Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 08:16 AM EST

PDB ID	:	1T4R
Title	:	arginase-descarboxy-nor-NOHA complex
Authors	:	Cama, E.; Pethe, S.; Boucher, J.-L.; Shoufa, H.; Emig, F.A.; Ash, D.E.; Viola, R.E.; Mansuy, D.; Christianson, D.W.
Deposited on	:	2004-04-30
Resolution	:	2.60 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 (i)) were used in the production of this report:

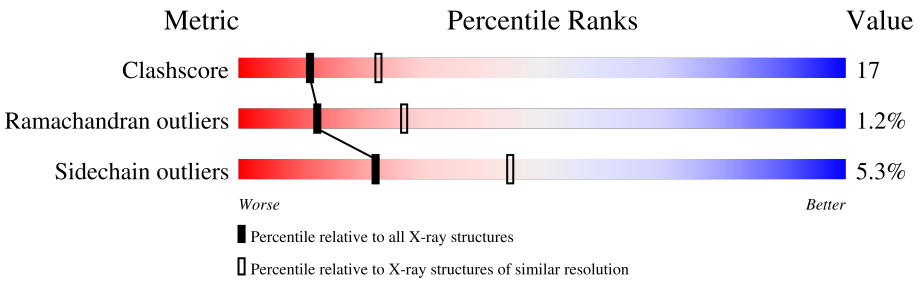
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	69% 25% 6%
1	B	314	67% 28% 5%
1	C	314	74% 22% .

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7391 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.

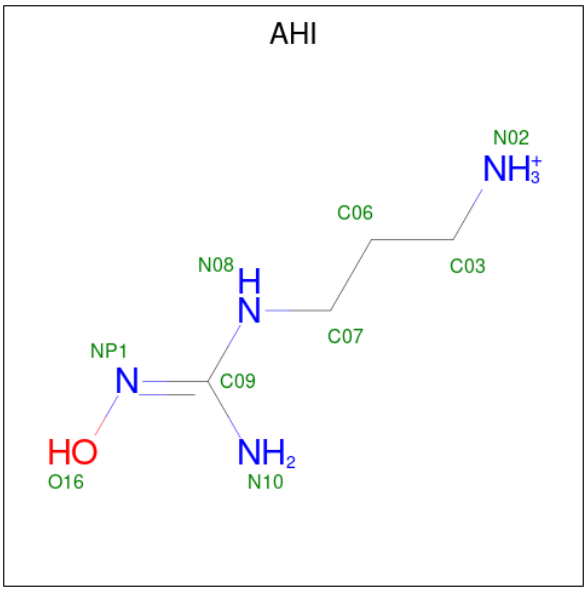
- Molecule 1 is a protein called Arginase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2396	1528	405	456	7	0	0	0
1	B	314	2396	1528	405	456	7	0	0	0
1	C	314	2396	1528	405	456	7	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0

- Molecule 3 is 3-{[(E)-AMINO(HYDROXYIMINO)METHYL]AMINO}PROPAN-1-AMINIUM (three-letter code: AHI) (formula: $C_4H_{13}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	9	4	4	1	0	0
			Total	C	N	O		
3	B	1	9	4	4	1	0	0
			Total	C	N	O		
3	C	1	9	4	4	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	46	46	46	0	0
			Total	O		
4	B	56	56	56	0	0
			Total	O		
4	C	68	68	68	0	0

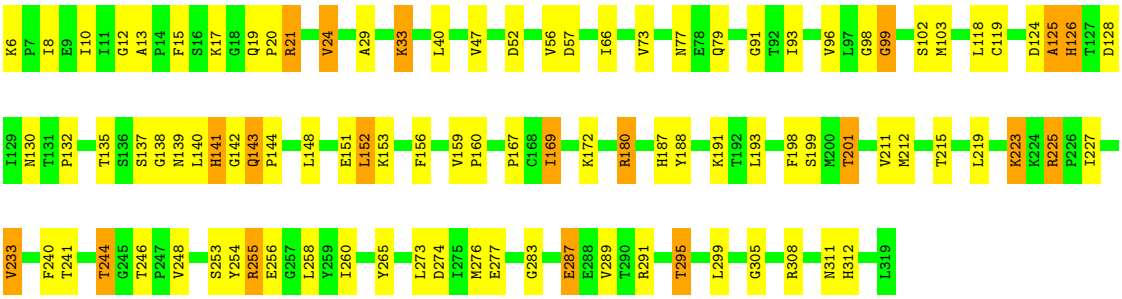
3 Residue-property plots (i)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

