Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:50 am BST

PDB ID	:	1E5R
Title	:	Proline 3-hydroxylase (type II) -apo form
Authors	:	Clifton, I.J.; Hsueh, L.C.; Baldwin, J.E.; Schofield, C.J.; Harlos, K.
Deposited on	:	2000-07-28
Resolution	:	2.30 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:

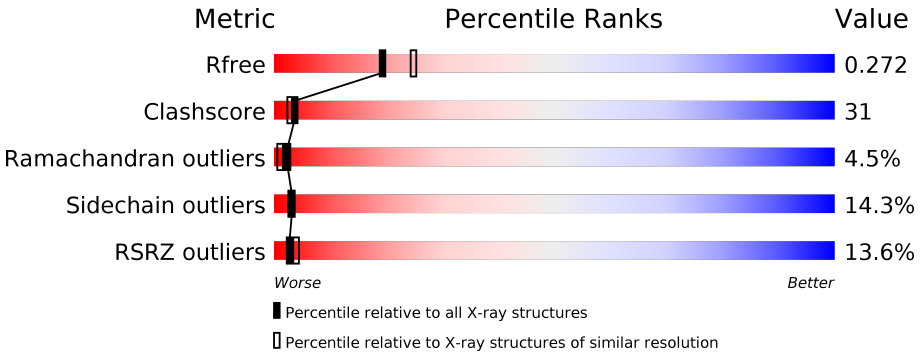
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 >=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	290	12% 46% 32% 9% • 10%
1	B	290	12% 50% 30% 10% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4474 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 PROLINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2110	1357	363	384	6			
1	B	262	Total	C	N	O	S	0	0	0
			2106	1354	363	383	6			

- Molecule 2 is water.

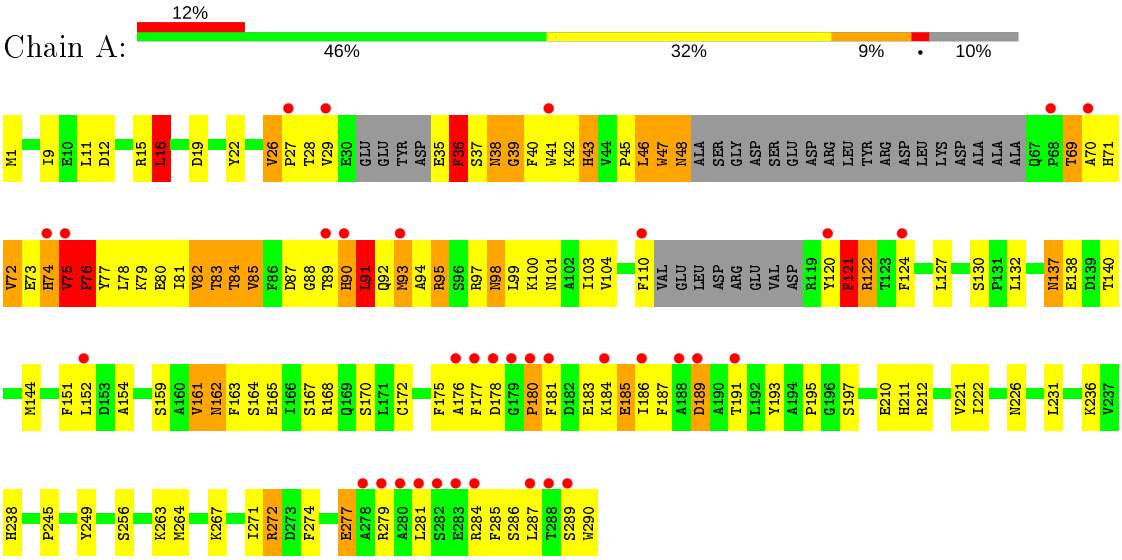
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total	O	0	0
			148	148		
2	B	110	Total	O	0	0
			110	110		

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.

