Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 03:41 PM EDT

PDB ID	:	1DQW
Title	:	CRYSTAL STRUCTURE OF OROTIDINE 5'-PHOSPHATE DECARBOXY-LASE
Authors	:	Milburn, M.V.; Miller, B.G.; Hassell, A.M.; Wolfenden, R.; Short, S.A.
Deposited on	:	2000-01-05
Resolution	:	2.10 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

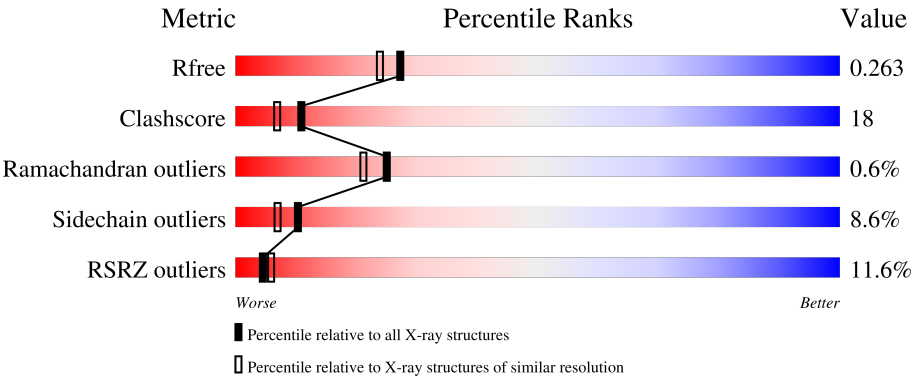
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	267	12% 64% 31% .
1	B	267	12% 60% 36% .
1	C	267	11% 62% 33% .
1	D	267	12% 60% 36% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9110 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 OROTIDINE 5'-PHOSPHATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2059	1299	357	393	10			
1	B	267	Total	C	N	O	S	0	0	0
			2059	1299	357	393	10			
1	C	267	Total	C	N	O	S	0	0	0
			2059	1299	357	393	10			
1	D	267	Total	C	N	O	S	0	0	0
			2059	1299	357	393	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	HIS	SER	engineered mutation	UNP P03962
A	267	ASP	ASN	engineered mutation	UNP P03962
B	2	HIS	SER	engineered mutation	UNP P03962
B	267	ASP	ASN	engineered mutation	UNP P03962
C	2	HIS	SER	engineered mutation	UNP P03962
C	267	ASP	ASN	engineered mutation	UNP P03962
D	2	HIS	SER	engineered mutation	UNP P03962
D	267	ASP	ASN	engineered mutation	UNP P03962

- Molecule 2 is water.

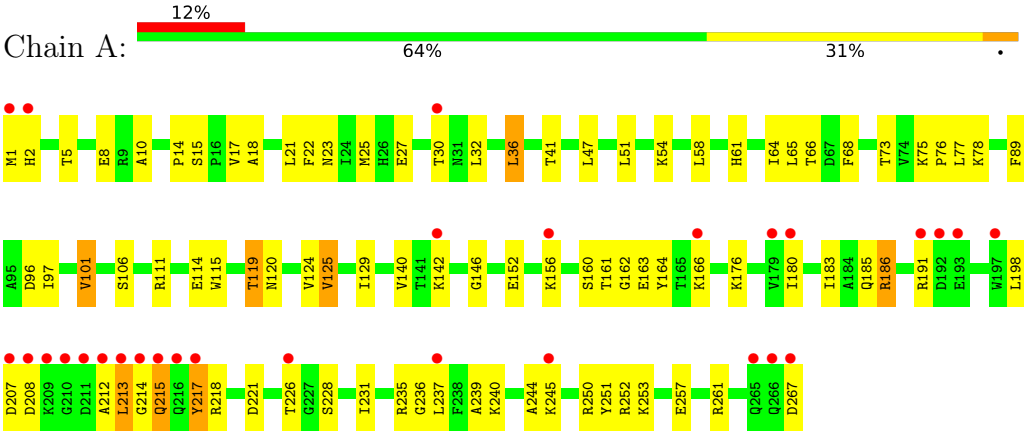
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	232	Total	O	0	0
			232	232		
2	B	232	Total	O	0	0
			232	232		
2	C	219	Total	O	0	0
			219	219		
2	D	191	Total	O	0	0
			191	191		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

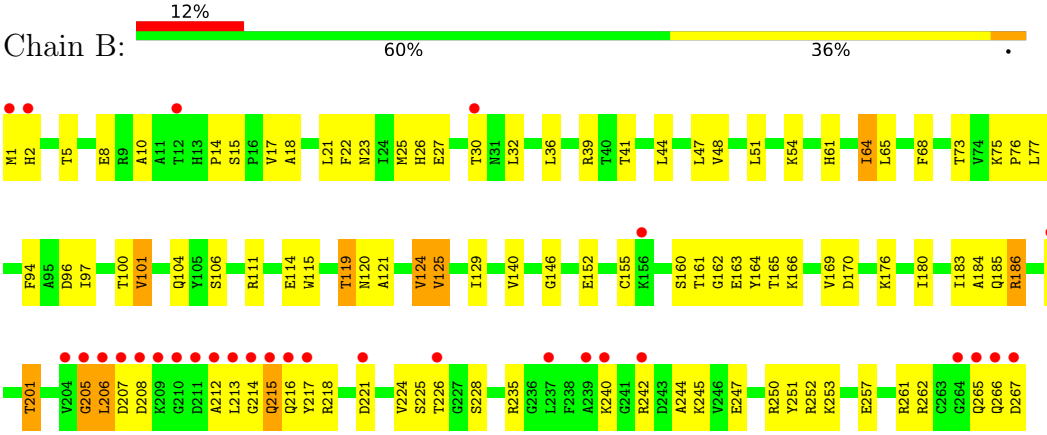
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain A:



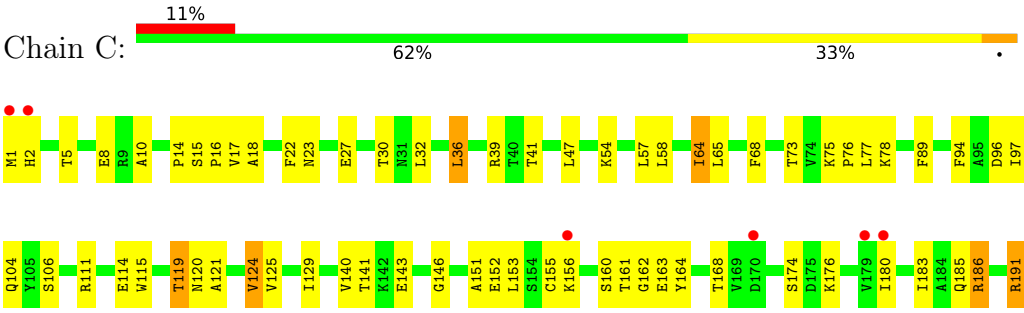
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain B:



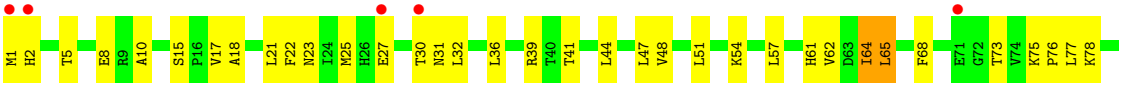
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

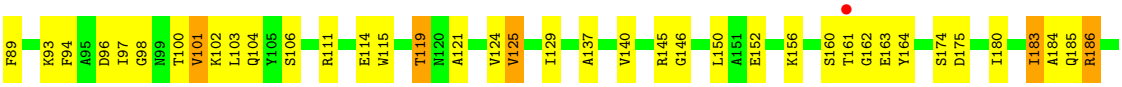
Chain C:

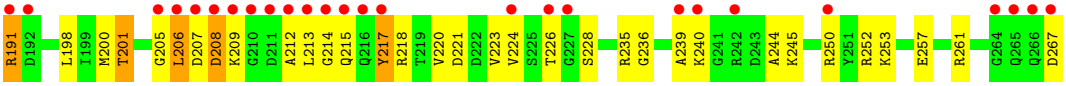


• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.06Å 116.22Å 116.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 19.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.1 (50.00-2.10) 94.7 (19.97-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 2.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.255 0.229 , 0.263	Depositor DCC
R_{free} test set	5746 reflections (8.18%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 67.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9110	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.45	1/2093 (0.0%)	1.39	7/2819 (0.2%)
1	B	0.46	2/2093 (0.1%)	1.38	7/2819 (0.2%)
1	C	0.47	1/2093 (0.0%)	1.40	7/2819 (0.2%)
1	D	0.46	1/2093 (0.0%)	1.38	7/2819 (0.2%)
All	All	0.46	5/8372 (0.1%)	1.39	28/11276 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	TYR	C-N	-9.45	1.12	1.34
1	A	217	TYR	C-N	-7.39	1.17	1.34
1	B	217	TYR	C-N	-7.31	1.17	1.34
1	D	217	TYR	C-N	-6.86	1.18	1.34
1	B	205	GLY	C-N	5.94	1.47	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	GLY	O-C-N	-63.58	20.98	122.70
1	C	205	GLY	O-C-N	-63.49	21.11	122.70
1	D	205	GLY	O-C-N	-61.94	23.60	122.70
1	B	205	GLY	O-C-N	-60.16	26.44	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	217	TYR	O-C-N	-13.77	100.67	122.70
1	D	217	TYR	O-C-N	-11.22	104.75	122.70
1	C	217	TYR	O-C-N	-10.39	106.08	122.70
1	B	217	TYR	C-N-CA	10.27	147.39	121.70
1	B	217	TYR	CA-C-N	9.58	138.28	117.20
1	B	205	GLY	CA-C-N	-9.30	96.74	117.20
1	A	217	TYR	O-C-N	-9.19	108.00	122.70
1	D	205	GLY	CA-C-N	-8.95	97.52	117.20
1	D	217	TYR	C-N-CA	8.28	142.41	121.70
1	C	217	TYR	C-N-CA	8.02	141.75	121.70
1	D	217	TYR	CA-C-N	8.02	134.84	117.20
1	C	205	GLY	CA-C-N	-7.70	100.26	117.20
1	A	205	GLY	CA-C-N	-7.25	101.25	117.20
1	C	217	TYR	CA-C-N	7.20	133.04	117.20
1	A	217	TYR	C-N-CA	6.88	138.89	121.70
1	B	205	GLY	C-N-CA	-6.66	105.05	121.70
1	A	217	TYR	CA-C-N	6.57	131.65	117.20
1	D	205	GLY	C-N-CA	-6.02	106.66	121.70
1	C	183	ILE	N-CA-C	-5.79	95.37	111.00
1	A	183	ILE	N-CA-C	-5.76	95.45	111.00
1	B	183	ILE	N-CA-C	-5.66	95.71	111.00
1	C	205	GLY	C-N-CA	-5.58	107.76	121.70
1	D	183	ILE	N-CA-C	-5.55	96.02	111.00
1	A	205	GLY	C-N-CA	-5.23	108.62	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	GLY	Mainchain
1	B	205	GLY	Mainchain
1	C	205	GLY	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2059	0	2077	71	0
1	B	2059	0	2077	78	0
1	C	2059	0	2077	79	0
1	D	2059	0	2077	78	0
2	A	232	0	0	7	0
2	B	232	0	0	7	0
2	C	219	0	0	11	0
2	D	191	0	0	6	0
All	All	9110	0	8308	301	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 18.