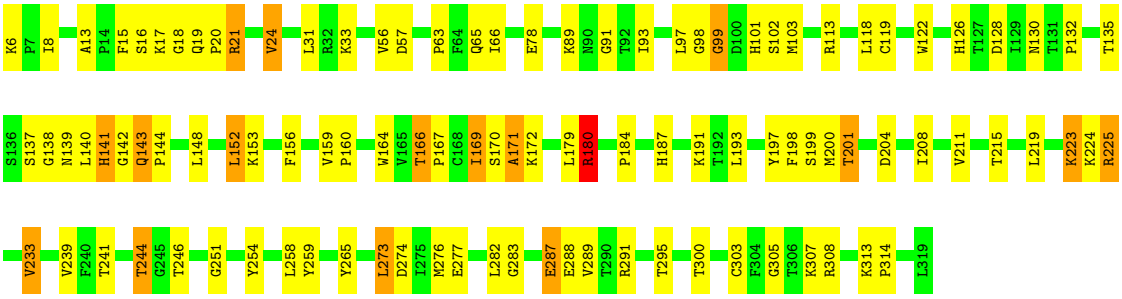
• Molecule 1: Arginase 1

Chain A: 69% 25% 6%



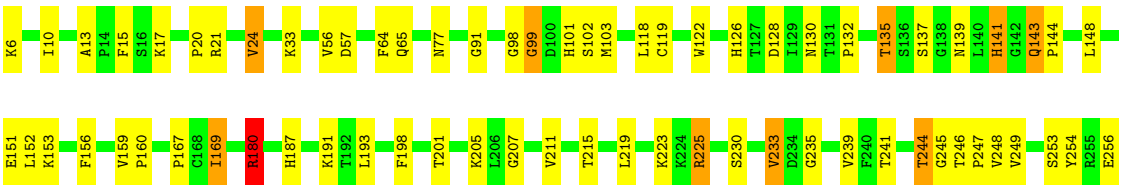
• Molecule 1: Arginase 1

Chain B: 67% 28% 5%



• Molecule 1: Arginase 1

Chain C: 74% 22%



G257
L258
E262
L273
D274
E277
E287
E288
R291
T295
R308
E309
G310
Y318
L319

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	88.30Å 88.30Å 113.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.90 – 2.60	Depositor
% Data completeness (in resolution range)	94.0 (28.90-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7391	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, AHI

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	0.61	7/2449 (0.3%)	0.71	3/3325 (0.1%)
1	B	0.66	6/2449 (0.2%)	0.78	5/3325 (0.2%)
1	C	0.61	4/2449 (0.2%)	0.80	5/3325 (0.2%)
All	All	0.63	17/7347 (0.2%)	0.77	13/9975 (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	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	ARG	CZ-NH1	-10.85	1.19	1.33
1	A	126	HIS	C-O	9.29	1.41	1.23
1	A	255	ARG	CG-CD	9.06	1.74	1.51
1	B	180	ARG	CZ-NH1	-8.72	1.21	1.33
1	B	180	ARG	CZ-NH2	-8.34	1.22	1.33
1	B	223	LYS	CD-CE	-7.07	1.33	1.51
1	A	125	ALA	C-O	6.97	1.36	1.23
1	A	79	GLN	CD-NE2	-6.78	1.16	1.32
1	A	79	GLN	CD-OE1	-6.56	1.09	1.24
1	B	223	LYS	CB-CG	-6.31	1.35	1.52
1	B	223	LYS	CE-NZ	-6.31	1.33	1.49
1	A	223	LYS	CB-CG	-6.17	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	LYS	CE-NZ	6.14	1.64	1.49
1	C	180	ARG	CZ-NH1	-5.87	1.25	1.33
1	C	223	LYS	CB-CG	-5.86	1.36	1.52
1	C	180	ARG	CZ-NH2	-5.37	1.26	1.33
1	A	21	ARG	CZ-NH1	-5.03	1.26	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	21	ARG	NE-CZ-NH2	16.89	128.74	120.30
1	B	180	ARG	NE-CZ-NH2	10.12	125.36	120.30
1	B	180	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	B	180	ARG	NH1-CZ-NH2	-8.76	109.77	119.40
1	B	21	ARG	NE-CZ-NH2	7.75	124.17	120.30
1	A	21	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	C	180	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	B	33	LYS	CD-CE-NZ	-6.61	96.50	111.70
1	C	21	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	A	255	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	126	HIS	O-C-N	6.13	132.51	122.70
1	C	180	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	C	180	ARG	NH1-CZ-NH2	-5.79	113.03	119.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	GLY	Peptide
1	B	98	GLY	Peptide
1	C	98	GLY	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	2396	0	2420	89	0
1	B	2396	0	2420	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2396	0	2420	74	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	9	0	12	4	0
3	B	9	0	12	4	0
3	C	9	0	12	4	0
4	A	46	0	0	6	0
4	B	56	0	0	10	0
4	C	68	0	0	6	0
All	All	7391	0	7296	252	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 17.