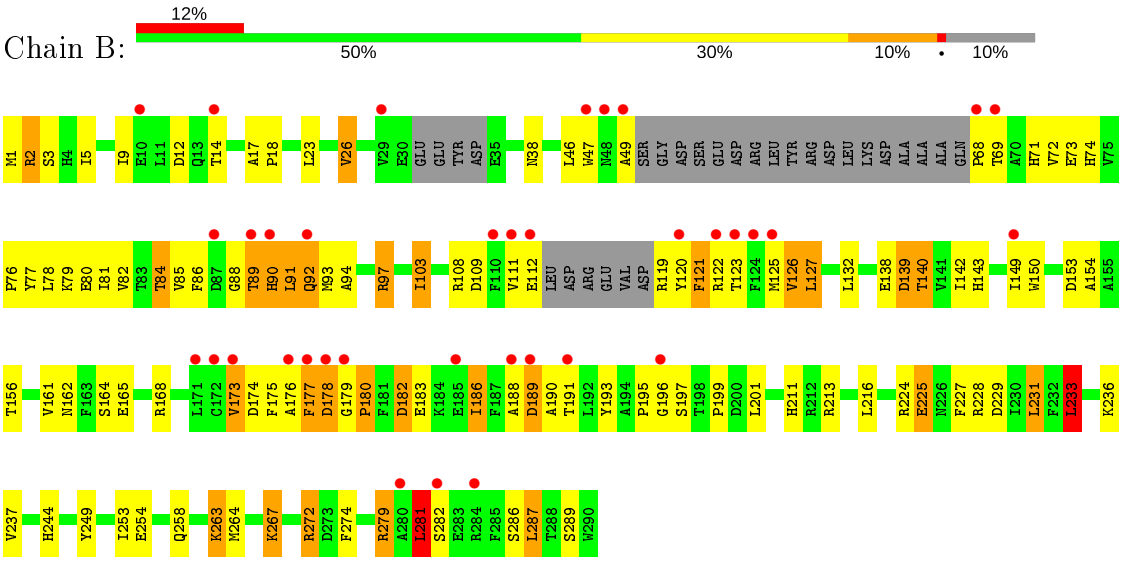
- Molecule 1: PROLINE OXIDASE

Chain A:



- Molecule 1: PROLINE OXIDASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	72.54Å 72.54Å 223.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.53 – 2.30 28.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.53-2.30) 99.3 (28.51-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.275 0.215 , 0.272	Depositor DCC
R_{free} test set	1252 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 74.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.065 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4474	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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

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	0.94	2/2167 (0.1%)	1.00	6/2941 (0.2%)
1	B	0.91	2/2161 (0.1%)	0.94	4/2933 (0.1%)
All	All	0.92	4/4328 (0.1%)	0.97	10/5874 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	LYS	CD-CE	5.71	1.65	1.51
1	A	210	GLU	CG-CD	5.63	1.60	1.51
1	A	161	VAL	CB-CG1	5.59	1.64	1.52
1	B	237	VAL	CB-CG2	5.26	1.63	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	233	LEU	CA-CB-CG	8.45	134.72	115.30
1	A	75	VAL	C-N-CD	-6.50	106.29	120.60
1	B	263	LYS	CD-CE-NZ	6.37	126.34	111.70
1	A	76	PRO	N-CA-C	6.28	128.41	112.10
1	A	36	PHE	N-CA-C	-5.83	95.26	111.00
1	B	231	LEU	CA-CB-CG	5.73	128.49	115.30
1	A	91	LEU	CA-CB-CG	5.47	127.88	115.30
1	B	281	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	16	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	75	VAL	C-N-CA	5.16	143.68	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	TYR	Sidechain

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	2110	0	2040	143	0
1	B	2106	0	2036	117	0
2	A	148	0	0	9	0
2	B	110	0	0	9	0
All	All	4474	0	4076	260	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 31.