All (301) 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:D:96:ASP:HB3	1:D:101:VAL:HG13	1.42	0.98
1:B:30:THR:HG22	1:B:32:LEU:H	1.29	0.97
1:A:96:ASP:HB3	1:A:101:VAL:HG13	1.47	0.94
1:D:30:THR:HG22	1:D:32:LEU:H	1.30	0.94
1:B:96:ASP:HB3	1:B:101:VAL:HG13	1.49	0.93
1:C:30:THR:HG22	1:C:32:LEU:H	1.29	0.93
1:C:15:SER:OG	1:C:180:ILE:HD11	1.69	0.92
1:A:30:THR:HG22	1:A:32:LEU:H	1.37	0.90
1:B:15:SER:OG	1:B:180:ILE:HD11	1.72	0.88
1:D:15:SER:OG	1:D:180:ILE:HD11	1.78	0.83
1:C:96:ASP:HB3	1:C:101:VAL:HG13	1.58	0.83
1:A:15:SER:OG	1:A:180:ILE:HD11	1.77	0.83
1:A:94:PHE:HE1	1:A:119:THR:HG21	1.46	0.80
1:D:75:LYS:HB3	1:D:76:PRO:HD3	1.64	0.80
1:A:161:THR:HG22	1:A:163:GLU:H	1.47	0.79
1:B:161:THR:HG22	1:B:163:GLU:H	1.46	0.79
1:C:94:PHE:HE1	1:C:119:THR:HG21	1.48	0.78
1:D:94:PHE:HE1	1:D:119:THR:HG21	1.47	0.78
1:C:75:LYS:HB3	1:C:76:PRO:HD3	1.67	0.75
1:C:18:ALA:HB2	1:C:180:ILE:HG13	1.69	0.75
1:B:75:LYS:HB3	1:B:76:PRO:HD3	1.68	0.74
1:A:75:LYS:HB3	1:A:76:PRO:HD3	1.70	0.74
1:C:161:THR:HG22	1:C:163:GLU:H	1.53	0.74
1:D:18:ALA:HB2	1:D:180:ILE:HG13	1.71	0.72
1:D:253:LYS:O	1:D:257:GLU:HG3	1.89	0.72
1:D:161:THR:HG22	1:D:163:GLU:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HG2	1:B:267:ASP:OD2	1.90	0.71
1:B:18:ALA:HB2	1:B:180:ILE:HG13	1.72	0.71
1:B:94:PHE:HE1	1:B:119:THR:HG21	1.56	0.71
1:C:97:ILE:HG23	1:C:125:VAL:HG22	1.73	0.71
1:D:201:THR:HG23	1:D:228:SER:OG	1.90	0.70
1:B:124:VAL:HG13	1:B:164:TYR:HE2	1.57	0.69
1:B:214:GLY:N	1:B:235:ARG:HB2	2.08	0.69
1:C:124:VAL:HG13	1:C:164:TYR:HE2	1.59	0.68
1:D:1:MET:HG2	1:D:267:ASP:OD2	1.94	0.68
1:A:30:THR:HG21	1:A:54:LYS:O	1.94	0.67
1:A:124:VAL:HG13	1:A:164:TYR:HE2	1.57	0.67
1:A:213:LEU:HD12	1:A:213:LEU:H	1.58	0.67
1:B:97:ILE:HG23	1:B:125:VAL:CG2	2.24	0.67
1:C:97:ILE:HG23	1:C:125:VAL:CG2	2.25	0.66
1:A:18:ALA:HB2	1:A:180:ILE:HG13	1.78	0.66
1:B:97:ILE:HG23	1:B:125:VAL:HG22	1.76	0.66
1:B:30:THR:HG21	1:B:54:LYS:O	1.95	0.66
1:C:30:THR:HG21	1:C:54:LYS:O	1.96	0.65
1:C:1:MET:HG2	1:C:267:ASP:OD2	1.96	0.65
1:A:214:GLY:N	1:A:235:ARG:HB2	2.12	0.64
1:A:161:THR:HG22	1:A:162:GLY:N	2.12	0.64
1:C:161:THR:HG22	1:C:162:GLY:N	2.12	0.64
1:A:124:VAL:HG13	1:A:164:TYR:CE2	2.33	0.64
1:A:94:PHE:CE1	1:A:119:THR:HG21	2.31	0.63
1:A:201:THR:HG23	1:A:228:SER:OG	1.98	0.63
1:A:5:THR:OG1	1:A:8:GLU:HG3	1.99	0.63
1:C:185:GLN:HE21	1:C:218:ARG:HH11	1.47	0.62
1:D:213:LEU:HD12	1:D:213:LEU:H	1.64	0.62
1:B:161:THR:HG22	1:B:162:GLY:N	2.14	0.62
1:C:5:THR:OG1	1:C:8:GLU:HG3	1.97	0.62
1:D:41:THR:OG1	1:D:73:THR:HG22	1.99	0.62
1:D:185:GLN:HE21	1:D:218:ARG:HH11	1.48	0.62
1:A:1:MET:HG2	1:A:267:ASP:OD2	2.00	0.62
1:D:5:THR:OG1	1:D:8:GLU:HG3	2.00	0.62
1:C:94:PHE:CE1	1:C:119:THR:HG21	2.34	0.62
1:A:61:HIS:HD2	2:A:288:HOH:O	1.82	0.61
1:A:124:VAL:CG1	1:A:164:TYR:HE2	2.13	0.61
1:B:201:THR:HG23	1:B:228:SER:OG	2.01	0.61
1:A:185:GLN:HE21	1:A:218:ARG:HH11	1.49	0.61
1:C:201:THR:HG23	1:C:228:SER:OG	2.01	0.60
1:D:97:ILE:HG23	1:D:125:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:LEU:HD12	2:C:324:HOH:O	2.00	0.60
1:B:124:VAL:HG13	1:B:164:TYR:CE2	2.37	0.60
1:D:94:PHE:CE1	1:D:119:THR:HG21	2.35	0.60
1:B:1:MET:HG3	2:B:494:HOH:O	2.02	0.59
1:B:185:GLN:HE21	1:B:218:ARG:HH11	1.50	0.59
1:B:235:ARG:HG3	1:B:235:ARG:HH11	1.65	0.59
1:B:213:LEU:HD12	1:B:213:LEU:H	1.67	0.59
1:A:68:PHE:HA	1:A:73:THR:HG21	1.84	0.59
1:B:100:THR:O	1:B:104:GLN:HG3	2.03	0.59