All (252) 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:255:ARG:CD	1:A:255:ARG:CG	1.74	1.58
3:C:1002:AHI:H032	4:C:680:HOH:O	1.61	0.98
3:B:1001:AHI:H032	4:B:685:HOH:O	1.64	0.96
1:C:246:THR:HG21	3:C:1002:AHI:H102	1.41	0.85
3:A:1000:AHI:H032	4:A:762:HOH:O	1.76	0.84
1:B:246:THR:HG23	4:B:717:HOH:O	1.77	0.84
1:A:143:GLN:N	1:A:144:PRO:HD3	1.95	0.82
1:C:128:ASP:HB3	1:C:144:PRO:HD2	1.64	0.80
1:A:255:ARG:CD	1:A:255:ARG:CB	2.58	0.80
1:B:135:THR:HB	1:B:137:SER:O	1.83	0.78
1:B:143:GLN:N	1:B:144:PRO:HD3	1.99	0.78
1:C:20:PRO:HD3	1:C:139:ASN:OD1	1.85	0.76
1:A:143:GLN:H	1:A:144:PRO:HD3	1.49	0.76
1:B:198:PHE:CE1	1:B:215:THR:HG22	2.23	0.74
1:A:128:ASP:HB3	1:A:144:PRO:HD2	1.69	0.73
1:B:63:PRO:HG3	4:B:742:HOH:O	1.88	0.73
1:C:143:GLN:N	1:C:144:PRO:HD3	2.03	0.73
1:C:135:THR:HB	1:C:137:SER:O	1.88	0.72
1:C:211:VAL:O	1:C:215:THR:HG23	1.89	0.72
1:A:135:THR:HB	1:A:137:SER:O	1.89	0.72
1:B:128:ASP:HB3	1:B:144:PRO:HD2	1.71	0.72
1:B:20:PRO:HD3	1:B:139:ASN:OD1	1.90	0.72
1:A:187:HIS:O	1:A:191:LYS:HG2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLY:HA3	4:A:723:HOH:O	1.91	0.71
1:A:153:LYS:HD2	1:A:167:PRO:HG2	1.73	0.71
1:A:291:ARG:O	1:A:295:THR:HG22	1.91	0.71
1:A:96:VAL:HG23	4:A:719:HOH:O	1.92	0.70
1:C:187:HIS:O	1:C:191:LYS:HG2	1.90	0.70
1:C:198:PHE:CE1	1:C:215:THR:HG22	2.26	0.70
1:C:246:THR:CG2	3:C:1002:AHI:H102	2.03	0.70
1:B:246:THR:HG21	3:B:1001:AHI:H102	1.57	0.70
1:B:143:GLN:H	1:B:144:PRO:HD3	1.56	0.70
1:C:180:ARG:NH1	1:C:248:VAL:O	2.26	0.69
1:A:143:GLN:N	1:A:144:PRO:CD	2.55	0.69
1:B:152:LEU:HD13	1:B:193:LEU:HD21	1.75	0.69
1:C:291:ARG:O	1:C:295:THR:HG22	1.92	0.69
1:B:187:HIS:O	1:B:191:LYS:HG2	1.94	0.68
1:C:153:LYS:HD2	1:C:167:PRO:HG2	1.75	0.68
1:C:6:LYS:N	4:C:710:HOH:O	2.26	0.67
1:A:180:ARG:NH1	1:A:248:VAL:O	2.28	0.67
1:A:246:THR:HG21	3:A:1000:AHI:H102	1.59	0.66
1:C:130:ASN:HB3	1:C:135:THR:HG23	1.76	0.65
1:C:246:THR:HG23	4:C:759:HOH:O	1.96	0.65
1:A:152:LEU:HD13	1:A:193:LEU:HD21	1.78	0.65
1:B:153:LYS:HD2	1:B:167:PRO:HG2	1.78	0.65
1:C:15:PHE:CZ	1:C:17:LYS:HB2	2.32	0.65
1:B:223:LYS:HE3	1:B:225:ARG:HD2	1.78	0.65
1:A:198:PHE:CE1	1:A:215:THR:HG22	2.31	0.64
1:A:118:LEU:O	1:A:118:LEU:HD12	1.98	0.64
1:B:143:GLN:N	1:B:144:PRO:CD	2.61	0.63
1:A:188:TYR:CD2	1:C:318:TYR:HB2	2.32	0.63
1:C:287:GLU:OE2	1:C:291:ARG:NH2	2.32	0.63