All (260) 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:19:ASP:OD1	1:A:75:VAL:HG12	1.62	0.99
1:A:92:GLN:HE21	1:A:176:ALA:HB2	1.23	0.97
1:A:274:PHE:HB2	1:A:281:LEU:HD13	1.46	0.96
1:A:90:HIS:CD2	1:A:90:HIS:H	1.79	0.95
1:A:90:HIS:HD2	1:A:90:HIS:H	1.14	0.95
1:A:69:THR:HG23	1:A:71:HIS:H	1.32	0.95
1:A:78:LEU:O	1:A:82:VAL:HG12	1.65	0.95
1:A:97:ARG:CD	1:A:172:CYS:SG	2.57	0.92
1:A:151:PHE:O	1:A:152:LEU:HD12	1.73	0.88
1:A:37:SER:O	1:A:38:ASN:HB3	1.73	0.88
1:B:267:LYS:HE3	1:B:286:SER:O	1.74	0.88
1:A:193:TYR:CD1	1:A:195:PRO:HD3	2.10	0.87
1:A:97:ARG:HD3	1:A:172:CYS:SG	2.17	0.85
1:A:97:ARG:HD2	1:A:172:CYS:SG	2.16	0.83
1:A:193:TYR:HE1	1:A:195:PRO:HG3	1.43	0.83
1:B:126:VAL:HB	2:B:2047:HOH:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:HD3	1:B:168:ARG:HH22	1.44	0.82
1:B:138:GLU:HG2	1:B:156:THR:HB	1.61	0.82
1:A:98:ASN:HD21	1:A:168:ARG:H	1.26	0.81
1:A:16:LEU:HB3	1:A:77:TYR:CD2	2.14	0.81
1:A:74:HIS:C	1:A:75:VAL:HG23	2.02	0.80
1:B:175:PHE:HE2	1:B:186:ILE:HG23	1.47	0.80
1:B:182:ASP:O	1:B:183:GLU:HB3	1.83	0.78
1:A:90:HIS:CD2	1:A:90:HIS:N	2.48	0.77
1:B:80:GLU:O	1:B:84:THR:HG23	1.86	0.76
1:B:175:PHE:CE2	1:B:186:ILE:HG23	2.22	0.74
1:A:16:LEU:HB3	1:A:77:TYR:HD2	1.51	0.74
1:B:92:GLN:NE2	1:B:176:ALA:HB2	2.03	0.73
1:B:177:PHE:HD1	1:B:177:PHE:O	1.72	0.73
1:B:47:TRP:CZ3	1:B:82:VAL:HG11	2.24	0.73
1:B:49:ALA:HB2	1:B:92:GLN:O	1.89	0.72
1:B:173:VAL:HG23	1:B:175:PHE:CE1	2.25	0.72
1:A:90:HIS:HD1	1:A:177:PHE:HZ	1.38	0.71
1:B:125:MET:HE2	1:B:127:LEU:HD11	1.71	0.71
1:B:97:ARG:CD	1:B:168:ARG:HH22	2.04	0.71
1:A:91:LEU:HD12	1:A:92:GLN:N	2.04	0.71
1:A:36:PHE:CE1	1:A:287:LEU:HD11	2.26	0.70
1:B:189:ASP:OD1	1:B:191:THR:HB	1.90	0.70
1:A:90:HIS:O	1:A:176:ALA:N	2.24	0.70
1:A:47:TRP:O	1:A:93:MET:HA	1.92	0.69
1:A:15:ARG:NH2	1:A:80:GLU:OE2	2.21	0.69
1:A:43:HIS:HD2	1:A:95:ARG:NH1	1.90	0.69
1:A:163:PHE:HE1	1:A:236:LYS:HD2	1.57	0.69
1:B:109:ASP:OD2	1:B:154:ALA:HB1	1.94	0.68
1:B:175:PHE:CD2	1:B:186:ILE:HG13	2.28	0.68
1:B:249:TYR:CB	1:B:272:ARG:HG3	2.24	0.68
1:A:193:TYR:CE1	1:A:195:PRO:HG3	2.26	0.68
1:B:12:ASP:OD1	1:B:14:THR:HG22	1.93	0.68
1:B:188:ALA:O	1:B:189:ASP:HB2	1.93	0.67
1:B:175:PHE:CE2	1:B:186:ILE:HG13	2.29	0.67
1:B:123:THR:OG1	1:B:173:VAL:HG22	1.94	0.67
1:B:38:ASN:HD21	1:B:103:ILE:H	1.42	0.67
1:A:16:LEU:CB	1:A:77:TYR:HD2	2.08	0.67
1:B:165:GLU:CD	1:B:165:GLU:H	1.98	0.66
1:B:81:ILE:O	1:B:85:VAL:HG23	1.94	0.66
1:A:162:ASN:ND2	1:A:164:SER:H	1.93	0.66
1:B:193:TYR:CE1	1:B:195:PRO:HD3	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PRO:O	1:A:79:LYS:N	2.29	0.66
1:A:37:SER:HB3	1:A:41:TRP:CZ3	2.31	0.66
1:A:191:THR:OG1	2:A:2070:HOH:O	2.14	0.64
1:B:46:LEU:O	1:B:69:THR:HG23	1.98	0.64
1:A:271:ILE:HD11	1:A:287:LEU:HD21	1.80	0.64
1:B:38:ASN:HB2	2:B:2017:HOH:O	1.98	0.64
1:A:92:GLN:HE21	1:A:176:ALA:CB	2.07	0.63
1:A:39:GLY:O	1:A:41:TRP:CE3	2.51	0.63
1:B:97:ARG:HD3	1:B:168:ARG:NH2	2.11	0.63
