1.83	0.60
1:B:185:HIS:HD2	2:B:850:HOH:O	1.85	0.59
1:A:148:TYR:N	1:A:245:HIS:HE1	1.98	0.59
1:D:185:HIS:HD2	2:D:850:HOH:O	1.85	0.59
1:A:207:ALA:O	1:A:245:HIS:HD2	1.86	0.58
1:B:148:TYR:H	1:B:245:HIS:CE1	2.18	0.58
1:B:31:GLN:HA	1:B:34:GLN:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:GLU:OE1	1:D:349:HIS:HE1	1.86	0.58
1:B:4:LYS:NZ	1:B:79:ARG:O	2.36	0.58
1:B:307:ASP:OD1	1:B:499:HIS:HE1	1.87	0.58
1:C:307:ASP:OD1	1:C:499:HIS:HE1	1.86	0.58
1:A:468:HIS:HE1	2:B:836:HOH:O	1.87	0.58
1:D:148:TYR:H	1:D:245:HIS:HE1	1.50	0.58
1:B:189:ASN:H	1:B:194:HIS:CD2	2.22	0.57
1:D:111:GLN:HE22	1:D:304:ASN:HD21	1.52	0.57
1:A:15:LYS:HE3	2:A:664:HOH:O	1.98	0.57
1:B:188:SER:H	1:B:194:HIS:HD2	1.52	0.57
1:A:121:ASP:OD1	1:A:123:THR:HG23	2.04	0.57
1:A:253:GLY:O	1:A:257:THR:HG23	2.04	0.57
1:C:148:TYR:H	1:C:245:HIS:HE1	1.51	0.57
1:A:111:GLN:HE22	1:A:304:ASN:ND2	1.97	0.56
1:A:155:ASP:OD1	1:A:185:HIS:HE1	1.87	0.56
1:A:148:TYR:H	1:A:245:HIS:CE1	2.20	0.56
1:C:148:TYR:N	1:C:245:HIS:HE1	2.04	0.56
1:C:541:HIS:HD2	1:D:437:GLU:OE2	1.89	0.56
1:B:399:HIS:HD2	2:B:644:HOH:O	1.89	0.55
1:C:230:THR:HG21	2:C:721:HOH:O	2.06	0.55
1:B:325:LEU:HA	1:B:328:VAL:HG22	1.89	0.55
1:D:148:TYR:N	1:D:245:HIS:HE1	2.04	0.55
1:A:424:HIS:HE1	1:B:227:SER:OG	1.89	0.55
1:C:468:HIS:HD2	1:D:367:VAL:HG11	1.61	0.55
1:B:173:GLU:OE1	1:B:349:HIS:HE1	1.90	0.54
1:B:194:HIS:HE1	2:B:759:HOH:O	1.90	0.54
1:C:207:ALA:O	1:C:245:HIS:HD2	1.90	0.54
1:A:111:GLN:NE2	1:A:304:ASN:HD21	1.96	0.54
1:D:8:LYS:CE	1:D:375:ASP:O	2.56	0.54
1:D:257:THR:HG22	1:D:263:PRO:HD3	1.90	0.54
1:A:437:GLU:OE2	1:B:541:HIS:HD2	1.91	0.53
1:B:111:GLN:HE22	1:B:304:ASN:ND2	1.99	0.53
1:A:173:GLU:OE1	1:A:349:HIS:HE1	1.92	0.53
2:A:760:HOH:O	1:B:468:HIS:HE1	1.90	0.53
1:A:123:THR:OG1	1:A:124:PRO:HD3	2.09	0.52
1:B:207:ALA:O	1:B:245:HIS:HD2	1.90	0.52
1:D:367:VAL:HG12	2:D:658:HOH:O	2.10	0.52
1:B:332:ASN:HD21	1:B:508:TRP:HE1	1.57	0.52
1:C:112:ASN:ND2	1:C:127:ASN:HD21	2.08	0.51
1:D:247:VAL:CG1	1:D:267:PHE:HE1	2.21	0.51
1:B:148:TYR:N	1:B:245:HIS:HE1	2.04	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:HIS:HD2	2:C:888:HOH:O	1.93	0.51
1:C:226:THR:O	1:C:230:THR:HG23	2.10	0.51
1:D:319:ALA:HB3	1:D:320:PRO:HD3	1.93	0.50
1:B:46:ARG:NH1	1:B:54:GLU:OE1	2.44	0.50
1:B:62:ASN:HD21	1:B:478:ASN:ND2	2.10	0.50
1:A:15:LYS:NZ	2:A:664:HOH:O	2.41	0.49
1:D:416:HIS:HE1	1:D:485:PHE:O	1.95	0.49
1:C:531:GLU:OE1	1:C:541:HIS:CE1	2.59	0.49
1:C:332:ASN:HD21	1:C:508:TRP:HE1	1.59	0.49
1:C:468:HIS:HE1	2:D:805:HOH:O	1.95	0.49
1:D:534:ASP:OD1	1:D:535:GLY:N	2.46	0.49
1:C:319:ALA:HB3	1:C:320:PRO:HD3	1.95	0.48
1:C:155:ASP:OD2	1:C:185:HIS:HE1	1.95	0.48
1:A:391:GLN:HA	1:A:395:TYR:CD1	2.49	0.48
1:A:332:ASN:ND2	1:A:508:TRP:HE1	2.10	0.48
1:D:454:LYS:C	1:D:456:GLY:H	2.16	0.48
1:B:399:HIS:HE1	1:B:435:GLN:OE1	1.96	0.48
1:B:332:ASN:ND2	1:B:508:TRP:HE1	2.12	0.47
1:C:391:GLN:HA	1:C:395:TYR:CD1	2.49	0.47
1:A:251:THR:O	1:A:251:THR:CG2	2.63	0.47
1:D:247:VAL:HG12	1:D:248:ALA:N	2.29	0.47
