Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 08:44 PM EDT

PDB ID	:	5M98
Title	:	Crystal structure of urate oxidase from zebrafish
Authors	:	Zanotti, G.; Cendron, l.; Percudani, R.; Berni, R.
Deposited on	:	2016-11-01
Resolution	:	2.80 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

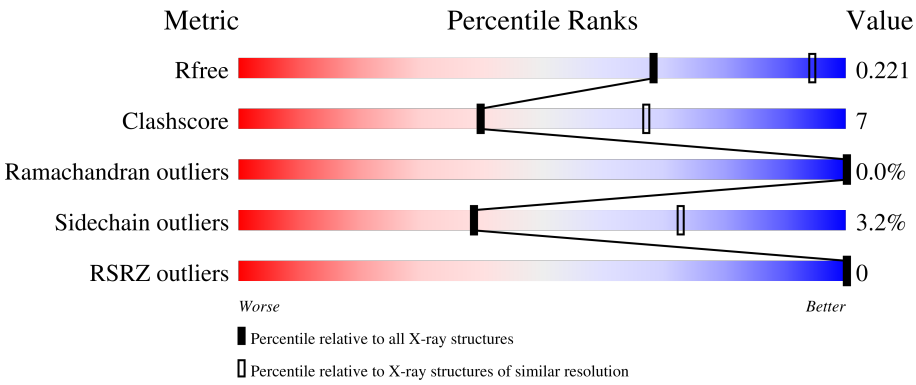
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	298	78% 17% • •
1	B	298	79% 16% • •
1	C	298	81% 14% • •
1	D	298	80% 16% •
1	E	298	79% 16% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	298	74% 21%
1	G	298	76% 18%
1	H	298	78% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18677 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 Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2322	1482	405	426	9	0	0	0
1	B	287	2322	1482	405	426	9	0	0	0
1	C	287	2322	1482	405	426	9	0	0	0
1	D	287	2322	1482	405	426	9	0	0	0
1	E	287	2322	1482	405	426	9	0	0	0
1	F	287	2322	1482	405	426	9	0	0	0
1	G	287	2322	1482	405	426	9	0	0	0
1	H	287	2322	1482	405	426	9	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	13	13	13	0	0
2	B	15	15	15	0	0
2	C	23	23	23	0	0
2	D	15	15	15	0	0
2	E	5	5	5	0	0
2	F	9	9	9	0	0

Continued on next page...

Continued from previous page...

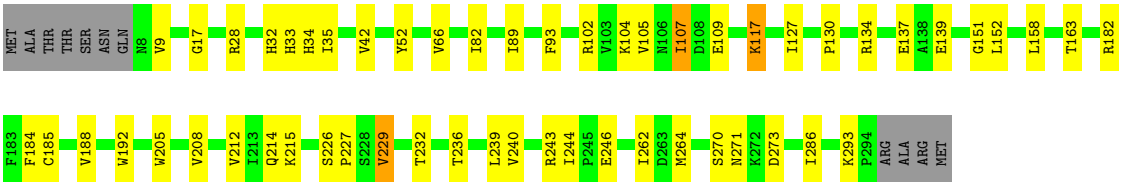
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	G	7	7	7	0	0
			Total	O		
2	H	14	14	14	0	0

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.

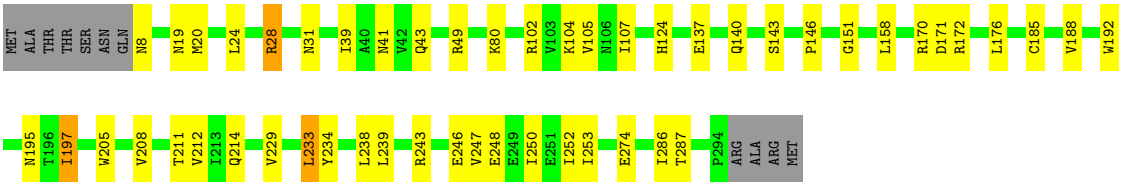
• Molecule 1: Uricase

Chain A:



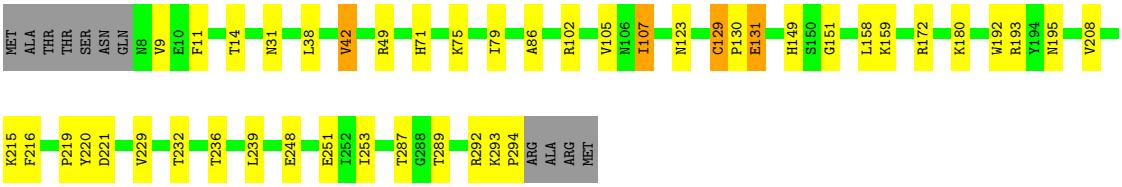
• Molecule 1: Uricase

Chain B:



