Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:07 AM GMT

PDB ID	:	2PHA
Title	:	Crystal structure of native, unliganded human arginase at 1.90 resolution
Authors	:	Di Costanzo, L.; Pique, M.E.; Christianson, D.W.
Deposited on	:	2007-04-10
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/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:

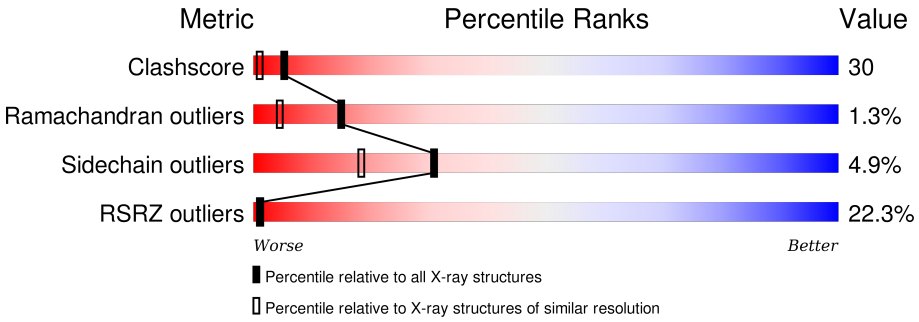
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	322	14% 60% 35%
1	B	322	29% 45% 49%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5032 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
1	A	314	Total	C	N	O	S	0	0	0
			2387	1522	406	453	6			
1	B	314	Total	C	N	O	S	0	0	0
			2387	1522	406	453	6			

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

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

- Molecule 3 is water.

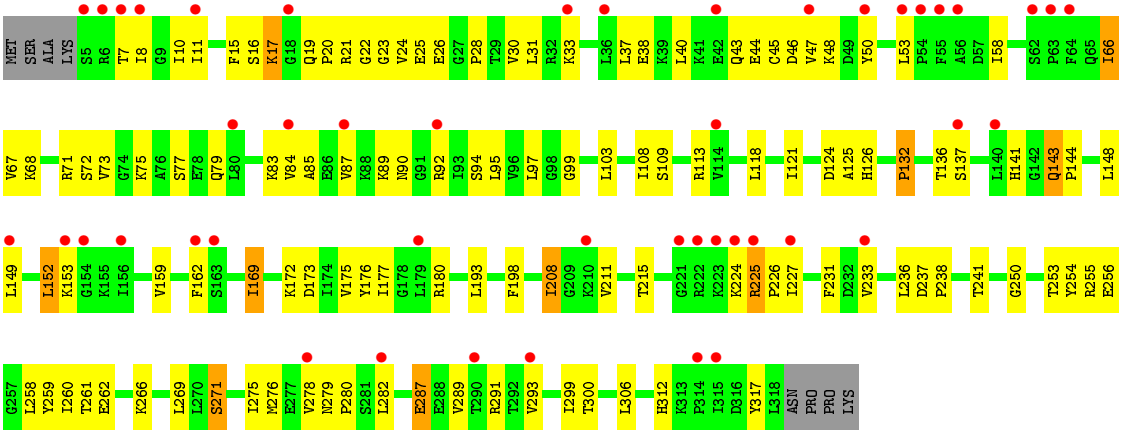
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	112	Total	O	0	0
			112	112		

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 errors 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.