1:A:186:ILE:HG13	1:A:187:PHE:N	2.14	0.62
1:B:125:MET:CE	1:B:127:LEU:HD11	2.28	0.62
1:A:277:GLU:OE1	1:A:277:GLU:HA	1.98	0.62
1:A:84:THR:OG1	1:A:85:VAL:N	2.33	0.62
1:A:193:TYR:CE1	1:A:195:PRO:HD3	2.34	0.62
1:A:88:GLY:HA2	1:A:91:LEU:HB3	1.82	0.61
1:B:249:TYR:HB3	1:B:272:ARG:HG3	1.81	0.61
1:A:151:PHE:C	1:A:152:LEU:HD12	2.20	0.61
1:A:69:THR:CG2	1:A:71:HIS:H	2.12	0.61
1:B:103:ILE:HD13	1:B:236:LYS:HG3	1.83	0.60
1:A:285:PHE:HA	2:A:2137:HOH:O	1.99	0.60
1:A:98:ASN:HD22	1:A:99:LEU:H	1.47	0.60
1:B:213:ARG:NE	2:B:2075:HOH:O	2.14	0.60
1:A:120:TYR:O	1:A:121:PHE:O	2.20	0.60
1:B:138:GLU:CG	1:B:156:THR:HB	2.29	0.60
1:A:238:HIS:CD2	1:A:245:PRO:HB3	2.37	0.60
1:B:26:VAL:HG11	1:B:71:HIS:CE1	2.38	0.59
1:B:274:PHE:CD1	1:B:281:LEU:HD22	2.37	0.59
1:B:1:MET:HE3	1:B:3:SER:HB2	1.84	0.59
1:B:121:PHE:HB3	1:B:175:PHE:HB2	1.85	0.59
1:A:16:LEU:C	1:A:16:LEU:HD13	2.24	0.58
1:B:47:TRP:HB2	1:B:94:ALA:HB3	1.86	0.58
1:A:26:VAL:HG21	1:A:71:HIS:CE1	2.37	0.58
1:A:47:TRP:HB2	1:A:94:ALA:HB3	1.86	0.58
1:B:76:PRO:O	1:B:79:LYS:HB3	2.04	0.58
1:A:193:TYR:CE1	1:A:195:PRO:CG	2.87	0.57
1:A:9:ILE:C	1:A:9:ILE:HD12	2.24	0.57
1:B:227:PHE:CD2	1:B:264:MET:HG2	2.40	0.57
1:A:189:ASP:OD1	1:A:189:ASP:C	2.44	0.57
1:B:97:ARG:HH11	1:B:97:ARG:HG3	1.69	0.57
1:A:16:LEU:HB3	1:A:77:TYR:CE2	2.40	0.56
1:A:73:GLU:HG2	2:A:2025:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PRO:O	1:B:197:SER:N	2.37	0.56
1:B:92:GLN:HE22	1:B:176:ALA:HB2	1.70	0.56
1:B:1:MET:HB2	1:B:140:THR:HG23	1.88	0.56
1:A:69:THR:O	1:A:72:VAL:HG23	2.06	0.56
1:A:163:PHE:CE1	1:A:236:LYS:HD2	2.41	0.56
1:A:26:VAL:O	1:A:42:LYS:NZ	2.31	0.56
1:A:183:GLU:HG3	1:A:193:TYR:HE2	1.71	0.55
1:B:173:VAL:HG23	1:B:175:PHE:HE1	1.71	0.55
1:B:88:GLY:C	1:B:90:HIS:H	2.09	0.55
1:B:225:GLU:CD	1:B:225:GLU:H	2.10	0.55
1:B:174:ASP:C	1:B:175:PHE:HD1	2.10	0.55
1:B:249:TYR:HB2	1:B:272:ARG:HG3	1.88	0.55
1:A:74:HIS:C	1:A:75:VAL:CG2	2.74	0.55
1:A:42:LYS:HD3	2:A:2010:HOH:O	2.08	0.54
1:A:183:GLU:HG3	1:A:193:TYR:CE2	2.43	0.54
1:A:98:ASN:ND2	1:A:168:ARG:H	2.01	0.53
1:A:92:GLN:NE2	1:A:176:ALA:HB2	2.08	0.53
1:A:12:ASP:HB3	1:A:15:ARG:HB2	1.89	0.53
1:A:98:ASN:ND2	1:A:99:LEU:H	2.06	0.53
1:B:272:ARG:HD2	2:B:2104:HOH:O	2.09	0.53
1:B:86:PHE:CZ	1:B:149:ILE:HD13	2.44	0.53
1:A:46:LEU:O	1:A:47:TRP:CE3	2.62	0.53
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.24	0.53
1:B:9:ILE:HG13	1:B:9:ILE:O	2.09	0.53
1:A:212:ARG:HG2	2:A:2095:HOH:O	2.09	0.52
1:A:92:GLN:O	1:A:93:MET:HB2	2.10	0.52
1:A:37:SER:O	1:A:38:ASN:CB	2.50	0.52
1:A:189:ASP:OD1	1:A:191:THR:OG1	2.24	0.52
1:A:45:PRO:O	1:A:69:THR:HG21	2.08	0.52
1:A:76:PRO:O	1:A:77:TYR:C	2.49	0.52
1:B:175:PHE:HE2	1:B:186:ILE:CG2	2.20	0.52
1:B:139:ASP:OD2	1:B:244:HIS:HD2	1.93	0.51
1:A:274:PHE:CD2	1:A:281:LEU:HB2	2.45	0.51
1:A:121:PHE:O	1:A:122:ARG:CB	2.59	0.50
1:A:87:ASP:OD1	1:A:89:THR:HG23	2.11	0.50
1:B:125:MET:HE2	1:B:127:LEU:CD1	2.39	0.50
1:A:263:LYS:HD3	1:A:290:TRP:O	2.10	0.50