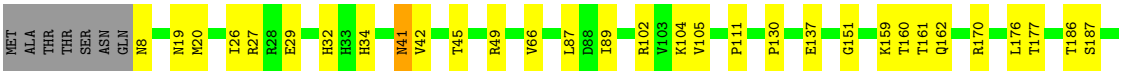
• Molecule 1: Uricase

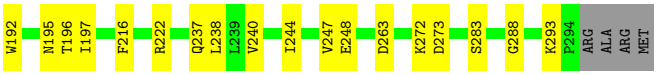
Chain C:



• Molecule 1: Uricase

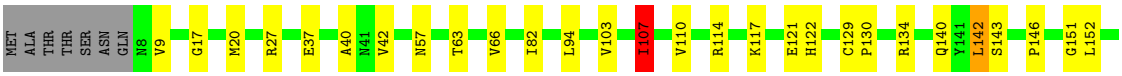
Chain D:

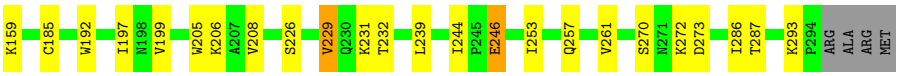




• Molecule 1: Uricase

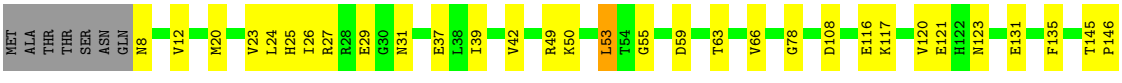
Chain E:





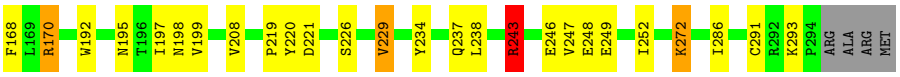
• Molecule 1: Uricase

Chain F:



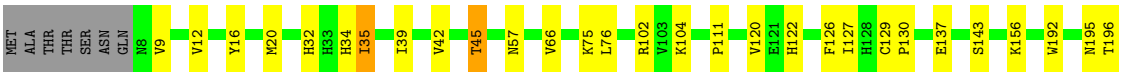
• Molecule 1: Uricase

Chain G:



• Molecule 1: Uricase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.34Å 127.42Å 132.60Å 90.00° 102.21° 90.00°	Depositor
Resolution (Å)	83.20 – 2.80 78.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.9 (83.20-2.80) 94.9 (78.05-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.204 , 0.242 0.206 , 0.221	Depositor DCC
R_{free} test set	3240 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 27.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18677	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.32 % 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 1.7963e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.71	0/2374	0.88	2/3217 (0.1%)
1	B	0.72	0/2374	0.85	2/3217 (0.1%)
1	C	0.73	0/2374	0.87	1/3217 (0.0%)
1	D	0.73	0/2374	0.86	3/3217 (0.1%)
1	E	0.71	0/2374	0.86	2/3217 (0.1%)
1	F	0.68	0/2374	0.82	2/3217 (0.1%)
1	G	0.73	0/2374	0.86	4/3217 (0.1%)
1	H	0.71	0/2374	0.86	0/3217
All	All	0.72	0/18992	0.86	16/25736 (0.1%)

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	E	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	170	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	C	102	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	B	233	LEU	CB-CG-CD1	-6.50	99.95	111.00
1	B	28	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	G	243	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	F	27	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	263	ASP	CB-CG-OD1	5.47	123.22	118.30
1	E	27	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	273	ASP	CB-CG-OD1	5.37	123.13	118.30
1	D	49	ARG	NE-CZ-NH2	-5.33	117.63	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	107	ILE	CG1-CB-CG2	-5.30	99.75	111.40
1	A	182	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	176	LEU	CA-CB-CG	5.26	127.39	115.30
1	G	27	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	G	102	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	F	53	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	142	LEU	Peptide

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	2322	0	2325	39	0
1	B	2322	0	2325	33	0
1	C	2322	0	2325	35	0
1	D	2322	0	2325	29	0
1	E	2322	0	2325	39	0
1	F	2322	0	2325	49	0
1	G	2322	0	2325	44	0
1	H	2322	0	2325	38	0
2	A	13	0	0	0	0
2	B	15	0	0	0	0
2	C	23	0	0	1	0
2	D	15	0	0	0	0
2	E	5	0	0	0	0
2	F	9	0	0	0	0
2	G	7	0	0	1	0
2	H	14	0	0	0	0
All	All	18677	0	18600	272	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 7.