1:D:30:THR:HG21	1:D:54:LYS:O	2.03	0.59
1:B:5:THR:OG1	1:B:8:GLU:HG3	2.02	0.59
1:B:253:LYS:O	1:B:257:GLU:HG3	2.03	0.59
1:D:161:THR:HG22	1:D:162:GLY:N	2.17	0.58
1:B:186:ARG:HD3	1:B:186:ARG:C	2.23	0.58
1:C:209:LYS:HB3	2:C:471:HOH:O	2.02	0.58
1:C:214:GLY:N	1:C:235:ARG:HB2	2.18	0.58
1:D:124:VAL:HG13	1:D:164:TYR:HE2	1.68	0.58
1:D:214:GLY:N	1:D:235:ARG:HB2	2.18	0.58
1:D:78:LYS:HD3	1:D:115:TRP:HB2	1.87	0.57
1:A:245:LYS:HE3	2:A:368:HOH:O	2.03	0.57
1:C:213:LEU:HD12	1:C:213:LEU:H	1.70	0.57
1:C:206:LEU:HD23	1:C:250:ARG:CZ	2.34	0.57
1:A:27:GLU:HG3	2:A:351:HOH:O	2.04	0.56
1:D:124:VAL:HG13	1:D:164:TYR:CE2	2.40	0.56
1:A:119:THR:HG22	1:A:120:ASN:H	1.70	0.56
1:B:265:GLN:HB3	2:B:494:HOH:O	2.04	0.56
1:C:161:THR:CG2	1:C:162:GLY:N	2.69	0.56
1:B:68:PHE:HA	1:B:73:THR:HG21	1.87	0.56
1:A:152:GLU:HA	1:A:160:SER:OG	2.05	0.56
1:B:161:THR:CG2	1:B:162:GLY:N	2.67	0.56
1:A:161:THR:CG2	1:A:162:GLY:N	2.69	0.56
1:D:221:ASP:OD2	1:D:261:ARG:NH1	2.38	0.56
1:A:36:LEU:HD22	1:A:58:LEU:HD11	1.89	0.55
1:A:206:LEU:HD23	1:A:250:ARG:CZ	2.36	0.55
1:C:253:LYS:O	1:C:257:GLU:HG3	2.06	0.55
1:C:41:THR:OG1	1:C:73:THR:HG22	2.05	0.55
1:B:184:ALA:O	1:B:201:THR:HG22	2.08	0.55
1:D:124:VAL:CG1	1:D:164:TYR:HE2	2.18	0.55
1:B:41:THR:OG1	1:B:73:THR:HG22	2.08	0.54
1:A:235:ARG:HG3	1:A:235:ARG:HH11	1.71	0.54
1:D:68:PHE:HA	1:D:73:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:THR:HG22	1:A:226:THR:O	2.08	0.54
1:B:221:ASP:OD2	1:B:261:ARG:NH1	2.41	0.54
1:C:121:ALA:HB1	1:C:129:ILE:HD13	1.90	0.54
1:C:212:ALA:HA	2:C:324:HOH:O	2.07	0.54
1:C:152:GLU:HA	1:C:160:SER:OG	2.08	0.53
1:A:23:ASN:O	1:A:27:GLU:HG2	2.09	0.53
1:C:186:ARG:HD3	1:C:186:ARG:C	2.29	0.53
1:C:235:ARG:HD3	2:C:345:HOH:O	2.08	0.53
1:C:235:ARG:HH11	1:C:235:ARG:HG3	1.74	0.53
1:B:235:ARG:HG3	1:B:235:ARG:NH1	2.24	0.52
1:D:161:THR:CG2	1:D:162:GLY:N	2.72	0.52
1:B:10:ALA:HB2	1:B:22:PHE:HB3	1.92	0.52
1:C:68:PHE:HA	1:C:73:THR:HG21	1.91	0.52
1:D:97:ILE:HG23	1:D:125:VAL:CG2	2.39	0.52
1:D:180:ILE:HG23	1:D:198:LEU:HD12	1.91	0.52
1:C:180:ILE:HG23	1:C:198:LEU:HD12	1.91	0.52
1:B:96:ASP:HB3	1:B:101:VAL:CG1	2.32	0.52
1:C:124:VAL:HG13	1:C:164:TYR:CE2	2.41	0.52
1:D:184:ALA:O	1:D:201:THR:HG22	2.10	0.52
1:A:36:LEU:HD22	1:A:58:LEU:CD1	2.40	0.52
1:A:253:LYS:O	1:A:257:GLU:HG3	2.11	0.51
1:C:16:PRO:HD2	2:C:323:HOH:O	2.10	0.51
1:C:156:LYS:O	1:C:156:LYS:HG3	2.09	0.51
1:B:214:GLY:H	1:B:235:ARG:HB2	1.74	0.51
1:B:124:VAL:CG1	1:B:164:TYR:HE2	2.24	0.51
1:A:186:ARG:HD3	1:A:186:ARG:C	2.30	0.51
1:D:44:LEU:O	1:D:48:VAL:HG23	2.11	0.51
1:A:92:ARG:HG3	1:A:92:ARG:HH11	1.75	0.51
1:A:213:LEU:HD23	2:A:380:HOH:O	2.10	0.50
1:D:245:LYS:HE3	2:D:409:HOH:O	2.12	0.50
1:B:152:GLU:HA	1:B:160:SER:OG	2.11	0.50
1:D:57:LEU:HD23	1:D:200:MET:HE1	1.93	0.50
1:A:97:ILE:CD1	1:B:155:CYS:HB3	2.42	0.50
1:B:94:PHE:CE1	1:B:119:THR:HG21	2.43	0.50
1:C:221:ASP:OD2	1:C:261:ARG:NH1	2.45	0.50
1:B:78:LYS:HD3	1:B:115:TRP:HB2	1.94	0.49
1:A:111:ARG:NH1	1:A:114:GLU:OE2	2.45	0.49
1:D:186:ARG:C	1:D:186:ARG:HD3	2.32	0.49
1:B:23:ASN:O	1:B:27:GLU:HG2	2.11	0.49
1:D:10:ALA:HB2	1:D:22:PHE:HB3	1.93	0.49
1:A:176:LYS:HE3	2:A:423:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ASP:O	1:C:101:VAL:HG11	2.12	0.49
1:C:226:THR:O	1:C:226:THR:HG22	2.13	0.49
1:A:166:LYS:HB3	2:A:322:HOH:O	2.14	0.48
1:B:97:ILE:CG2	1:B:125:VAL:HG22	2.43	0.48
1:C:78:LYS:HD3	1:C:115:TRP:HB2	1.94	0.48