1:B:274:PHE:HB2	1:B:281:LEU:HD13	1.94	0.50
1:A:16:LEU:C	1:A:16:LEU:CD1	2.80	0.50
1:A:9:ILE:HD11	1:A:11:LEU:CD2	2.41	0.50
1:B:119:ARG:HA	2:B:2042:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:TRP:O	1:B:93:MET:HB2	2.12	0.50
1:A:15:ARG:HH22	1:A:80:GLU:CD	2.13	0.50
1:B:199:PRO:HG2	1:B:201:LEU:HG	1.93	0.50
1:B:38:ASN:ND2	2:B:2017:HOH:O	2.44	0.50
1:B:125:MET:CE	1:B:127:LEU:CD1	2.90	0.49
1:A:74:HIS:O	1:A:75:VAL:HG23	2.12	0.49
1:A:12:ASP:OD2	1:A:15:ARG:HG3	2.12	0.49
1:A:90:HIS:HE1	1:A:185:GLU:O	1.94	0.49
1:B:274:PHE:HA	1:B:279:ARG:O	2.13	0.49
1:A:132:LEU:HB3	1:A:163:PHE:HB2	1.95	0.49
1:A:274:PHE:HD2	1:A:281:LEU:HB2	1.77	0.49
1:A:222:ILE:HD13	1:A:264:MET:HE3	1.94	0.49
1:B:174:ASP:O	1:B:175:PHE:HD1	1.96	0.49
1:B:88:GLY:HA2	1:B:91:LEU:HB2	1.95	0.48
1:A:277:GLU:C	1:A:279:ARG:H	2.16	0.48
1:A:38:ASN:O	1:A:39:GLY:O	2.30	0.48
1:B:111:VAL:HG23	1:B:112:GLU:H	1.78	0.48
1:B:86:PHE:CD1	1:B:175:PHE:HZ	2.31	0.48
1:A:1:MET:HG2	1:A:151:PHE:CE2	2.49	0.48
1:A:101:ASN:ND2	1:A:165:GLU:HB3	2.29	0.48
1:A:189:ASP:OD1	1:A:189:ASP:O	2.31	0.48
1:A:39:GLY:O	1:A:41:TRP:HE3	1.96	0.48
1:B:132:LEU:HD12	1:B:164:SER:HB3	1.96	0.48
1:B:69:THR:H	1:B:72:VAL:HG23	1.78	0.48
1:A:1:MET:HG2	1:A:151:PHE:HE2	1.79	0.47
1:B:191:THR:O	1:B:191:THR:HG22	2.14	0.47
1:A:181:PHE:CD1	1:A:181:PHE:N	2.82	0.47
1:A:19:ASP:HA	1:A:75:VAL:CG1	2.44	0.47
1:A:222:ILE:HG23	1:A:264:MET:HE1	1.95	0.47
1:B:179:GLY:O	1:B:180:PRO:C	2.53	0.47
1:B:224:ARG:NH2	1:B:263:LYS:HD2	2.29	0.47
1:B:77:TYR:O	1:B:81:ILE:HG13	2.14	0.47
1:A:22:TYR:HB2	1:A:75:VAL:HG21	1.95	0.47
1:A:162:ASN:C	1:A:162:ASN:HD22	2.18	0.47
1:B:253:ILE:HD12	1:B:272:ARG:CZ	2.45	0.47
1:A:162:ASN:HD22	1:A:163:PHE:N	2.13	0.47
1:A:193:TYR:CE1	1:A:195:PRO:CD	2.98	0.47
1:B:2:ARG:HB3	1:B:153:ASP:HB2	1.97	0.47
1:A:137:ASN:O	1:A:140:THR:HG22	2.14	0.46
1:B:123:THR:HA	1:B:150:TRP:O	2.15	0.46
1:A:193:TYR:HD1	1:A:195:PRO:HD3	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PHE:N	1:A:175:PHE:CD1	2.83	0.46
1:A:286:SER:OG	1:A:289:SER:N	2.48	0.46
1:A:37:SER:HB3	1:A:41:TRP:CH2	2.50	0.46
1:B:1:MET:HE2	1:B:3:SER:O	2.16	0.46
1:B:91:LEU:HD13	1:B:92:GLN:N	2.31	0.46
1:A:36:PHE:HE1	1:A:287:LEU:HD11	1.80	0.46
1:B:224:ARG:CZ	1:B:263:LYS:HD2	2.46	0.46
1:A:184:LYS:O	1:A:186:ILE:N	2.49	0.45
1:B:23:LEU:HD11	1:B:78:LEU:HD11	1.97	0.45
1:A:80:GLU:O	1:A:81:ILE:C	2.54	0.45
1:A:98:ASN:HD22	1:A:99:LEU:N	2.14	0.45
1:B:177:PHE:CD1	1:B:177:PHE:O	2.61	0.45
1:A:35:GLU:HB2	2:A:2015:HOH:O	2.16	0.45
1:B:274:PHE:HB2	1:B:281:LEU:CD1	2.47	0.45
1:A:222:ILE:CG2	1:A:264:MET:HE1	2.47	0.45
1:B:287:LEU:HD12	1:B:287:LEU:HA	1.74	0.45
1:A:91:LEU:CD1	1:A:92:GLN:N	2.78	0.45
1:A:274:PHE:CD1	1:A:274:PHE:C	2.90	0.45
1:B:233:LEU:C	1:B:233:LEU:HD12	2.38	0.44
1:B:254:GLU:HB2	2:B:2093:HOH:O	2.16	0.44
1:B:91:LEU:C	1:B:91:LEU:HD13	2.37	0.44
1:B:165:GLU:OE1	1:B:165:GLU:N	2.42	0.44
1:B:193:TYR:CE1	1:B:195:PRO:CD	2.99	0.44