All (272) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:VAL:HG21	1:H:238:LEU:HD11	1.55	0.88
1:B:229:VAL:HG21	1:B:286:ILE:HD13	1.56	0.87
1:F:229:VAL:HG21	1:F:286:ILE:HD13	1.56	0.87
1:G:20:MET:HA	1:G:39:ILE:HD11	1.61	0.82
1:H:241:LEU:HD23	1:H:247:VAL:HG23	1.63	0.81
1:A:151:GLY:O	1:A:205:TRP:HZ3	1.64	0.80
1:A:215:LYS:HB3	1:A:236:THR:HG22	1.62	0.79
1:H:215:LYS:HB3	1:H:236:THR:HG22	1.64	0.79
1:D:170:ARG:HH22	1:D:177:THR:HA	1.48	0.78
1:D:20:MET:H	1:D:41:ASN:HD22	1.30	0.76
1:C:38:LEU:HD22	1:C:107:ILE:HD11	1.65	0.75
1:F:158:LEU:HD13	1:F:185:CYS:HB2	1.70	0.72
1:B:28:ARG:NH2	1:D:273:ASP:O	2.22	0.72
1:A:158:LEU:HD13	1:A:185:CYS:HB2	1.72	0.72
1:B:151:GLY:O	1:B:205:TRP:HZ3	1.71	0.72
1:E:151:GLY:O	1:E:205:TRP:HZ3	1.72	0.71
1:F:253:ILE:HG12	1:F:287:THR:HG22	1.73	0.70
1:D:20:MET:H	1:D:41:ASN:ND2	1.89	0.70
1:E:20:MET:HB3	1:F:281:ASN:HD22	1.56	0.70
1:F:151:GLY:O	1:F:205:TRP:HZ3	1.73	0.70
1:A:117:LYS:HE3	1:C:220:TYR:CZ	2.27	0.69
1:B:19:ASN:HD22	1:B:41:ASN:CG	1.99	0.67
1:E:229:VAL:CG2	1:E:286:ILE:HG13	2.25	0.67
1:C:42:VAL:HB	1:C:105:VAL:HG12	1.77	0.67
1:A:42:VAL:HG12	1:A:105:VAL:HG22	1.77	0.66
1:G:238:LEU:HD11	1:H:9:VAL:HG21	1.76	0.66
1:D:244:ILE:CG2	1:D:247:VAL:HG13	2.25	0.66
1:A:214:GLN:NE2	1:H:120:VAL:HG22	2.11	0.66
1:G:27:ARG:NH2	1:G:34:HIS:CD2	2.65	0.65
1:H:156:LYS:NZ	1:H:257:GLN:OE1	2.30	0.65
1:C:129:CYS:O	1:C:129:CYS:SG	2.55	0.64
1:G:243:ARG:HG3	1:G:243:ARG:HH11	1.63	0.64
1:B:49:ARG:HG3	1:B:49:ARG:HH11	1.62	0.64
1:F:42:VAL:HG11	1:F:66:VAL:HG22	1.80	0.63
1:C:49:ARG:HG2	1:C:49:ARG:HH11	1.63	0.63
1:A:229:VAL:CG2	1:A:286:ILE:HG13	2.29	0.63
1:G:146:PRO:O	1:G:197:ILE:HD11	1.99	0.63
1:F:20:MET:SD	1:F:39:ILE:HD11	2.39	0.62
1:D:151:GLY:HA2	1:D:192:TRP:CZ3	2.35	0.62
1:H:42:VAL:HG22	1:H:66:VAL:HG11	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:ARG:NH2	1:G:34:HIS:HD2	1.98	0.61
1:E:229:VAL:HG21	1:E:286:ILE:HG13	1.82	0.61
1:F:31:ASN:O	1:F:123:ASN:HB3	2.01	0.60
1:H:234:TYR:CE2	1:H:238:LEU:HD22	2.37	0.59
1:F:25:HIS:CE1	1:F:78:GLY:HA2	2.38	0.59
1:A:42:VAL:HG11	1:A:89:ILE:HG21	1.85	0.59
1:C:215:LYS:HG2	1:C:236:THR:HG22	1.85	0.58
1:H:111:PRO:HG3	1:H:130:PRO:HB3	1.85	0.58
1:E:94:LEU:HD22	1:E:142:LEU:HB2	1.86	0.58
1:B:211:THR:O	1:B:214:GLN:HB3	2.03	0.58
1:B:229:VAL:CG2	1:B:286:ILE:HD13	2.30	0.58
1:B:104:LYS:HD2	1:B:137:GLU:OE2	2.04	0.57
1:A:192:TRP:CZ3	1:A:208:VAL:HG11	2.40	0.57
1:B:253:ILE:HG12	1:B:287:THR:HG22	1.87	0.57
1:E:229:VAL:HG23	1:E:286:ILE:HG21	1.87	0.57
1:G:20:MET:CA	1:G:39:ILE:HD11	2.32	0.57