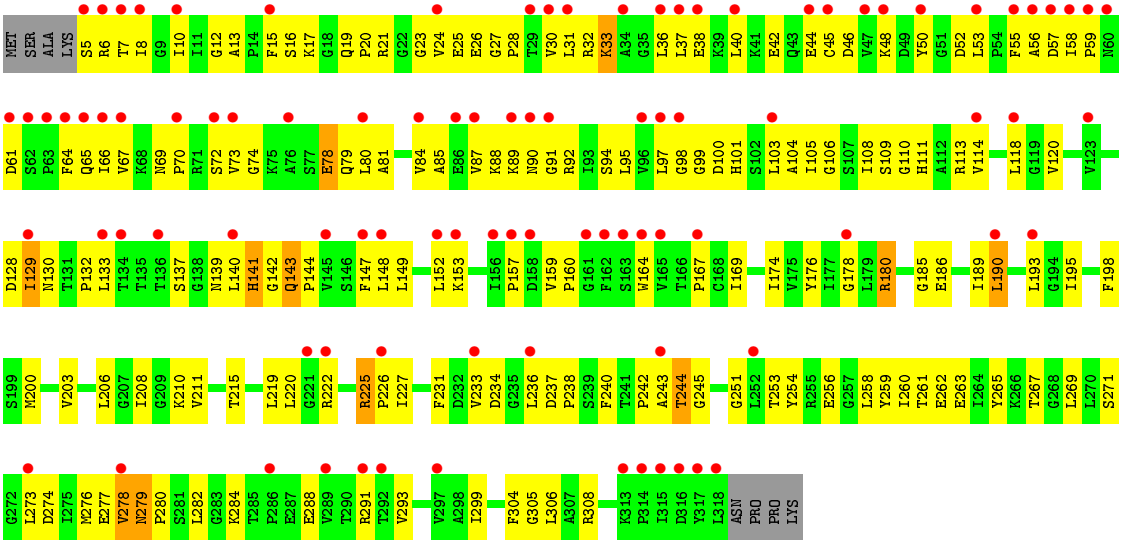
- Molecule 1: Arginase-1

Chain A:



- Molecule 1: Arginase-1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	90.77Å 90.77Å 69.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.03 – 1.90 18.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (18.03-1.90) 97.8 (18.03-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.244 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 103.6	EDS
Estimated twinning fraction	0.470 for -h,-k,l 0.128 for h,-h-k,-l 0.128 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 49512 reflections	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	5032	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/2437	0.70	1/3307 (0.0%)
1	B	0.40	0/2437	0.68	0/3307
All	All	0.43	0/4874	0.69	1/6614 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	GLY	N-CA-C	-5.45	99.47	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2387	0	2432	110	0
1	B	2387	0	2432	183	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	142	0	0	5	0
3	B	112	0	0	6	0
All	All	5032	0	4864	292	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 30.