1:A:221:ASP:OD2	1:A:261:ARG:NH1	2.47	0.48
1:A:142:LYS:HD2	2:A:446:HOH:O	2.12	0.48
1:C:10:ALA:HB2	1:C:22:PHE:HB3	1.96	0.48
1:B:161:THR:HG22	1:B:163:GLU:N	2.23	0.48
1:B:206:LEU:HD23	1:B:250:ARG:CZ	2.44	0.48
1:C:97:ILE:CG2	1:C:125:VAL:HG22	2.43	0.48
1:B:21:LEU:O	1:B:25:MET:HG3	2.13	0.48
1:D:152:GLU:HA	1:D:160:SER:OG	2.14	0.48
1:B:44:LEU:O	1:B:48:VAL:HG23	2.14	0.48
1:B:17:VAL:HG11	1:B:146:GLY:HA3	1.97	0.47
1:D:121:ALA:HB1	1:D:129:ILE:HD13	1.97	0.47
1:C:111:ARG:NH1	1:C:114:GLU:OE2	2.47	0.47
1:D:23:ASN:O	1:D:27:GLU:HG2	2.14	0.47
1:A:97:ILE:HG23	1:A:125:VAL:HG22	1.97	0.47
1:D:191:ARG:HD3	1:D:191:ARG:HA	1.80	0.47
1:A:96:ASP:O	1:A:101:VAL:HG11	2.15	0.47
1:A:51:LEU:CD2	1:A:244:ALA:HB1	2.45	0.47
1:A:235:ARG:HG3	1:A:235:ARG:NH1	2.29	0.47
1:D:206:LEU:HD23	1:D:250:ARG:CZ	2.45	0.47
1:C:124:VAL:CG1	1:C:164:TYR:HE2	2.27	0.47
1:D:235:ARG:HB3	1:D:239:ALA:HB2	1.96	0.47
1:B:225:SER:HB3	2:B:497:HOH:O	2.15	0.46
1:D:156:LYS:HG3	1:D:156:LYS:O	2.15	0.46
1:D:174:SER:O	1:D:175:ASP:HB3	2.14	0.46
1:A:14:PRO:HG3	1:A:176:LYS:HD2	1.96	0.46
1:C:15:SER:CB	1:C:180:ILE:HD11	2.43	0.46
1:C:36:LEU:HD22	1:C:58:LEU:CD1	2.45	0.46
1:C:186:ARG:HB3	2:C:410:HOH:O	2.15	0.46
1:C:14:PRO:HG3	1:C:176:LYS:HD2	1.97	0.46
1:D:57:LEU:CD2	1:D:200:MET:HE1	2.45	0.46
1:B:170:ASP:HB2	2:B:305:HOH:O	2.16	0.46
1:B:186:ARG:HD3	1:B:186:ARG:O	2.15	0.46
1:D:235:ARG:HG3	1:D:235:ARG:HH11	1.81	0.46
1:D:51:LEU:CD2	1:D:244:ALA:HB1	2.46	0.46
1:D:214:GLY:H	1:D:235:ARG:HB2	1.79	0.46
1:A:21:LEU:O	1:A:25:MET:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ASN:O	1:C:27:GLU:HG2	2.15	0.46
1:C:191:ARG:HD3	1:C:191:ARG:HA	1.81	0.46
1:B:90:GLU:O	1:B:119:THR:HG23	2.16	0.46
1:C:57:LEU:CD2	1:C:200:MET:HE1	2.46	0.46
1:C:106:SER:HB2	1:C:140:VAL:HG11	1.98	0.46
1:A:10:ALA:HB2	1:A:22:PHE:HB3	1.98	0.45
1:B:121:ALA:HB1	1:B:129:ILE:HD13	1.97	0.45
1:D:209:LYS:HE2	2:D:382:HOH:O	2.16	0.45
1:C:64:ILE:HG13	1:D:103:LEU:HD12	1.98	0.45
1:B:96:ASP:O	1:B:101:VAL:HG11	2.16	0.45
1:B:214:GLY:O	1:B:215:GLN:HB2	2.16	0.45
1:D:10:ALA:HB2	1:D:22:PHE:CB	2.47	0.45
1:A:78:LYS:HD3	1:A:115:TRP:HB2	1.98	0.45
1:B:165:THR:O	1:B:169:VAL:HG23	2.17	0.45
1:D:245:LYS:HB3	1:D:245:LYS:HE2	1.79	0.45
1:D:98:GLY:O	1:D:102:LYS:HG3	2.17	0.44
1:D:21:LEU:O	1:D:25:MET:HG3	2.16	0.44
1:A:90:GLU:O	1:A:119:THR:HG23	2.18	0.44
1:D:111:ARG:NH1	1:D:114:GLU:OE2	2.50	0.44
1:D:220:VAL:O	1:D:224:VAL:HG23	2.17	0.44
1:C:174:SER:HB3	2:C:373:HOH:O	2.17	0.44
1:A:125:VAL:CG1	1:A:129:ILE:HB	2.47	0.44
1:A:237:LEU:O	1:A:244:ALA:HA	2.16	0.44
1:B:125:VAL:CG1	1:B:129:ILE:HB	2.46	0.44
1:C:64:ILE:HG13	1:D:103:LEU:CD1	2.48	0.44
1:C:239:ALA:HB3	2:C:324:HOH:O	2.16	0.44
1:D:97:ILE:C	1:D:101:VAL:HG22	2.38	0.44
1:D:223:VAL:HG23	1:D:224:VAL:N	2.33	0.44
1:A:235:ARG:HB3	1:A:239:ALA:HB2	2.00	0.44
1:C:121:ALA:HB1	1:C:129:ILE:CD1	2.47	0.44
1:C:214:GLY:H	1:C:235:ARG:HB2	1.81	0.44
1:D:201:THR:CG2	1:D:228:SER:OG	2.65	0.44
1:C:119:THR:HG22	1:C:120:ASN:H	1.83	0.43
1:D:62:VAL:O	1:D:65:LEU:HB2	2.17	0.43
1:B:226:THR:HG22	1:B:226:THR:O	2.18	0.43
1:C:266:GLN:HA	2:C:380:HOH:O	2.18	0.43
1:B:266:GLN:O	1:B:267:ASP:CB	2.67	0.43
1:A:97:ILE:HG23	1:A:125:VAL:CG2	2.48	0.43
1:A:106:SER:HB2	1:A:140:VAL:HG11	1.99	0.43
1:D:183:ILE:HD13	1:D:200:MET:HB2	2.00	0.43
1:A:214:GLY:H	1:A:235:ARG:HB2	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASP:HA	2:D:425:HOH:O	2.18	0.43