1:G:21:VAL:HA	2:G:304:HOH:O	2.06	0.56
1:C:38:LEU:HD13	1:C:107:ILE:HD12	1.87	0.56
1:D:27:ARG:NH2	1:D:34:HIS:HD1	2.03	0.56
1:H:45:THR:CG2	1:H:102:ARG:HE	2.18	0.56
1:H:45:THR:HG23	1:H:102:ARG:HE	1.70	0.56
1:A:293:LYS:HZ3	1:B:8:ASN:N	2.03	0.56
1:H:215:LYS:CB	1:H:236:THR:HG22	2.33	0.56
1:E:20:MET:HB3	1:F:281:ASN:ND2	2.21	0.56
1:E:199:VAL:HG13	1:E:246:GLU:HG3	1.87	0.56
1:F:233:LEU:HD11	1:F:252:ILE:HB	1.88	0.56
1:B:253:ILE:HG23	1:B:287:THR:HG22	1.88	0.55
1:A:264:MET:HE3	1:A:271:ASN:HB2	1.87	0.55
1:G:170:ARG:HG3	1:G:170:ARG:HH11	1.70	0.55
1:F:50:LYS:HD2	1:F:59:ASP:OD2	2.07	0.55
1:A:229:VAL:HG21	1:A:286:ILE:HG13	1.88	0.55
1:F:146:PRO:HG2	1:F:197:ILE:HG21	1.89	0.54
1:A:102:ARG:NH1	1:A:139:GLU:OE2	2.41	0.54
1:G:39:ILE:HG23	1:G:108:ASP:HB2	1.88	0.54
1:H:20:MET:SD	1:H:39:ILE:HD11	2.48	0.54
1:B:158:LEU:HD13	1:B:185:CYS:HB2	1.90	0.54
1:F:42:VAL:HG11	1:F:66:VAL:CG2	2.38	0.54
1:F:160:THR:CG2	1:H:35:ILE:HD11	2.38	0.54
1:G:129:CYS:O	1:G:129:CYS:SG	2.64	0.53
1:C:253:ILE:HG12	1:C:287:THR:HG22	1.89	0.53
1:F:25:HIS:HD2	1:F:26:ILE:N	2.06	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:ARG:HH11	1:G:243:ARG:CG	2.21	0.53
1:H:207:ALA:HB3	1:H:244:ILE:HD11	1.91	0.53
1:H:111:PRO:CG	1:H:130:PRO:HB3	2.38	0.53
1:B:140:GLN:NE2	1:B:146:PRO:HD3	2.24	0.53
1:D:111:PRO:HG3	1:D:130:PRO:HB3	1.90	0.52
1:G:229:VAL:HG21	1:G:286:ILE:HD13	1.88	0.52
1:C:219:PRO:C	1:C:221:ASP:H	2.13	0.52
1:F:270:SER:O	1:H:75:LYS:HE2	2.09	0.52
1:A:229:VAL:HG23	1:A:286:ILE:HG21	1.92	0.52
1:E:82:ILE:HB	1:E:107:ILE:HG13	1.91	0.52
1:A:117:LYS:HE3	1:C:220:TYR:OH	2.08	0.52
1:F:24:LEU:HD12	1:F:37:GLU:HB2	1.92	0.52
1:F:207:ALA:CB	1:F:244:ILE:HD11	2.39	0.52
1:B:20:MET:SD	1:B:39:ILE:HD11	2.50	0.52
1:B:188:VAL:HG11	1:B:212:VAL:HG11	1.91	0.51
1:E:226:SER:OG	1:E:232:THR:OG1	2.24	0.51
1:A:262:ILE:O	1:A:271:ASN:ND2	2.41	0.51
1:E:17:GLY:HA3	1:E:42:VAL:O	2.09	0.51
1:E:192:TRP:CZ3	1:E:208:VAL:HG11	2.45	0.51
1:A:134:ARG:HA	1:A:205:TRP:CH2	2.44	0.51
1:C:195:ASN:HB3	1:C:248:GLU:HB2	1.92	0.51
1:F:156:LYS:O	1:H:127:ILE:HD12	2.10	0.51
1:H:192:TRP:CZ3	1:H:208:VAL:HG11	2.46	0.50
1:A:117:LYS:CE	1:C:220:TYR:OH	2.59	0.50
1:A:188:VAL:HG11	1:A:212:VAL:HG11	1.92	0.50
1:E:146:PRO:HG2	1:E:197:ILE:HG21	1.92	0.50
1:D:104:LYS:HE2	1:D:137:GLU:OE2	2.12	0.50
1:E:57:ASN:O	1:F:168:PHE:HA	2.11	0.50
1:D:186:THR:OG1	1:D:187:SER:N	2.45	0.50
1:G:22:LYS:HG2	1:G:39:ILE:HD13	1.94	0.50
1:H:222:ARG:NH1	1:H:222:ARG:HB3	2.27	0.49
1:C:38:LEU:HD21	1:C:79:ILE:HD13	1.92	0.49