All (292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:VAL:HG21	1:B:278:VAL:HG13	1.38	1.00
1:B:129:ILE:HD12	1:B:189:ILE:HG21	1.43	0.97
1:A:66:ILE:H	1:A:66:ILE:HD13	1.33	0.92
1:B:30:VAL:HG13	1:B:33:LYS:NZ	1.88	0.89
1:B:48:LYS:HG3	1:B:92:ARG:HE	1.37	0.89
1:A:53:LEU:HD21	1:A:83:LYS:HG2	1.51	0.89
1:A:30:VAL:HG13	1:A:33:LYS:HE2	1.55	0.86
1:B:208:ILE:HD11	1:B:260:ILE:HD11	1.57	0.86
1:B:178:GLY:HA2	1:B:200:MET:CE	2.06	0.84
1:B:304:PHE:HB2	3:B:375:HOH:O	1.77	0.84
1:A:233:VAL:HG23	1:A:276:MET:O	1.78	0.83
1:A:22:GLY:O	1:A:25:GLU:HG3	1.78	0.83
1:B:89:LYS:NZ	1:B:89:LYS:HB2	1.96	0.80
1:A:233:VAL:HG21	1:A:278:VAL:HG23	1.61	0.80
1:B:30:VAL:HG13	1:B:33:LYS:HZ3	1.45	0.80
1:A:21:ARG:HD2	1:A:282:LEU:HD11	1.63	0.79
1:B:16:SER:HB3	1:B:25:GLU:HG3	1.61	0.79
1:A:87:VAL:HG21	1:A:94:SER:HB3	1.63	0.79
1:B:211:VAL:O	1:B:215:THR:HG23	1.84	0.78
1:A:208:ILE:HD11	1:A:260:ILE:HD13	1.66	0.77
1:B:33:LYS:HD2	1:B:33:LYS:C	2.05	0.77
1:A:143:GLN:N	1:A:144:PRO:HD2	2.01	0.76
1:A:19:GLN:HB2	1:A:20:PRO:HD2	1.67	0.75
1:A:208:ILE:HD11	1:A:260:ILE:CD1	2.17	0.75
1:A:208:ILE:HD12	1:A:259:TYR:HD2	1.52	0.74
1:B:7:THR:HG23	1:B:46:ASP:O	1.87	0.74
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.22	0.73
1:A:275:ILE:HD13	1:A:300:THR:OG1	1.88	0.72
1:B:70:PRO:HB2	1:B:160:PRO:O	1.90	0.71
1:A:211:VAL:O	1:A:215:THR:HG23	1.92	0.70
1:B:88:LYS:HB2	1:B:114:VAL:HG21	1.74	0.69
1:B:48:LYS:HG3	1:B:92:ARG:NE	2.07	0.69
1:B:129:ILE:HG22	1:B:186:GLU:HB3	1.75	0.69
1:B:178:GLY:HA2	1:B:200:MET:HE1	1.75	0.68
1:B:178:GLY:HA2	1:B:200:MET:HE3	1.74	0.68
1:A:10:ILE:CD1	1:A:95:LEU:HD13	2.24	0.68
1:A:79:GLN:O	1:A:83:LYS:HD3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LYS:HZ2	1:B:89:LYS:HB2	1.59	0.68
1:A:256:GLU:O	1:A:260:ILE:HG12	1.93	0.68
1:A:233:VAL:HG21	1:A:278:VAL:CG2	2.24	0.67
1:B:31:LEU:HD13	1:B:97:LEU:HD22	1.76	0.66
1:B:236:LEU:HD11	1:B:299:ILE:HD11	1.77	0.66
1:B:36:LEU:O	1:B:40:LEU:HG	1.95	0.66
1:A:224:LYS:N	1:A:224:LYS:HD2	2.10	0.66
1:A:40:LEU:O	1:A:45:CYS:HB2	1.95	0.65
1:B:10:ILE:CD1	1:B:95:LEU:HD13	2.27	0.65
1:B:28:PRO:HG3	1:B:97:LEU:O	1.95	0.65
1:A:121:ILE:HD13	1:A:227:ILE:HG23	1.79	0.65
1:A:233:VAL:HG12	1:A:241:THR:HB	1.80	0.64
1:A:24:VAL:HG12	1:A:279:ASN:HB2	1.78	0.64
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.32	0.64
1:B:128:ASP:HB3	1:B:144:PRO:HD2	1.80	0.64
1:B:143:GLN:N	1:B:144:PRO:CD	2.61	0.63
1:B:233:VAL:HG23	1:B:276:MET:O	1.99	0.63
1:A:66:ILE:HD13	1:A:66:ILE:N	2.11	0.63
1:A:159:VAL:HG22	3:A:434:HOH:O	1.99	0.62