1:A:191:ARG:HD3	1:A:191:ARG:HA	1.80	0.43
1:B:224:VAL:O	1:B:262:ARG:HD3	2.19	0.43
1:C:245:LYS:HE2	1:C:245:LYS:HB3	1.84	0.43
1:A:156:LYS:HG3	1:A:156:LYS:O	2.19	0.43
1:D:61:HIS:HD2	2:D:273:HOH:O	2.02	0.43
1:A:206:LEU:HD13	1:A:251:TYR:CE2	2.54	0.43
1:B:51:LEU:CD2	1:B:244:ALA:HB1	2.48	0.43
1:B:206:LEU:HD13	1:B:251:TYR:CE2	2.54	0.43
1:B:212:ALA:HB3	1:B:216:GLN:CD	2.39	0.43
1:A:180:ILE:HG23	1:A:198:LEU:HD12	2.01	0.42
1:D:100:THR:O	1:D:104:GLN:HG3	2.19	0.42
1:D:209:LYS:HA	2:D:372:HOH:O	2.18	0.42
1:A:92:ARG:HG3	1:A:92:ARG:NH1	2.35	0.42
1:A:231:ILE:HG13	1:A:231:ILE:O	2.19	0.42
1:B:97:ILE:HG23	1:B:125:VAL:HG21	1.98	0.42
1:A:15:SER:HG	1:A:180:ILE:HD11	1.80	0.42
1:B:214:GLY:HA2	1:B:235:ARG:HG2	2.01	0.42
1:A:214:GLY:O	1:A:215:GLN:HB2	2.19	0.42
1:C:36:LEU:HD22	1:C:58:LEU:HD11	2.01	0.42
1:C:100:THR:O	1:C:104:GLN:HG3	2.19	0.42
1:D:212:ALA:HB1	1:D:236:GLY:N	2.35	0.42
1:A:23:ASN:HD22	1:A:23:ASN:HA	1.72	0.42
1:B:180:ILE:HG23	1:B:198:LEU:HD12	2.00	0.42
1:D:106:SER:HB2	1:D:140:VAL:HG11	2.01	0.42
1:A:17:VAL:HG11	1:A:146:GLY:HA3	2.01	0.42
1:B:39:ARG:NH1	1:B:64:ILE:O	2.53	0.42
1:B:61:HIS:HD2	2:B:286:HOH:O	2.01	0.42
1:B:106:SER:HB2	1:B:140:VAL:HG11	2.02	0.42
1:B:242:ARG:HB3	1:B:247:GLU:HG3	2.01	0.42
1:C:103:LEU:HD12	1:D:64:ILE:HG13	2.01	0.42
1:C:212:ALA:HB1	1:C:236:GLY:N	2.35	0.42
1:B:26:HIS:HD2	2:B:316:HOH:O	2.02	0.42
1:C:151:ALA:HA	1:C:168:THR:HG21	2.02	0.42
1:C:97:ILE:HG23	1:C:125:VAL:HG21	2.01	0.42
1:A:41:THR:OG1	1:A:73:THR:HG22	2.20	0.41
1:B:162:GLY:O	1:B:166:LYS:HG3	2.20	0.41
1:C:214:GLY:O	1:C:215:GLN:HB2	2.19	0.41
1:A:213:LEU:HD12	1:A:213:LEU:N	2.30	0.41
1:B:14:PRO:HG3	1:B:176:LYS:HD2	2.02	0.41
1:B:184:ALA:O	1:B:201:THR:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ARG:HG3	1:C:235:ARG:NH1	2.34	0.41
1:C:235:ARG:HB3	1:C:239:ALA:HB2	2.02	0.41
1:D:214:GLY:O	1:D:215:GLN:HB2	2.20	0.41
1:A:212:ALA:HB1	1:A:236:GLY:N	2.36	0.41
1:C:17:VAL:HG11	1:C:146:GLY:HA3	2.03	0.41
1:C:192:ASP:HB2	2:C:475:HOH:O	2.21	0.41
1:D:125:VAL:CG1	1:D:129:ILE:HB	2.51	0.41
1:B:166:LYS:HB3	2:B:452:HOH:O	2.20	0.41
1:C:102:LYS:HE3	2:C:403:HOH:O	2.19	0.41
1:D:39:ARG:NH1	1:D:64:ILE:O	2.54	0.41
1:D:235:ARG:HG3	1:D:235:ARG:NH1	2.36	0.41
1:C:141:THR:HB	1:C:143:GLU:H	1.86	0.41
1:C:39:ARG:NH1	1:C:64:ILE:O	2.54	0.41
1:B:245:LYS:HB3	1:B:245:LYS:HE2	1.80	0.40
1:B:111:ARG:NH1	1:B:114:GLU:OE2	2.55	0.40
1:A:51:LEU:HD21	1:A:244:ALA:HB1	2.02	0.40
1:B:161:THR:CG2	1:B:162:GLY:H	2.34	0.40
1:D:30:THR:HG22	1:D:31:ASN:N	2.37	0.40
1:D:137:ALA:HB1	1:D:145:ARG:HG3	2.04	0.40
1:D:191:ARG:HG2	2:D:403:HOH:O	2.20	0.40
1:B:10:ALA:HB2	1:B:22:PHE:CB	2.50	0.40
1:C:97:ILE:C	1:C:101:VAL:HG22	2.42	0.40
1:C:209:LYS:H	1:C:209:LYS:HG3	1.68	0.40
1:C:212:ALA:HB3	1:C:216:GLN:HG2	2.04	0.40
1:B:119:THR:HG22	1:B:120:ASN:H	1.87	0.40
1:C:153:LEU:HD23	1:D:125:VAL:HA	2.03	0.40
1:D:17:VAL:HG11	1:D:146:GLY:HA3	2.03	0.40
1:D:93:LYS:HG2	1:D:150:LEU:HD11	2.04	0.40
1:D:226:THR:HG22	1:D:226:THR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/267 (99%)	245 (92%)	18 (7%)	2 (1%)	19	15
1	B	265/267 (99%)	241 (91%)	22 (8%)	2 (1%)	19	15
1	C	265/267 (99%)	244 (92%)	20 (8%)	1 (0%)	34	32
1	D	265/267 (99%)	243 (92%)	21 (8%)	1 (0%)	34	32
All	All	1060/1068 (99%)	973 (92%)	81 (8%)	6 (1%)	25	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	LYS
1	B	215	GLN
1	B	240	LYS
1	D	240	LYS
1	A	215	GLN
1	C	215	GLN