1:A:6:LYS:HE2	1:A:91:GLY:O	1.99	0.62
1:A:254:TYR:CE2	1:A:258:LEU:HD11	2.35	0.62
1:B:211:VAL:O	1:B:215:THR:HG23	2.00	0.62
1:B:246:THR:CG2	3:B:1001:AHI:H102	2.13	0.62
1:A:211:VAL:O	1:A:215:THR:HG23	1.99	0.61
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.35	0.61
1:A:276:MET:HA	4:A:741:HOH:O	1.99	0.60
1:A:20:PRO:HD3	1:A:139:ASN:OD1	2.00	0.60
1:A:308:ARG:O	1:B:180:ARG:HA	2.01	0.60
1:C:225:ARG:NH2	4:C:728:HOH:O	2.33	0.60
1:A:283:GLY:HA3	1:A:289:VAL:HG23	1.83	0.59
1:A:246:THR:CG2	3:A:1000:AHI:H102	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:SER:HB3	1:B:141:HIS:HA	1.85	0.59
1:C:152:LEU:HD13	1:C:193:LEU:HD21	1.85	0.58
1:C:6:LYS:HE2	1:C:91:GLY:O	2.04	0.58
1:C:143:GLN:N	1:C:144:PRO:CD	2.66	0.58
1:B:130:ASN:HB3	1:B:135:THR:HG22	1.86	0.57
1:B:180:ARG:HD2	1:B:200:MET:HG3	1.86	0.57
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.40	0.56
1:A:130:ASN:HB3	1:A:135:THR:HG22	1.86	0.56
1:A:265:TYR:HD1	4:A:733:HOH:O	1.87	0.56
1:C:15:PHE:O	1:C:99:GLY:HA3	2.05	0.56
1:C:118:LEU:HD12	1:C:118:LEU:O	2.05	0.56
1:C:151:GLU:OE1	1:C:151:GLU:N	2.38	0.56
1:A:148:LEU:O	1:A:169:ILE:HD13	2.06	0.55
1:C:180:ARG:HD2	1:C:248:VAL:HG12	1.88	0.55
1:C:239:VAL:HG12	1:C:239:VAL:O	2.07	0.55
1:A:102:SER:HB3	1:A:141:HIS:HA	1.88	0.55
1:B:15:PHE:O	1:B:99:GLY:HA3	2.07	0.54
1:C:126:HIS:CE1	1:C:246:THR:OG1	2.60	0.54
1:C:254:TYR:CE2	1:C:258:LEU:HD11	2.42	0.54
1:A:15:PHE:O	1:A:99:GLY:HA3	2.07	0.54
1:B:19:GLN:HB2	1:B:20:PRO:HD2	1.91	0.53
1:C:143:GLN:H	1:C:144:PRO:HD3	1.72	0.53
1:A:118:LEU:HD12	1:A:118:LEU:C	2.29	0.52
1:B:130:ASN:HB3	1:B:135:THR:CG2	2.39	0.52
1:A:188:TYR:CD1	1:C:318:TYR:HD2	2.28	0.52
1:A:169:ILE:HD13	1:A:169:ILE:H	1.75	0.52
1:B:152:LEU:CD1	1:B:193:LEU:HD21	2.40	0.52
1:B:199:SER:OG	1:B:201:THR:HG23	2.10	0.51
1:A:180:ARG:HD2	1:A:248:VAL:HG12	1.92	0.51
1:A:311:ASN:O	1:B:184:PRO:HA	2.11	0.51
1:C:233:VAL:HG12	1:C:244:THR:HG21	1.92	0.51
1:C:148:LEU:O	1:C:169:ILE:HD13	2.10	0.51
1:A:244:THR:HG22	1:A:277:GLU:HB3	1.93	0.51
1:B:118:LEU:HD12	1:B:118:LEU:O	2.11	0.51
1:A:201:THR:HG22	1:C:308:ARG:HB2	1.92	0.50
1:B:223:LYS:CE	1:B:225:ARG:HD2	2.40	0.50
1:B:180:ARG:NH2	1:B:251:GLY:HA3	2.27	0.50
1:A:24:VAL:HB	1:A:99:GLY:HA2	1.93	0.50
1:C:77:ASN:OD1	1:C:103:MET:HA	2.12	0.50
1:C:198:PHE:CD2	1:C:211:VAL:HG13	2.47	0.50