1:B:143:GLN:H	1:B:144:PRO:CD	2.13	0.62
1:A:83:LYS:HD2	1:A:83:LYS:N	2.15	0.62
1:A:87:VAL:CG2	1:A:94:SER:HB3	2.29	0.62
1:B:149:LEU:HA	1:B:169:ILE:O	2.00	0.61
1:B:258:LEU:O	1:B:262:GLU:HG3	2.01	0.61
1:A:46:ASP:OD1	1:A:48:LYS:HE2	2.01	0.61
1:B:200:MET:CE	1:B:200:MET:HA	2.30	0.60
1:B:200:MET:HE2	1:B:200:MET:HA	1.82	0.60
1:B:220:LEU:HD21	1:B:227:ILE:HD11	1.84	0.60
1:A:143:GLN:N	1:A:144:PRO:CD	2.66	0.59
1:A:83:LYS:O	1:A:87:VAL:HG13	2.03	0.59
1:B:100:ASP:O	1:B:103:LEU:HD12	2.03	0.59
1:B:153:LYS:HD2	1:B:167:PRO:HG2	1.83	0.59
1:B:30:VAL:CG1	1:B:293:VAL:HG21	2.32	0.59
1:A:126:HIS:HB3	3:A:342:HOH:O	2.02	0.59
1:A:208:ILE:O	1:A:208:ILE:HD13	2.02	0.59
1:B:13:ALA:HB1	1:B:103:LEU:HD22	1.85	0.59
1:A:258:LEU:O	1:A:262:GLU:HG3	2.03	0.58
1:B:30:VAL:HG13	1:B:33:LYS:HZ1	1.68	0.58
1:B:40:LEU:O	1:B:45:CYS:HB2	2.03	0.58
1:B:265:TYR:CZ	1:B:305:GLY:HA2	2.37	0.58
1:B:20:PRO:HG2	1:B:21:ARG:HH21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ILE:HG21	1:B:190:LEU:CD2	2.33	0.58
1:B:200:MET:HE2	1:B:203:VAL:HG21	1.86	0.58
1:B:253:THR:HG22	1:B:254:TYR:N	2.19	0.58
1:A:253:THR:HG22	1:A:254:TYR:N	2.19	0.57
1:A:136:THR:HG23	3:A:382:HOH:O	2.03	0.57
1:A:53:LEU:CD2	1:A:83:LYS:HG2	2.30	0.57
1:B:80:LEU:HD23	1:B:103:LEU:HB3	1.86	0.57
1:B:19:GLN:HB2	1:B:20:PRO:HD2	1.87	0.57
1:A:16:SER:HB3	1:A:25:GLU:HG2	1.86	0.57
1:B:111:HIS:CE1	1:B:271:SER:HB2	2.41	0.56
1:A:85:ALA:O	1:A:89:LYS:HG3	2.05	0.56
1:A:75:LYS:O	1:A:79:GLN:HG3	2.05	0.56
1:A:253:THR:HG22	1:A:255:ARG:H	1.70	0.56
1:B:109:SER:O	1:B:113:ARG:HG3	2.06	0.56
1:A:30:VAL:HG21	1:A:280:PRO:HG3	1.87	0.56
1:A:231:PHE:CZ	1:A:299:ILE:HD13	2.41	0.56
1:B:244:THR:C	1:B:282:LEU:HD13	2.26	0.55
1:A:176:TYR:C	1:A:177:ILE:HD12	2.26	0.55
1:A:159:VAL:HB	1:A:162:PHE:CD1	2.41	0.55
1:A:149:LEU:HA	1:A:169:ILE:O	2.07	0.55
1:B:78:GLU:HG2	1:B:164:TRP:CE2	2.42	0.55
1:A:208:ILE:HD12	1:A:259:TYR:CD2	2.37	0.55
1:B:279:ASN:HB3	1:B:282:LEU:HD12	1.88	0.55
1:B:240:PHE:CD1	1:B:254:TYR:HB2	2.41	0.54
1:A:11:ILE:HD12	1:A:83:LYS:HB3	1.89	0.54
1:B:48:LYS:HE3	1:B:92:ARG:HH21	1.73	0.54
1:B:129:ILE:HG23	1:B:129:ILE:O	2.07	0.54
1:B:8:ILE:HD12	1:B:304:PHE:CE1	2.44	0.53
1:B:129:ILE:HG22	1:B:186:GLU:CB	2.37	0.53
1:B:32:ARG:NH1	1:B:52:ASP:OD1	2.42	0.53
1:B:147:PHE:CZ	1:B:159:VAL:HG21	2.43	0.53
1:A:250:GLY:HA3	3:A:433:HOH:O	2.07	0.53
1:B:38:GLU:O	1:B:42:GLU:HG3	2.09	0.53
1:A:30:VAL:HG11	1:A:293:VAL:HG21	1.91	0.53
1:A:17:LYS:HD2	1:A:72:SER:HB3	1.90	0.53
1:A:233:VAL:HG12	1:A:241:THR:CB	2.38	0.53
1:A:17:LYS:HD2	1:A:72:SER:CB	2.38	0.53