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	216/216 (100%)	197 (91%)	19 (9%)	10	6
1	B	216/216 (100%)	198 (92%)	18 (8%)	11	7
1	C	216/216 (100%)	197 (91%)	19 (9%)	10	6
1	D	216/216 (100%)	198 (92%)	18 (8%)	11	7
All	All	864/864 (100%)	790 (91%)	74 (9%)	10	7

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	36	LEU
1	A	47	LEU
1	A	64	ILE
1	A	65	LEU

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Mol	Chain	Res	Type
1	A	66	THR
1	A	77	LEU
1	A	89	PHE
1	A	101	VAL
1	A	119	THR
1	A	125	VAL
1	A	186	ARG
1	A	201	THR
1	A	206	LEU
1	A	207	ASP
1	A	208	ASP
1	A	213	LEU
1	A	217	TYR
1	A	252	ARG
1	B	2	HIS
1	B	36	LEU
1	B	47	LEU
1	B	64	ILE
1	B	65	LEU
1	B	77	LEU
1	B	89	PHE
1	B	101	VAL
1	B	119	THR
1	B	124	VAL
1	B	125	VAL
1	B	186	ARG
1	B	191	ARG
1	B	201	THR
1	B	206	LEU
1	B	207	ASP
1	B	208	ASP
1	B	252	ARG
1	C	2	HIS
1	C	36	LEU
1	C	47	LEU
1	C	64	ILE
1	C	65	LEU
1	C	77	LEU
1	C	89	PHE
1	C	101	VAL
1	C	119	THR
1	C	124	VAL