1:H:35:ILE:HD12	1:H:126:PHE:CE1	2.47	0.49
1:D:240:VAL:HG12	1:D:247:VAL:HG21	1.95	0.49
1:G:146:PRO:HG2	1:G:197:ILE:HG12	1.93	0.49
1:C:149:HIS:NE2	1:C:193:ARG:HB2	2.28	0.49
1:D:159:LYS:HG3	1:D:216:PHE:CZ	2.48	0.49
1:D:244:ILE:HG22	1:D:247:VAL:HG13	1.92	0.49
1:E:134:ARG:HG3	1:E:205:TRP:CE3	2.48	0.49
1:E:273:ASP:HB3	1:G:28:ARG:NH2	2.27	0.49
1:C:71:HIS:HD2	2:C:320:HOH:O	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:HIS:HD2	1:D:34:HIS:NE2	2.11	0.49
1:E:151:GLY:HA2	1:E:192:TRP:CZ3	2.48	0.49
1:E:159:LYS:HA	1:G:124:HIS:O	2.13	0.49
1:F:63:THR:HA	1:F:66:VAL:HG12	1.94	0.49
1:G:19:ASN:CG	1:G:41:ASN:HD22	2.16	0.49
1:B:49:ARG:HG3	1:B:49:ARG:NH1	2.28	0.48
1:E:140:GLN:HB2	1:E:146:PRO:HB3	1.94	0.48
1:B:105:VAL:HG12	1:B:107:ILE:CD1	2.44	0.48
1:C:158:LEU:HD23	1:C:159:LYS:N	2.28	0.48
1:D:45:THR:HB	1:D:102:ARG:HB3	1.95	0.48
1:A:32:HIS:HD2	1:A:34:HIS:CE1	2.30	0.48
1:D:161:THR:OG1	1:D:162:GLN:N	2.47	0.48
1:E:244:ILE:HG22	1:E:246:GLU:HG2	1.95	0.48
1:H:214:GLN:HE22	1:H:243:ARG:HH22	1.61	0.48
1:C:151:GLY:HA2	1:C:192:TRP:CZ3	2.49	0.47
1:C:251:GLU:HG3	1:C:289:THR:OG1	2.13	0.47
1:E:40:ALA:HA	1:E:107:ILE:HG22	1.96	0.47
1:B:233:LEU:HD11	1:B:252:ILE:CG2	2.44	0.47
1:B:31:ASN:HD21	1:D:222:ARG:HH11	1.61	0.47
1:E:63:THR:HA	1:E:66:VAL:HG12	1.97	0.47
1:D:195:ASN:HB3	1:D:248:GLU:HB2	1.97	0.47
1:E:205:TRP:CD1	1:E:206:LYS:N	2.83	0.47
1:G:192:TRP:CZ3	1:G:208:VAL:HG11	2.49	0.47
1:C:11:PHE:CD2	1:C:49:ARG:HD3	2.50	0.47
1:G:168:PHE:HA	1:H:57:ASN:O	2.15	0.47
1:G:199:VAL:HG13	1:G:246:GLU:HG3	1.97	0.47
1:G:82:ILE:HD11	1:G:134:ARG:HG2	1.97	0.46
1:H:20:MET:HA	1:H:39:ILE:HD11	1.97	0.46
1:C:292:ARG:O	1:C:294:PRO:HD3	2.15	0.46
1:E:293:LYS:HD2	1:F:8:ASN:N	2.30	0.46
1:B:146:PRO:HG2	1:B:197:ILE:HG21	1.96	0.46
1:B:274:GLU:O	1:D:26:ILE:HG22	2.15	0.46
1:F:229:VAL:HG23	1:F:286:ILE:HG21	1.97	0.46
1:A:17:GLY:HA3	1:A:42:VAL:O	2.15	0.46
1:A:232:THR:O	1:A:236:THR:HG23	2.14	0.46
1:G:18:LYS:C	1:G:19:ASN:HD22	2.18	0.46
1:H:249:GLU:HG3	1:H:291:CYS:HB3	1.97	0.46
1:B:105:VAL:HG12	1:B:107:ILE:HD12	1.98	0.46
1:E:9:VAL:HG21	1:F:238:LEU:HD11	1.97	0.46
1:G:195:ASN:HB3	1:G:248:GLU:HB2	1.97	0.46
1:G:122:HIS:HE1	1:G:124:HIS:CD2	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:231:LYS:HE3	1:H:235:ASP:OD2	2.16	0.45
1:A:130:PRO:HD2	1:C:130:PRO:HD2	1.97	0.45
1:E:205:TRP:CD1	1:E:205:TRP:C	2.89	0.45
1:A:28:ARG:HG2	1:A:33:HIS:CD2	2.51	0.45
1:B:229:VAL:HG23	1:B:286:ILE:HG21	1.98	0.45
1:D:20:MET:N	1:D:41:ASN:HD22	2.07	0.45