1:A:255:ARG:CG	1:A:255:ARG:NE	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:HA	1:A:144:PRO:HG3	1.92	0.50
1:C:152:LEU:CD1	1:C:193:LEU:HD21	2.42	0.50
1:B:239:VAL:HG12	1:B:239:VAL:O	2.11	0.49
1:C:244:THR:HG22	1:C:277:GLU:O	2.12	0.49
1:C:13:ALA:O	1:C:15:PHE:N	2.44	0.49
1:A:233:VAL:HG12	1:A:244:THR:CG2	2.43	0.49
1:A:312:HIS:HA	1:B:184:PRO:HB3	1.93	0.49
1:A:180:ARG:HG3	1:A:248:VAL:HG11	1.94	0.49
1:C:20:PRO:CD	1:C:139:ASN:OD1	2.59	0.49
1:B:118:LEU:HD12	1:B:118:LEU:C	2.33	0.49
1:B:169:ILE:HD13	1:B:169:ILE:H	1.77	0.49
1:B:179:LEU:HD12	1:B:197:TYR:HB2	1.94	0.49
1:C:180:ARG:NH2	1:C:235:GLY:O	2.46	0.49
1:C:246:THR:OG1	3:C:1002:AHI:N10	2.46	0.49
1:B:6:LYS:HE2	1:B:91:GLY:O	2.13	0.49
1:A:258:LEU:HD23	1:A:299:LEU:HD23	1.95	0.48
1:B:24:VAL:HB	1:B:99:GLY:HA2	1.94	0.48
1:C:101:HIS:CE1	1:C:122:TRP:CZ2	3.01	0.48
1:A:77:ASN:OD1	1:A:103:MET:HA	2.13	0.48
1:A:151:GLU:OE1	1:A:151:GLU:N	2.45	0.48
1:B:244:THR:HG22	1:B:277:GLU:HB3	1.95	0.48
1:B:244:THR:HG22	1:B:277:GLU:O	2.13	0.48
1:C:24:VAL:HB	1:C:99:GLY:HA2	1.95	0.48
1:B:180:ARG:CZ	1:B:251:GLY:HA3	2.43	0.48
1:A:12:GLY:HA3	1:A:52:ASP:OD1	2.14	0.48
1:B:287:GLU:OE2	1:B:291:ARG:NH2	2.46	0.48
1:B:287:GLU:HG3	1:B:288:GLU:N	2.29	0.48
1:B:102:SER:HA	1:B:144:PRO:HG3	1.96	0.47
1:B:259:TYR:OH	1:C:205:LYS:HB2	2.14	0.47
1:A:135:THR:HG21	1:A:143:GLN:NE2	2.29	0.47
1:A:198:PHE:CD2	1:A:211:VAL:HG13	2.49	0.47
1:B:135:THR:CB	1:B:137:SER:O	2.60	0.47
1:A:19:GLN:HB2	1:A:20:PRO:HD2	1.95	0.47
1:A:212:MET:SD	1:A:260:ILE:HG12	2.54	0.47
1:C:239:VAL:O	1:C:239:VAL:CG1	2.62	0.47
1:C:102:SER:HA	1:C:144:PRO:HG3	1.96	0.47
1:C:169:ILE:HD13	1:C:169:ILE:H	1.80	0.47
1:C:56:VAL:HG23	1:C:56:VAL:O	2.15	0.46
1:A:40:LEU:HB3	1:A:47:VAL:HG21	1.97	0.46
1:A:172:LYS:HD2	1:A:172:LYS:HA	1.52	0.46
1:B:246:THR:OG1	3:B:1001:AHI:N10	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:753:HOH:O	1:C:249:VAL:HG11	2.16	0.46
1:B:223:LYS:N	4:B:664:HOH:O	2.38	0.46
1:C:253:SER:OG	1:C:256:GLU:HG3	2.16	0.46
1:B:233:VAL:HG22	1:B:241:THR:HG21	1.98	0.45
1:C:233:VAL:HG12	1:C:244:THR:CG2	2.45	0.45
1:C:118:LEU:HD12	1:C:118:LEU:C	2.36	0.45
1:B:8:ILE:HD13	1:B:93:ILE:HB	1.98	0.45
1:B:140:LEU:C	1:B:142:GLY:N	2.70	0.45
1:C:102:SER:HB3	1:C:141:HIS:HA	1.98	0.45
1:C:244:THR:HG22	1:C:277:GLU:HB3	1.98	0.45