1:B:15:LYS:HE2	2:B:689:HOH:O	2.15	0.47
1:B:257:THR:HG22	1:B:263:PRO:HD3	1.96	0.47
2:C:651:HOH:O	1:D:468:HIS:HE1	1.97	0.47
1:A:257:THR:HG22	1:A:263:PRO:CD	2.39	0.47
1:D:93:LYS:NZ	1:D:118:ASN:HD21	2.13	0.46
1:A:62:ASN:HD21	1:A:478:ASN:ND2	2.14	0.46
1:D:111:GLN:HE22	1:D:304:ASN:ND2	2.14	0.46
1:B:356:GLN:O	1:B:360:MET:HB2	2.16	0.46
1:D:332:ASN:ND2	1:D:508:TRP:HE1	2.12	0.46
1:C:148:TYR:H	1:C:245:HIS:CE1	2.32	0.45
1:C:69:PHE:CE2	1:C:73:LEU:HD11	2.51	0.45
1:D:8:LYS:HE2	1:D:375:ASP:O	2.16	0.45
1:C:416:HIS:HE1	1:C:485:PHE:O	2.00	0.45
1:C:544:SER:HB2	1:D:60:SER:OG	2.15	0.45
2:A:641:HOH:O	1:B:468:HIS:HD2	1.98	0.45
1:C:391:GLN:HA	1:C:395:TYR:CG	2.51	0.45
1:D:367:VAL:O	1:D:367:VAL:CG1	2.62	0.45
1:B:461:ALA:HA	1:B:464:LYS:HG2	1.99	0.45
1:A:112:ASN:ND2	1:A:127:ASN:HD21	2.15	0.45
1:D:96:PHE:CE1	1:D:369:ARG:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:CD2	1:B:13:TYR:CG	2.98	0.44
1:C:181:HIS:H	1:C:181:HIS:CD2	2.34	0.44
1:A:157:ILE:HD12	1:A:157:ILE:N	2.33	0.44
1:D:279:LEU:HD12	1:D:279:LEU:C	2.38	0.44
1:C:181:HIS:HD2	2:C:615:HOH:O	2.01	0.44
1:C:222:ILE:O	1:C:226:THR:HG23	2.18	0.44
1:B:535:GLY:O	1:C:454:LYS:HE2	2.18	0.44
1:A:166:LEU:HD12	1:A:357:GLN:OE1	2.18	0.44
1:A:519:GLU:HG2	1:A:523:GLN:NE2	2.32	0.43
1:B:291:ILE:HD12	1:B:295:ASN:HB3	2.01	0.43
1:C:214:LYS:NZ	1:C:251:THR:HG21	2.33	0.43
1:C:482:VAL:HG21	1:C:489:THR:HB	1.99	0.43
1:A:468:HIS:HD2	2:B:695:HOH:O	2.00	0.43
1:C:62:ASN:HD21	1:C:478:ASN:ND2	2.15	0.43
1:C:388:THR:O	1:C:391:GLN:HB3	2.19	0.43
1:D:391:GLN:HA	1:D:395:TYR:CD1	2.53	0.42
1:C:214:LYS:HZ3	1:C:251:THR:HG21	1.84	0.42
1:A:190:ILE:O	1:B:424:HIS:HD2	2.02	0.42
1:C:452:LEU:HD21	1:C:469:LYS:HE3	2.01	0.42
1:B:455:SER:O	1:B:457:MET:N	2.51	0.42
1:C:356:GLN:O	1:C:360:MET:HB2	2.19	0.42
1:D:515:GLN:O	1:D:518:VAL:HG22	2.19	0.42
1:B:249:LEU:HD13	1:B:283:ILE:HA	2.01	0.42
1:C:464:LYS:HB3	1:C:464:LYS:HE3	1.74	0.42
1:A:251:THR:HG22	1:A:251:THR:O	2.19	0.42
1:D:454:LYS:C	1:D:456:GLY:N	2.72	0.41
1:A:416:HIS:HE1	1:A:485:PHE:O	2.03	0.41
1:D:148:TYR:H	1:D:245:HIS:CE1	2.34	0.41
1:A:252:ASN:ND2	1:A:255:LYS:HG3	2.36	0.41
1:C:257:THR:HG22	1:C:263:PRO:HB3	2.01	0.41
1:D:62:ASN:HD21	1:D:478:ASN:HD21	1.66	0.41
1:A:356:GLN:O	1:A:360:MET:HB2	2.21	0.41
1:B:177:PRO:HG3	1:B:347:TYR:CE2	2.56	0.41
1:A:391:GLN:HA	1:A:395:TYR:CG	2.56	0.40
1:B:103:LEU:HB2	1:B:272:TRP:CE3	2.56	0.40
1:B:96:PHE:CE1	1:B:369:ARG:HA	2.57	0.40
1:C:450:ALA:O	1:C:454:LYS:HG3	2.21	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	551/556 (99%)	534 (97%)	17 (3%)	0	100	100
1	B	553/556 (100%)	532 (96%)	21 (4%)	0	100	100
1	C	552/556 (99%)	535 (97%)	17 (3%)	0	100	100
1	D	551/556 (99%)	533 (97%)	18 (3%)	0	100	100
All	All	2207/2224 (99%)	2134 (97%)	73 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	459/462 (99%)	455 (99%)	4 (1%)	78	61
1	B	461/462 (100%)	456 (99%)	5 (1%)	73	53
1	C	460/462 (100%)	457 (99%)	3 (1%)	84	69
1	D	459/462 (99%)	453 (99%)	6 (1%)	69	44
All	All	1839/1848 (100%)	1821 (99%)	18 (1%)	76	57