1:A:82:ILE:HG21	1:A:109:GLU:HB2	1.97	0.45
1:C:31:ASN:O	1:C:123:ASN:HB3	2.17	0.45
1:C:86:ALA:HA	1:C:105:VAL:HG21	1.98	0.45
1:E:270:SER:O	1:G:75:LYS:HE2	2.16	0.45
1:A:102:ARG:HH12	1:A:104:LYS:HD2	1.80	0.45
1:G:114:ARG:HD2	1:G:121:GLU:HB3	1.97	0.45
1:B:124:HIS:HB2	1:D:160:THR:OG1	2.17	0.45
1:F:25:HIS:HE1	1:F:78:GLY:HA2	1.80	0.45
1:A:226:SER:HA	1:A:227:PRO:HD3	1.79	0.45
1:C:14:THR:OG1	1:C:49:ARG:NH1	2.40	0.45
1:C:232:THR:O	1:C:236:THR:HG23	2.16	0.45
1:G:249:GLU:HG3	1:G:291:CYS:HB3	1.97	0.45
1:B:192:TRP:CZ3	1:B:208:VAL:HG11	2.52	0.44
1:E:20:MET:HE2	1:F:281:ASN:HD21	1.82	0.44
1:G:272:LYS:HB2	1:G:272:LYS:HE3	1.74	0.44
1:F:117:LYS:O	1:F:120:VAL:HG12	2.17	0.44
1:F:158:LEU:O	1:H:126:PHE:N	2.48	0.44
1:A:151:GLY:O	1:A:205:TRP:CZ3	2.56	0.44
1:A:163:THR:HG21	1:A:184:PHE:HB2	1.99	0.44
1:C:107:ILE:HD13	1:C:107:ILE:HG21	1.72	0.44
1:B:24:LEU:C	1:B:24:LEU:HD23	2.38	0.44
1:C:159:LYS:HB2	1:C:216:PHE:CZ	2.52	0.44
1:E:231:LYS:HG3	1:F:55:GLY:N	2.33	0.44
1:B:195:ASN:HB3	1:B:248:GLU:HB2	1.99	0.44
1:D:244:ILE:HG21	1:D:247:VAL:HG13	2.00	0.44
1:A:127:ILE:HD13	1:C:131:GLU:HG2	2.00	0.44
1:C:9:VAL:HG21	1:D:238:LEU:HD11	1.99	0.44
1:E:122:HIS:CD2	1:G:220:TYR:HA	2.52	0.44
1:H:32:HIS:CD2	1:H:34:HIS:HE2	2.36	0.44
1:G:17:GLY:HA3	1:G:42:VAL:O	2.18	0.43
1:F:205:TRP:CD1	1:F:206:LYS:N	2.86	0.43
1:F:207:ALA:HB1	1:F:244:ILE:HD11	1.99	0.43
1:F:293:LYS:HA	1:F:294:PRO:HD2	1.81	0.43
1:G:45:THR:CG2	1:G:102:ARG:HH21	2.31	0.43
1:G:237:GLN:HG3	1:G:252:ILE:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:GLN:NE2	1:D:288:GLY:O	2.51	0.43
1:F:151:GLY:HA2	1:F:192:TRP:CZ3	2.52	0.43
1:A:264:MET:CE	1:A:271:ASN:HB2	2.48	0.43
1:F:163:THR:HG21	1:F:184:PHE:HB2	2.00	0.43
1:G:192:TRP:HB2	1:G:247:VAL:HG13	2.00	0.43
1:H:129:CYS:O	1:H:129:CYS:SG	2.76	0.43
1:F:156:LYS:NZ	1:F:257:GLN:OE1	2.48	0.43
1:D:87:LEU:HD21	1:D:197:ILE:HD11	2.01	0.43
1:G:45:THR:HG23	1:G:102:ARG:HE	1.83	0.43
1:F:214:GLN:HE22	1:F:243:ARG:HH22	1.65	0.43
1:A:240:VAL:HG13	1:A:244:ILE:HD12	2.00	0.43
1:B:239:LEU:O	1:B:243:ARG:HG3	2.19	0.43
1:E:114:ARG:HD2	1:E:121:GLU:HB3	2.01	0.43
1:E:129:CYS:HA	1:E:130:PRO:HD3	1.88	0.43
1:F:199:VAL:HG22	1:F:246:GLU:HG3	1.99	0.43
1:E:134:ARG:HG3	1:E:205:TRP:CZ3	2.54	0.42
1:H:244:ILE:O	1:H:247:VAL:HG22	2.19	0.42
1:G:219:PRO:C	1:G:221:ASP:H	2.23	0.42
1:F:24:LEU:C	1:F:24:LEU:HD23	2.40	0.42
1:A:66:VAL:HG23	1:A:93:PHE:CZ	2.54	0.42
1:C:180:LYS:HB3	1:C:180:LYS:HE3	1.95	0.42
1:E:37:GLU:HB3	1:E:110:VAL:HB	2.00	0.42
1:F:31:ASN:O	1:F:123:ASN:CB	2.66	0.42