1:A:30:VAL:CG1	1:A:293:VAL:HG21	2.39	0.52
1:B:16:SER:HB3	1:B:25:GLU:CG	2.35	0.52
1:B:143:GLN:N	1:B:144:PRO:HD2	2.23	0.52
1:B:33:LYS:HD2	1:B:33:LYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:HG12	1:B:279:ASN:HB2	1.91	0.52
1:A:236:LEU:HD11	1:A:299:ILE:CD1	2.39	0.52
1:B:78:GLU:HG2	1:B:164:TRP:CD2	2.45	0.52
1:A:289:VAL:O	1:A:293:VAL:HG23	2.08	0.52
1:A:31:LEU:HD13	1:A:97:LEU:HD22	1.92	0.52
1:B:284:LYS:HB3	1:B:288:GLU:OE2	2.09	0.52
1:A:109:SER:O	1:A:113:ARG:HG3	2.10	0.52
1:B:87:VAL:CG2	1:B:94:SER:HB3	2.40	0.51
1:B:105:ILE:HA	1:B:148:LEU:HD21	1.92	0.51
1:B:258:LEU:CD1	1:B:308:ARG:HD3	2.40	0.51
1:B:240:PHE:CE1	1:B:254:TYR:HB2	2.46	0.51
1:B:85:ALA:HB2	1:B:110:GLY:O	2.11	0.51
1:B:7:THR:CG2	1:B:92:ARG:HG2	2.41	0.51
1:B:69:ASN:HB3	1:B:72:SER:HB2	1.92	0.51
1:B:30:VAL:HG11	1:B:293:VAL:HG21	1.92	0.51
1:B:13:ALA:HB3	1:B:98:GLY:HA2	1.93	0.51
1:B:23:GLY:C	1:B:279:ASN:ND2	2.64	0.51
1:A:108:ILE:HD12	1:A:148:LEU:HD13	1.92	0.51
1:B:256:GLU:O	1:B:260:ILE:HG12	2.12	0.50
1:A:121:ILE:HD13	1:A:227:ILE:CG2	2.40	0.50
1:B:130:ASN:HB2	1:B:142:GLY:O	2.12	0.50
1:B:306:LEU:HD23	1:B:306:LEU:C	2.32	0.50
1:A:66:ILE:CD1	1:A:66:ILE:H	2.14	0.50
1:B:15:PHE:CZ	1:B:73:VAL:HA	2.47	0.50
1:B:23:GLY:HA3	1:B:279:ASN:HD21	1.76	0.50
1:B:87:VAL:HG21	1:B:94:SER:HB3	1.92	0.50
1:A:121:ILE:N	1:A:121:ILE:HD12	2.27	0.50
1:B:226:PRO:HD3	3:B:397:HOH:O	2.11	0.50
1:B:129:ILE:HG21	1:B:190:LEU:HD23	1.94	0.50
1:A:262:GLU:O	1:A:266:LYS:HG3	2.12	0.49
1:A:38:GLU:H	1:A:38:GLU:CD	2.15	0.49
1:B:73:VAL:HG11	1:B:140:LEU:HD13	1.92	0.49
1:B:88:LYS:NZ	1:B:271:SER:HB3	2.27	0.49
1:B:50:TYR:OH	1:B:92:ARG:HD2	2.12	0.49
1:B:70:PRO:O	1:B:74:GLY:N	2.43	0.49
1:A:121:ILE:HG23	1:A:177:ILE:HD13	1.95	0.49
1:B:64:PHE:CD2	1:B:159:VAL:HG13	2.48	0.49
1:A:236:LEU:HD11	1:A:299:ILE:HD12	1.94	0.49
1:B:15:PHE:HB3	1:B:103:LEU:HD11	1.95	0.48
1:A:30:VAL:HA	1:A:33:LYS:HG2	1.95	0.48
1:B:198:PHE:CE1	1:B:215:THR:HG22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:O	1:B:225:ARG:HD2	2.13	0.48
1:A:58:ILE:N	1:A:58:ILE:HD12	2.28	0.48
1:B:87:VAL:HA	1:B:90:ASN:ND2	2.29	0.48
1:B:84:VAL:O	1:B:87:VAL:HG22	2.14	0.48
1:B:206:LEU:HB3	1:B:210:LYS:HB3	1.96	0.48
1:B:8:ILE:HD12	1:B:304:PHE:CD1	2.49	0.48
1:B:200:MET:CE	1:B:203:VAL:HG21	2.44	0.47
1:A:23:GLY:HA2	1:A:26:GLU:OE1	2.14	0.47
1:B:132:PRO:HD2	1:B:157:PRO:HD2	1.96	0.47
1:B:186:GLU:O	1:B:190:LEU:HD23	2.14	0.47
1:A:143:GLN:H	1:A:144:PRO:CD	2.27	0.47
1:B:263:GLU:O	1:B:267:THR:HG23	2.15	0.47
1:B:89:LYS:HZ3	1:B:89:LYS:HB2	1.79	0.47
1:B:234:ASP:C	1:B:234:ASP:OD1	2.52	0.47