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	68	THR

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Mol	Chain	Res	Type
1	A	108	ARG
1	A	216	PHE
1	B	28	ASN
1	B	108	ARG
1	B	194	HIS
1	B	216	PHE
1	B	421	ASN
1	C	108	ARG
1	C	216	PHE
1	C	262	ASP
1	D	108	ARG
1	D	123	THR
1	D	216	PHE
1	D	445	ASP
1	D	534	ASP
1	D	536	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	112	ASN
1	A	185	HIS
1	A	224	ASN
1	A	245	HIS
1	A	304	ASN
1	A	332	ASN
1	A	349	HIS
1	A	416	HIS
1	A	424	HIS
1	A	468	HIS
1	A	478	ASN
1	A	541	HIS
1	A	550	ASN
1	B	17	GLN
1	B	31	GLN
1	B	112	ASN
1	B	118	ASN
1	B	185	HIS
1	B	194	HIS
1	B	224	ASN
1	B	245	HIS

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Mol	Chain	Res	Type
1	B	304	ASN
1	B	332	ASN
1	B	349	HIS
1	B	399	HIS
1	B	424	HIS
1	B	468	HIS
1	B	478	ASN
1	B	499	HIS
1	B	533	GLN
1	B	541	HIS
1	B	550	ASN
1	C	6	ASN
1	C	28	ASN
1	C	112	ASN
1	C	181	HIS
1	C	185	HIS
1	C	224	ASN
1	C	245	HIS
1	C	295	ASN
1	C	304	ASN
1	C	332	ASN
1	C	349	HIS
1	C	416	HIS
1	C	424	HIS
1	C	468	HIS
1	C	478	ASN
1	C	499	HIS
1	C	541	HIS
1	C	550	ASN
1	D	41	ASN
1	D	111	GLN
1	D	118	ASN
1	D	185	HIS
1	D	224	ASN
1	D	245	HIS
1	D	332	ASN
1	D	339	HIS
1	D	349	HIS
1	D	416	HIS
1	D	424	HIS
1	D	468	HIS
1	D	478	ASN

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Mol	Chain	Res	Type
1	D	499	HIS
1	D	533	GLN
1	D	550	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 carbohydrates in this entry.

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

There are no ligands in this entry.

### 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	553/556 (99%)	-0.25	8 (1%) 75 79	10, 16, 32, 47	0
1	B	555/556 (99%)	-0.22	4 (0%) 87 90	11, 17, 31, 60	0
1	C	554/556 (99%)	-0.19	6 (1%) 80 84	10, 16, 30, 47	0
1	D	553/556 (99%)	-0.28	4 (0%) 87 90	10, 16, 28, 55	0
All	All	2215/2224 (99%)	-0.24	22 (0%) 82 85	10, 16, 31, 60	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	ALA	5.1
1	A	251	THR	4.0
1	B	458	ALA	3.6
1	A	535	GLY	3.3
1	C	535	GLY	3.3
1	C	456	GLY	3.1
1	D	460	GLU	3.0
1	A	456	GLY	2.7
1	A	454	LYS	2.7
1	B	25	ASP	2.5
1	C	119	GLY	2.5
1	C	118	ASN	2.4
1	D	534	ASP	2.4
1	A	254	GLU	2.3
1	B	460	GLU	2.3
1	D	535	GLY	2.3
1	A	457	MET	2.2
1	A	215	THR	2.2
1	C	454	LYS	2.2
1	B	464	LYS	2.2
1	C	234	GLU	2.0
1	A	257	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.