1:B:43:GLN:OE1	1:B:102:ARG:NH2	2.53	0.42
1:F:25:HIS:CD2	1:F:26:ILE:N	2.86	0.42
1:C:38:LEU:HD22	1:C:107:ILE:CD1	2.42	0.42
1:D:19:ASN:OD1	1:D:41:ASN:HB3	2.20	0.42
1:E:273:ASP:OD1	1:E:273:ASP:N	2.50	0.42
1:F:116:GLU:HG3	1:F:121:GLU:HG2	2.02	0.42
1:G:114:ARG:CD	1:G:121:GLU:HB3	2.50	0.41
1:E:20:MET:CE	1:F:281:ASN:HD21	2.33	0.41
1:F:192:TRP:CZ3	1:F:208:VAL:HG11	2.54	0.41
1:G:234:TYR:HA	1:G:237:GLN:OE1	2.20	0.41
1:E:253:ILE:HG12	1:E:287:THR:HG22	2.02	0.41
1:H:241:LEU:HD23	1:H:247:VAL:CG2	2.44	0.41
1:F:217:ALA:HB1	1:H:122:HIS:CD2	2.56	0.41
1:G:144:LYS:HA	1:G:144:LYS:HD3	1.93	0.41
1:D:272:LYS:O	1:D:272:LYS:CG	2.69	0.41
1:A:239:LEU:O	1:A:243:ARG:HG3	2.21	0.41
1:F:253:ILE:HG12	1:F:287:THR:CG2	2.48	0.41
1:G:122:HIS:CE1	1:G:124:HIS:CD2	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:LYS:HE2	1:H:137:GLU:OE2	2.21	0.41
1:C:86:ALA:HB1	1:C:105:VAL:CG2	2.50	0.41
1:F:31:ASN:O	1:F:123:ASN:CG	2.59	0.41
1:A:52:TYR:HB3	1:B:234:TYR:HB2	2.02	0.41
1:A:82:ILE:HB	1:A:107:ILE:HD11	2.02	0.41
1:B:170:ARG:NH2	1:B:176:LEU:O	2.54	0.41
1:C:158:LEU:HD23	1:C:158:LEU:C	2.41	0.41
1:E:185:CYS:HB3	1:E:257:GLN:O	2.20	0.41
1:H:239:LEU:HD12	1:H:239:LEU:HA	1.90	0.41
1:H:245:PRO:HA	1:H:292:ARG:NH2	2.36	0.41
1:B:233:LEU:HD11	1:B:252:ILE:HG22	2.02	0.40
1:D:42:VAL:HG22	1:D:66:VAL:HG11	2.02	0.40
1:E:152:LEU:HB3	1:E:205:TRP:CH2	2.56	0.40
1:F:226:SER:HA	1:F:227:PRO:HD3	1.87	0.40
1:H:195:ASN:OD1	1:H:196:THR:HG22	2.22	0.40
1:A:152:LEU:HB3	1:A:205:TRP:CH2	2.56	0.40
1:D:89:ILE:HB	1:D:105:VAL:HG21	2.04	0.40
1:G:111:PRO:HG3	1:G:133:LEU:CD2	2.50	0.40
1:H:273:ASP:N	1:H:273:ASP:OD1	2.55	0.40
1:A:104:LYS:NZ	1:A:137:GLU:OE2	2.51	0.40
1:H:232:THR:O	1:H:236:THR:HG23	2.21	0.40
1:C:192:TRP:CZ3	1:C:208:VAL:HG11	2.57	0.40
1:C:253:ILE:HG23	1:C:287:THR:HG22	2.04	0.40
1:F:108:ASP:OD1	1:F:135:PHE:HB3	2.22	0.40
1:A:9:VAL:HG11	1:B:238:LEU:HD11	2.04	0.40
1:G:35:ILE:HD12	1:G:35:ILE:HA	1.92	0.40
1:G:127:ILE:HG13	1:G:128:HIS:N	2.37	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	285/298 (96%)	277 (97%)	8 (3%)	0	100	100
1	B	285/298 (96%)	276 (97%)	9 (3%)	0	100	100
1	C	285/298 (96%)	275 (96%)	10 (4%)	0	100	100
1	D	285/298 (96%)	276 (97%)	9 (3%)	0	100	100
1	E	285/298 (96%)	275 (96%)	10 (4%)	0	100	100
1	F	285/298 (96%)	274 (96%)	11 (4%)	0	100	100
1	G	285/298 (96%)	272 (95%)	13 (5%)	0	100	100
1	H	285/298 (96%)	278 (98%)	6 (2%)	1 (0%)	34	66
All	All	2280/2384 (96%)	2203 (97%)	76 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	143	SER