1:A:287:GLU:OE2	1:A:291:ARG:NH2	2.49	0.45
1:B:204:ASP:HA	4:B:701:HOH:O	2.16	0.45
1:A:135:THR:HG21	1:A:143:GLN:CD	2.37	0.45
1:A:187:HIS:ND1	1:C:310:GLY:HA3	2.30	0.45
1:B:180:ARG:HD2	1:B:200:MET:CG	2.45	0.45
1:A:132:PRO:HD2	1:A:156:PHE:CD2	2.52	0.45
1:A:274:ASP:HB3	1:A:276:MET:SD	2.57	0.45
1:B:148:LEU:O	1:B:169:ILE:HD13	2.17	0.45
1:A:56:VAL:HG23	1:A:56:VAL:O	2.17	0.45
1:B:140:LEU:C	1:B:142:GLY:H	2.20	0.45
1:C:230:SER:HA	1:C:274:ASP:HB2	1.99	0.45
1:B:259:TYR:CZ	1:C:205:LYS:HB2	2.52	0.45
1:B:13:ALA:O	1:B:15:PHE:N	2.48	0.44
4:A:700:HOH:O	1:B:201:THR:HG21	2.17	0.44
1:B:233:VAL:HG12	1:B:244:THR:HG21	2.00	0.44
1:C:180:ARG:HG3	1:C:248:VAL:HG11	1.99	0.44
1:B:180:ARG:HB3	1:B:200:MET:HG2	1.99	0.44
1:B:313:LYS:HA	1:B:314:PRO:HD3	1.88	0.44
1:A:233:VAL:HG12	1:A:244:THR:HG21	1.99	0.44
1:B:283:GLY:HA3	1:B:289:VAL:HG23	1.99	0.44
1:B:101:HIS:CE1	1:B:122:TRP:CZ2	3.06	0.43
1:A:8:ILE:HD13	1:A:93:ILE:HB	2.00	0.43
1:B:21:ARG:HD3	1:B:282:LEU:HD11	2.00	0.43
1:B:78:GLU:HB2	1:B:164:TRP:CE2	2.52	0.43
1:A:199:SER:OG	1:A:201:THR:HG23	2.19	0.43
1:A:246:THR:OG1	3:A:1000:AHI:N10	2.51	0.43
1:B:307:LYS:HG2	4:B:747:HOH:O	2.18	0.43
1:B:101:HIS:CD2	1:B:276:MET:HG3	2.53	0.43
1:B:239:VAL:O	1:B:239:VAL:CG1	2.67	0.43
1:A:13:ALA:O	1:A:15:PHE:N	2.48	0.43
1:A:126:HIS:CE1	1:A:246:THR:OG1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:VAL:HG22	1:A:241:THR:HG21	2.01	0.43
1:B:166:THR:O	1:B:166:THR:HG22	2.18	0.43
1:B:244:THR:CG2	1:B:277:GLU:O	2.66	0.43
1:B:180:ARG:CZ	1:B:251:GLY:CA	2.96	0.43
1:B:198:PHE:CD2	1:B:211:VAL:HG13	2.54	0.43
1:B:246:THR:OG1	1:B:246:THR:O	2.36	0.43
1:A:198:PHE:CG	1:A:211:VAL:HG13	2.54	0.43
1:B:233:VAL:HG12	1:B:244:THR:CG2	2.48	0.43
1:C:245:GLY:HA3	4:C:659:HOH:O	2.19	0.43
1:A:152:LEU:CD1	1:A:193:LEU:HD21	2.47	0.43
1:C:10:ILE:HD12	1:C:10:ILE:N	2.33	0.43
1:C:258:LEU:O	1:C:262:GLU:HG3	2.19	0.43
1:B:126:HIS:CE1	1:B:246:THR:OG1	2.72	0.43
1:B:135:THR:HG21	1:B:143:GLN:CD	2.39	0.43
1:B:265:TYR:CZ	1:B:305:GLY:HA2	2.53	0.43
1:C:119:CYS:HB2	1:C:219:LEU:HD22	2.01	0.43
1:C:207:GLY:O	1:C:211:VAL:HG23	2.18	0.42
1:B:56:VAL:HG23	1:B:56:VAL:O	2.19	0.42
1:B:31:LEU:HD13	1:B:97:LEU:HD22	2.01	0.42
1:B:78:GLU:HB2	1:B:164:TRP:NE1	2.35	0.42
1:A:66:ILE:HG22	1:A:138:GLY:HA2	2.01	0.42
1:A:135:THR:CB	1:A:137:SER:O	2.65	0.42