1:A:137:ASN:C	1:A:137:ASN:HD22	2.21	0.44
1:A:46:LEU:O	1:A:47:TRP:CD2	2.70	0.44
1:B:188:ALA:O	1:B:189:ASP:CB	2.62	0.44
1:B:88:GLY:O	1:B:90:HIS:N	2.46	0.44
1:B:89:THR:O	1:B:90:HIS:CB	2.65	0.44
1:A:154:ALA:HA	2:A:2059:HOH:O	2.17	0.44
1:A:79:LYS:O	1:A:83:THR:OG1	2.21	0.44
1:B:161:VAL:HG22	1:B:162:ASN:N	2.33	0.43
1:A:256:SER:HA	1:A:264:MET:HE2	2.01	0.43
1:A:80:GLU:O	1:A:83:THR:N	2.51	0.43
1:A:221:VAL:HG22	1:A:221:VAL:O	2.17	0.43
1:B:38:ASN:ND2	1:B:103:ILE:H	2.15	0.43
1:B:173:VAL:O	1:B:173:VAL:CG2	2.67	0.43
1:B:91:LEU:CD1	1:B:91:LEU:C	2.87	0.43
1:B:233:LEU:HD13	2:B:2084:HOH:O	2.19	0.43
1:B:92:GLN:HE22	1:B:176:ALA:CB	2.32	0.43
1:A:19:ASP:HA	1:A:75:VAL:HG11	1.99	0.42
1:B:47:TRP:CD1	1:B:68:PRO:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:HG3	1:B:174:ASP:OD1	2.18	0.42
1:A:69:THR:O	1:A:71:HIS:N	2.52	0.42
1:A:26:VAL:HG21	1:A:71:HIS:ND1	2.35	0.42
1:A:26:VAL:HA	1:A:27:PRO:HD3	1.77	0.42
1:A:15:ARG:O	1:A:77:TYR:HB2	2.19	0.42
1:B:5:ILE:HG21	1:B:197:SER:HB2	2.02	0.42
1:B:23:LEU:HD11	1:B:78:LEU:CD1	2.50	0.42
1:A:249:TYR:HB3	1:A:272:ARG:CG	2.49	0.42
1:B:225:GLU:N	1:B:225:GLU:CD	2.73	0.42
1:B:17:ALA:N	1:B:18:PRO:HD2	2.35	0.42
1:A:285:PHE:C	1:A:285:PHE:CD1	2.93	0.42
1:A:40:PHE:CD1	1:A:100:LYS:HD3	2.54	0.42
1:A:271:ILE:HD11	1:A:287:LEU:CD2	2.48	0.41
1:A:281:LEU:HD21	1:A:285:PHE:CZ	2.55	0.41
1:A:183:GLU:O	1:A:186:ILE:HG12	2.20	0.41
1:A:267:LYS:NZ	2:A:2137:HOH:O	2.53	0.41
1:B:178:ASP:O	1:B:180:PRO:HD3	2.21	0.41
1:B:189:ASP:O	1:B:191:THR:N	2.53	0.41
1:B:139:ASP:HA	2:B:2066:HOH:O	2.20	0.41
1:B:91:LEU:HD22	1:B:175:PHE:CE1	2.55	0.41
1:B:69:THR:C	1:B:71:HIS:N	2.72	0.41
1:B:258:GLN:HB3	1:B:258:GLN:HE21	1.63	0.41
1:B:71:HIS:O	1:B:74:HIS:HB2	2.21	0.41
1:B:86:PHE:HZ	1:B:149:ILE:HD13	1.84	0.41
1:A:249:TYR:HB3	1:A:272:ARG:HG3	2.02	0.41
1:A:48:ASN:HA	1:A:48:ASN:HD22	1.64	0.41
1:A:87:ASP:O	1:A:90:HIS:NE2	2.54	0.41
1:B:78:LEU:O	1:B:79:LYS:C	2.59	0.41
1:A:277:GLU:HB3	1:A:279:ARG:CG	2.51	0.41
1:B:142:ILE:HG22	1:B:143:HIS:N	2.36	0.41
1:B:191:THR:CG2	1:B:191:THR:O	2.69	0.41
1:A:226:ASN:HA	2:A:2112:HOH:O	2.21	0.40
1:B:193:TYR:CZ	1:B:195:PRO:HD3	2.55	0.40
1:A:91:LEU:C	1:A:91:LEU:HD12	2.42	0.40
1:A:124:PHE:CD1	1:A:144:MET:SD	3.15	0.40
1:A:130:SER:HB2	1:A:167:SER:O	2.21	0.40
1:A:80:GLU:O	1:A:84:THR:HG23	2.21	0.40
1:A:103:ILE:HB	1:A:161:VAL:HG23	2.03	0.40
1:A:137:ASN:HD22	1:A:138:GLU:N	2.19	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	252/290 (87%)	219 (87%)	17 (7%)	16 (6%)	1 0
1	B	254/290 (88%)	228 (90%)	19 (8%)	7 (3%)	5 3
All	All	506/580 (87%)	447 (88%)	36 (7%)	23 (4%)	2 1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PHE
1	A	122	ARG
1	A	180	PRO
1	A	185	GLU
1	A	284	ARG
1	B	90	HIS
1	B	189	ASP
1	B	196	GLY
1	A	29	VAL
1	A	36	PHE
1	A	39	GLY
1	A	93	MET
1	B	182	ASP
1	B	190	ALA
1	A	28	THR
1	A	84	THR
1	B	89	THR
1	A	38	ASN
1	A	70	ALA
1	B	180	PRO
1	A	85	VAL
1	A	75	VAL
1	A	72	VAL