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	258/267 (97%)	252 (98%)	6 (2%)	50	82
1	B	258/267 (97%)	250 (97%)	8 (3%)	40	74
1	C	258/267 (97%)	249 (96%)	9 (4%)	36	70
1	D	258/267 (97%)	252 (98%)	6 (2%)	50	82
1	E	258/267 (97%)	249 (96%)	9 (4%)	36	70
1	F	258/267 (97%)	250 (97%)	8 (3%)	40	74
1	G	258/267 (97%)	248 (96%)	10 (4%)	32	66
1	H	258/267 (97%)	247 (96%)	11 (4%)	29	62
All	All	2064/2136 (97%)	1997 (97%)	67 (3%)	39	73

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	107	ILE
1	A	117	LYS
1	A	229	VAL
1	A	246	GLU
1	A	270	SER
1	B	80	LYS
1	B	143	SER
1	B	171	ASP
1	B	172	ARG
1	B	197	ILE
1	B	246	GLU
1	B	247	VAL
1	B	250	ILE
1	C	42	VAL
1	C	75	LYS
1	C	107	ILE
1	C	129	CYS
1	C	131	GLU
1	C	172	ARG
1	C	229	VAL
1	C	239	LEU
1	C	293	LYS
1	D	8	ASN
1	D	29	GLU
1	D	41	ASN
1	D	196	THR
1	D	283	SER
1	D	293	LYS
1	E	103	VAL
1	E	107	ILE
1	E	117	LYS
1	E	143	SER
1	E	229	VAL
1	E	239	LEU
1	E	246	GLU
1	E	261	VAL
1	E	272	LYS
1	F	12	VAL
1	F	23	VAL
1	F	29	GLU
1	F	49	ARG
1	F	53	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	131	GLU
1	F	145	THR
1	F	197	ILE
1	G	10	GLU
1	G	16	TYR
1	G	45	THR
1	G	145	THR
1	G	198	ASN
1	G	226	SER
1	G	229	VAL
1	G	243	ARG
1	G	272	LYS
1	G	293	LYS
1	H	12	VAL
1	H	16	TYR
1	H	35	ILE
1	H	45	THR
1	H	76	LEU
1	H	197	ILE
1	H	222	ARG
1	H	238	LEU
1	H	239	LEU
1	H	266	LYS
1	H	293	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	34	HIS
1	A	106	ASN
1	A	214	GLN
1	B	19	ASN
1	B	31	ASN
1	B	162	GLN
1	C	71	HIS
1	D	8	ASN
1	D	32	HIS
1	D	41	ASN
1	F	25	HIS
1	F	34	HIS
1	F	41	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	92	HIS
1	F	281	ASN
1	G	8	ASN
1	G	19	ASN
1	G	34	HIS
1	G	41	ASN
1	G	123	ASN
1	G	124	HIS
1	H	32	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	287/298 (96%)	-0.59	0	100	100	14, 29, 48, 78	0
1	B	287/298 (96%)	-0.62	0	100	100	12, 25, 46, 67	0
1	C	287/298 (96%)	-0.67	0	100	100	13, 25, 49, 63	0
1	D	287/298 (96%)	-0.67	0	100	100	13, 24, 44, 68	0
1	E	287/298 (96%)	-0.54	0	100	100	18, 31, 51, 85	0
1	F	287/298 (96%)	-0.58	0	100	100	17, 30, 50, 67	0
1	G	287/298 (96%)	-0.58	0	100	100	16, 32, 48, 75	0
1	H	287/298 (96%)	-0.45	0	100	100	17, 33, 53, 71	0
All	All	2296/2384 (96%)	-0.59	0	100	100	12, 28, 49, 85	0

There are no RSRZ outliers to report.

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.