1:A:240:PHE:CE2	1:A:253:SER:HA	2.54	0.42
1:A:244:THR:HG22	1:A:277:GLU:O	2.20	0.42
1:A:119:CYS:HB2	1:A:219:LEU:HD22	2.02	0.42
1:C:198:PHE:CG	1:C:211:VAL:HG13	2.54	0.42
1:B:273:LEU:HD22	1:B:274:ASP:N	2.35	0.42
1:C:247:PRO:HA	4:C:649:HOH:O	2.20	0.42
1:B:20:PRO:HD3	1:B:139:ASN:CG	2.40	0.42
1:A:253:SER:OG	1:A:256:GLU:HG3	2.20	0.42
1:B:16:SER:C	1:B:18:GLY:H	2.23	0.42
1:A:119:CYS:SG	1:A:227:ILE:HG12	2.59	0.41
1:A:10:ILE:HD12	1:A:10:ILE:N	2.34	0.41
1:B:171:ALA:O	4:B:757:HOH:O	2.22	0.41
1:B:170:SER:C	1:B:172:LYS:H	2.24	0.41
1:B:259:TYR:CE1	1:C:205:LYS:HB2	2.55	0.41
1:B:300:THR:O	1:B:303:CYS:HB2	2.20	0.41
1:B:132:PRO:HD2	1:B:156:PHE:CD2	2.55	0.41
1:B:119:CYS:HB2	1:B:219:LEU:HD22	2.02	0.41
1:C:132:PRO:HD2	1:C:156:PHE:CD2	2.56	0.41
1:B:159:VAL:HA	1:B:160:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ARG:O	1:C:180:ARG:HA	2.20	0.41
1:A:15:PHE:HE2	1:A:73:VAL:HG22	1.86	0.41
1:A:140:LEU:C	1:A:142:GLY:N	2.74	0.41
1:A:148:LEU:HB3	1:A:169:ILE:CD1	2.50	0.41
1:B:66:ILE:O	1:B:138:GLY:HA3	2.21	0.41
1:A:19:GLN:OE1	1:A:21:ARG:HB2	2.21	0.41
1:A:130:ASN:HB3	1:A:135:THR:CG2	2.48	0.41
1:A:265:TYR:CZ	1:A:305:GLY:HA2	2.55	0.41
1:A:287:GLU:OE2	1:A:291:ARG:NE	2.49	0.41
1:B:113:ARG:NH2	4:B:729:HOH:O	2.44	0.41
1:B:130:ASN:CB	1:B:135:THR:HG22	2.50	0.41
1:B:172:LYS:HA	1:B:172:LYS:HD2	1.55	0.41
1:C:64:PHE:O	1:C:65:GLN:HB2	2.21	0.41
1:C:159:VAL:HA	1:C:160:PRO:HD3	1.90	0.41
1:C:233:VAL:HG13	1:C:241:THR:HB	2.03	0.41
1:A:124:ASP:OD1	1:A:125:ALA:N	2.53	0.41
1:B:19:GLN:OE1	1:B:21:ARG:HB2	2.21	0.41
1:B:254:TYR:CE2	1:B:258:LEU:HD11	2.56	0.41
1:A:29:ALA:O	1:A:33:LYS:HB2	2.21	0.40
1:A:159:VAL:HA	1:A:160:PRO:HD3	1.93	0.40
1:C:148:LEU:HB3	1:C:169:ILE:CD1	2.50	0.40
1:B:208:ILE:HB	4:B:612:HOH:O	2.22	0.40
1:A:223:LYS:O	1:A:225:ARG:HD3	2.21	0.40
1:C:287:GLU:HG3	1:C:288:GLU:N	2.36	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	312/314 (99%)	293 (94%)	16 (5%)	3 (1%)	15 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	312/314 (99%)	292 (94%)	15 (5%)	5 (2%)	9	19
1	C	312/314 (99%)	291 (93%)	18 (6%)	3 (1%)	15	32
All	All	936/942 (99%)	876 (94%)	49 (5%)	11 (1%)	13	27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	GLY
1	B	99	GLY
1	C	99	GLY
1	A	180	ARG
1	B	171	ALA
1	B	180	ARG
1	B	65	GLN
1	B	143	GLN
1	A	143	GLN
1	C	143	GLN
1	C	180	ARG