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	226/256 (88%)	194 (86%)	32 (14%)	3 3
1	B	223/256 (87%)	191 (86%)	32 (14%)	3 3
All	All	449/512 (88%)	385 (86%)	64 (14%)	3 3

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	26	VAL
1	A	43	HIS
1	A	46	LEU
1	A	47	TRP
1	A	48	ASN
1	A	69	THR
1	A	74	HIS
1	A	75	VAL
1	A	76	PRO
1	A	82	VAL
1	A	83	THR
1	A	90	HIS
1	A	91	LEU
1	A	95	ARG
1	A	98	ASN
1	A	104	VAL
1	A	110	PHE
1	A	121	PHE
1	A	127	LEU
1	A	137	ASN
1	A	159	SER
1	A	162	ASN
1	A	170	SER
1	A	178	ASP
1	A	180	PRO
1	A	189	ASP

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Mol	Chain	Res	Type
1	A	197	SER
1	A	211	HIS
1	A	231	LEU
1	A	272	ARG
1	A	277	GLU
1	B	2	ARG
1	B	26	VAL
1	B	73	GLU
1	B	84	THR
1	B	91	LEU
1	B	92	GLN
1	B	97	ARG
1	B	103	ILE
1	B	108	ARG
1	B	121	PHE
1	B	126	VAL
1	B	127	LEU
1	B	139	ASP
1	B	140	THR
1	B	173	VAL
1	B	177	PHE
1	B	178	ASP
1	B	186	ILE
1	B	211	HIS
1	B	216	LEU
1	B	225	GLU
1	B	228	ARG
1	B	229	ASP
1	B	231	LEU
1	B	233	LEU
1	B	267	LYS
1	B	272	ARG
1	B	279	ARG
1	B	281	LEU
1	B	282	SER
1	B	287	LEU
1	B	289	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS

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Mol	Chain	Res	Type
1	A	48	ASN
1	A	92	GLN
1	A	98	ASN
1	A	101	ASN
1	A	137	ASN
1	A	162	ASN
1	B	13	GLN
1	B	38	ASN
1	B	48	ASN
1	B	74	HIS
1	B	101	ASN
1	B	143	HIS
1	B	211	HIS
1	B	220	GLN
1	B	258	GLN
1	B	270	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 carbohydrates 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

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^{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	260/290 (89%)	0.63	35 (13%)	3	4	21, 42, 89, 110	0
1	B	262/290 (90%)	0.59	36 (13%)	3	4	22, 48, 98, 111	0
All	All	522/580 (90%)	0.61	71 (13%)	3	4	21, 45, 95, 111	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	THR	7.7
1	A	178	ASP	7.0
1	A	110	PHE	6.3
1	B	179	GLY	6.0
1	B	177	PHE	6.0
1	B	49	ALA	5.7
1	B	111	VAL	5.6
1	A	180	PRO	5.6
1	A	179	GLY	5.5
1	B	89	THR	5.4
1	A	284	ARG	5.4
1	B	185	GLU	5.2
1	A	90	HIS	5.1
1	A	280	ALA	5.0
1	A	278	ALA	4.9
1	A	176	ALA	4.7
1	B	120	TYR	4.6
1	B	92	GLN	4.4
1	A	188	ALA	4.4
1	B	110	PHE	4.3
1	A	281	LEU	4.2
1	A	181	PHE	4.0
1	B	14	THR	3.9
1	B	112	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	189	ASP	3.8
1	A	283	GLU	3.7
1	A	279	ARG	3.7
1	B	90	HIS	3.6
1	A	184	LYS	3.4
1	B	68	PRO	3.3
1	A	186	ILE	3.3
1	B	125	MET	3.2
1	A	289	SER	3.1
1	A	89	THR	3.1
1	B	196	GLY	3.1
1	B	188	ALA	3.1
1	B	171	LEU	3.0
1	A	177	PHE	3.0
1	A	120	TYR	2.9
1	B	69	THR	2.8
1	B	122	ARG	2.8
1	B	178	ASP	2.8
1	B	176	ALA	2.8
1	A	75	VAL	2.8
1	A	282	SER	2.7
1	A	288	THR	2.7
1	B	124	PHE	2.7
1	A	74	HIS	2.7
1	B	87	ASP	2.6
1	B	173	VAL	2.6
1	A	152	LEU	2.6
1	A	191	THR	2.6
1	A	41	TRP	2.6
1	A	124	PHE	2.6
1	A	27	PRO	2.5
1	A	70	ALA	2.5
1	B	149	ILE	2.5
1	B	47	TRP	2.4
1	B	10	GLU	2.4
1	B	172	CYS	2.4
1	A	189	ASP	2.4
1	A	29	VAL	2.3
1	B	284	ARG	2.3
1	B	48	ASN	2.3
1	B	280	ALA	2.3
1	A	287	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	282	SER	2.1
1	B	123	THR	2.1
1	B	29	VAL	2.1
1	A	93	MET	2.0
1	A	68	PRO	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.