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Mol	Chain	Res	Type
1	C	155	CYS
1	C	186	ARG
1	C	191	ARG
1	C	201	THR
1	C	206	LEU
1	C	207	ASP
1	C	208	ASP
1	C	217	TYR
1	C	252	ARG
1	D	2	HIS
1	D	36	LEU
1	D	47	LEU
1	D	64	ILE
1	D	65	LEU
1	D	77	LEU
1	D	89	PHE
1	D	101	VAL
1	D	119	THR
1	D	125	VAL
1	D	186	ARG
1	D	191	ARG
1	D	201	THR
1	D	206	LEU
1	D	207	ASP
1	D	208	ASP
1	D	217	TYR
1	D	252	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	26	HIS
1	A	61	HIS
1	A	85	ASN
1	A	185	GLN
1	A	215	GLN
1	A	265	GLN
1	B	23	ASN
1	B	26	HIS
1	B	61	HIS
1	B	85	ASN

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Mol	Chain	Res	Type
1	B	185	GLN
1	B	215	GLN
1	B	265	GLN
1	C	23	ASN
1	C	61	HIS
1	C	85	ASN
1	C	185	GLN
1	C	215	GLN
1	C	265	GLN
1	D	23	ASN
1	D	26	HIS
1	D	85	ASN
1	D	185	GLN
1	D	215	GLN
1	D	265	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	A	1
1	B	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	217:TYR	C	218:ARG	N	1.18
1	A	217:TYR	C	218:ARG	N	1.17
1	B	217:TYR	C	218:ARG	N	1.17
1	C	217:TYR	C	218:ARG	N	1.12

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^{th} 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^2)	Q<0.9
1	A	267/267 (100%)	0.82	31 (11%)	4 6	13, 26, 56, 70	0
1	B	267/267 (100%)	0.93	32 (11%)	4 5	13, 26, 57, 70	0
1	C	267/267 (100%)	0.96	29 (10%)	5 7	14, 27, 57, 70	0
1	D	267/267 (100%)	0.91	32 (11%)	4 5	14, 28, 56, 70	0
All	All	1068/1068 (100%)	0.90	124 (11%)	4 6	13, 27, 60, 70	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	ASP	16.5
1	C	214	GLY	16.1
1	C	212	ALA	15.7
1	D	212	ALA	14.2
1	B	212	ALA	14.2
1	D	213	LEU	13.6
1	D	208	ASP	12.9
1	D	210	GLY	12.9
1	D	214	GLY	12.7
1	B	208	ASP	12.4
1	C	213	LEU	11.9
1	A	214	GLY	11.8
1	A	213	LEU	11.8
1	B	215	GLN	11.7
1	C	210	GLY	11.5
1	B	213	LEU	11.3
1	C	267	ASP	10.9
1	C	215	GLN	10.8
1	C	208	ASP	10.8
1	A	1	MET	10.7
1	A	207	ASP	10.7

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Mol	Chain	Res	Type	RSRZ
1	D	215	GLN	10.6
1	B	267	ASP	10.4
1	A	215	GLN	10.4
1	D	267	ASP	10.3
1	C	211	ASP	10.2
1	B	1	MET	10.1
1	A	212	ALA	10.0
1	A	210	GLY	9.8
1	A	267	ASP	9.7
1	C	1	MET	9.5
1	D	1	MET	9.4
1	A	209	LYS	9.3
1	A	211	ASP	9.1
1	B	207	ASP	8.8
1	B	266	GLN	8.6
1	C	216	GLN	8.5
1	C	209	LYS	8.4
1	B	216	GLN	8.2
1	D	216	GLN	8.2
1	D	211	ASP	8.1
1	A	208	ASP	8.0
1	C	217	TYR	7.5
1	C	266	GLN	7.4
1	B	214	GLY	7.3
1	B	210	GLY	7.3
1	A	216	GLN	7.2
1	D	207	ASP	6.7
1	B	217	TYR	6.5
1	D	266	GLN	6.2
1	C	2	HIS	6.1
1	B	209	LYS	6.1
1	C	207	ASP	6.1
1	B	265	GLN	5.9
1	D	265	GLN	5.8
1	D	209	LYS	5.5
1	C	206	LEU	5.2
1	B	264	GLY	5.1
1	D	217	TYR	5.0
1	A	217	TYR	5.0
1	B	2	HIS	4.8
1	D	2	HIS	4.7
1	A	206	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	2	HIS	4.2
1	B	242	ARG	4.1
1	D	206	LEU	4.0
1	B	206	LEU	3.8
1	D	226	THR	3.7
1	C	265	GLN	3.7
1	A	191	ARG	3.4
1	B	240	LYS	3.4
1	C	226	THR	3.3
1	D	264	GLY	3.2
1	A	266	GLN	3.1
1	C	192	ASP	3.1
1	C	237	LEU	3.1
1	A	192	ASP	3.0
1	D	205	GLY	3.0
1	B	30	THR	3.0
1	D	27	GLU	2.9
1	A	265	GLN	2.9
1	B	237	LEU	2.8
1	D	240	LYS	2.8
1	C	170	ASP	2.8
1	A	197	TRP	2.7
1	C	197	TRP	2.7
1	C	245	LYS	2.7
1	A	237	LEU	2.7
1	A	156	LYS	2.7
1	A	205	GLY	2.7
1	A	226	THR	2.6
1	D	161	THR	2.6
1	A	180	ILE	2.5
1	B	192	ASP	2.5
1	B	204	VAL	2.5
1	A	179	VAL	2.4
1	C	221	ASP	2.4
1	B	205	GLY	2.4
1	B	226	THR	2.3
1	D	192	ASP	2.3
1	C	205	GLY	2.3
1	C	193	GLU	2.3
1	D	227	GLY	2.3
1	A	166	LYS	2.3
1	B	12	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	224	VAL	2.2
1	A	142	LYS	2.2
1	C	180	ILE	2.2
1	D	71	GLU	2.2
1	B	198	LEU	2.2
1	A	193	GLU	2.2
1	C	179	VAL	2.2
1	B	239	ALA	2.2
1	B	191	ARG	2.2
1	D	239	ALA	2.1
1	A	245	LYS	2.1
1	D	30	THR	2.1
1	B	221	ASP	2.1
1	B	156	LYS	2.1
1	D	191	ARG	2.0
1	D	250	ARG	2.0
1	A	30	THR	2.0
1	C	156	LYS	2.0
1	D	242	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.