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	264/264 (100%)	251 (95%)	13 (5%)	25	48
1	B	264/264 (100%)	248 (94%)	16 (6%)	18	38
1	C	264/264 (100%)	251 (95%)	13 (5%)	25	48
All	All	792/792 (100%)	750 (95%)	42 (5%)	22	45

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	33	LYS
1	A	57	ASP

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Mol	Chain	Res	Type
1	A	141	HIS
1	A	152	LEU
1	A	169	ILE
1	A	201	THR
1	A	225	ARG
1	A	233	VAL
1	A	244	THR
1	A	273	LEU
1	A	287	GLU
1	A	295	THR
1	B	24	VAL
1	B	57	ASP
1	B	103	MET
1	B	141	HIS
1	B	152	LEU
1	B	166	THR
1	B	169	ILE
1	B	180	ARG
1	B	201	THR
1	B	224	LYS
1	B	225	ARG
1	B	233	VAL
1	B	244	THR
1	B	273	LEU
1	B	287	GLU
1	B	295	THR
1	C	24	VAL
1	C	33	LYS
1	C	57	ASP
1	C	135	THR
1	C	141	HIS
1	C	169	ILE
1	C	201	THR
1	C	225	ARG
1	C	233	VAL
1	C	244	THR
1	C	273	LEU
1	C	287	GLU
1	C	295	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	141	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)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AHI	C	1002	2	6,8,8	1.73	2 (33%)	3,8,8	1.91	1 (33%)
3	AHI	B	1001	2	6,8,8	1.73	2 (33%)	3,8,8	1.92	1 (33%)
3	AHI	A	1000	2	6,8,8	1.73	2 (33%)	3,8,8	1.92	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHI	C	1002	2	-	1/5/7/7	-
3	AHI	B	1001	2	-	1/5/7/7	-
3	AHI	A	1000	2	-	1/5/7/7	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	AHI	O16-NP1	-3.07	1.31	1.40
3	B	1001	AHI	O16-NP1	-3.07	1.31	1.40
3	A	1000	AHI	O16-NP1	-3.04	1.31	1.40
3	C	1002	AHI	C06-C03	2.31	1.62	1.51
3	A	1000	AHI	C06-C03	2.31	1.62	1.51
3	B	1001	AHI	C06-C03	2.30	1.62	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1000	AHI	C06-C07-N08	-2.26	105.76	112.21
3	B	1001	AHI	C06-C07-N08	-2.24	105.81	112.21
3	C	1002	AHI	C06-C07-N08	-2.22	105.86	112.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	AHI	N02-C03-C06-C07
3	B	1001	AHI	N02-C03-C06-C07
3	C	1002	AHI	N02-C03-C06-C07

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	AHI	4	0
3	B	1001	AHI	4	0
3	A	1000	AHI	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.