1:B:265:TYR:CE2	1:B:305:GLY:HA2	2.50	0.47
1:A:275:ILE:CD1	1:A:300:THR:OG1	2.59	0.47
1:A:84:VAL:O	1:A:87:VAL:HG22	2.15	0.47
1:B:67:VAL:HG13	1:B:140:LEU:HG	1.96	0.47
1:B:89:LYS:NZ	1:B:89:LYS:CB	2.74	0.46
1:B:120:VAL:HB	1:B:174:ILE:HG13	1.96	0.46
1:A:19:GLN:HB2	1:A:20:PRO:CD	2.43	0.46
1:B:137:SER:HB2	1:B:139:ASN:ND2	2.30	0.46
1:B:190:LEU:HD22	1:B:195:ILE:HD12	1.96	0.46
1:B:67:VAL:CG1	1:B:140:LEU:HG	2.46	0.46
1:A:136:THR:HB	1:B:222:ARG:HD3	1.97	0.46
1:A:8:ILE:CD1	1:A:40:LEU:HD13	2.45	0.46
1:A:153:LYS:HD3	3:A:429:HOH:O	2.14	0.46
1:A:312:HIS:HB2	1:A:317:TYR:CE2	2.50	0.46
1:B:233:VAL:HG21	1:B:278:VAL:CG1	2.28	0.46
1:A:28:PRO:HG3	1:A:97:LEU:O	2.15	0.46
1:B:89:LYS:C	1:B:91:GLY:H	2.19	0.46
1:B:242:PRO:CD	1:B:291:ARG:HD2	2.45	0.46
1:B:180:ARG:CZ	1:B:251:GLY:HA2	2.46	0.46
1:B:81:ALA:HB2	1:B:106:GLY:HA2	1.98	0.46
1:A:226:PRO:HB3	1:A:271:SER:OG	2.15	0.46
1:B:190:LEU:H	1:B:190:LEU:HD23	1.81	0.46
1:B:225:ARG:HA	3:B:397:HOH:O	2.14	0.46
1:B:53:LEU:HB2	1:B:55:PHE:CZ	2.51	0.45
1:B:108:ILE:HD12	1:B:148:LEU:HD13	1.98	0.45
1:A:15:PHE:HB3	1:A:103:LEU:HD11	1.97	0.45
1:B:261:THR:HG21	1:B:299:ILE:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PRO:CG	1:B:21:ARG:HH21	2.30	0.45
1:A:68:LYS:NZ	1:A:137:SER:O	2.31	0.45
1:B:129:ILE:HG21	1:B:190:LEU:HD21	1.98	0.45
1:A:143:GLN:H	1:A:144:PRO:HD2	1.77	0.45
1:B:220:LEU:HD22	1:B:269:LEU:CD1	2.47	0.45
1:B:48:LYS:CG	1:B:92:ARG:HE	2.18	0.45
1:B:80:LEU:CD2	1:B:103:LEU:HB3	2.46	0.45
1:B:64:PHE:O	1:B:65:GLN:HB2	2.17	0.45
1:A:7:THR:CG2	1:A:92:ARG:HG2	2.47	0.45
1:A:30:VAL:O	1:A:33:LYS:HG2	2.16	0.45
1:A:10:ILE:HG13	1:A:37:LEU:HD21	1.99	0.45
1:A:37:LEU:CD2	1:A:47:VAL:HG11	2.47	0.45
1:B:104:ALA:O	1:B:108:ILE:HG13	2.17	0.45
1:B:20:PRO:HG2	1:B:21:ARG:NH2	2.31	0.45
1:A:177:ILE:HD12	1:A:177:ILE:N	2.32	0.45
1:B:133:LEU:N	1:B:133:LEU:HD12	2.32	0.44
1:B:19:GLN:HB3	1:B:141:HIS:CG	2.52	0.44
1:B:133:LEU:H	1:B:133:LEU:HD12	1.82	0.44
1:A:19:GLN:NE2	1:A:21:ARG:O	2.43	0.44
1:A:224:LYS:HB3	1:A:269:LEU:HD11	1.98	0.44
1:B:90:ASN:HB3	1:B:92:ARG:HH11	1.82	0.44
1:B:13:ALA:HA	1:B:55:PHE:CZ	2.51	0.44
1:B:89:LYS:C	1:B:91:GLY:N	2.71	0.44
1:B:15:PHE:CE1	1:B:17:LYS:HB2	2.53	0.44
1:A:287:GLU:OE2	1:A:291:ARG:NH2	2.47	0.44
1:B:48:LYS:HG3	1:B:92:ARG:HH21	1.83	0.43
1:B:64:PHE:CE2	1:B:159:VAL:HG22	2.53	0.43
1:B:10:ILE:HG13	1:B:37:LEU:HD22	1.99	0.43
1:B:169:ILE:HG13	1:B:169:ILE:O	2.18	0.43
1:B:220:LEU:HD22	1:B:269:LEU:HD13	2.00	0.43
1:B:253:THR:HG22	1:B:254:TYR:H	1.83	0.43
1:A:172:LYS:HG3	1:A:173:ASP:OD1	2.17	0.43
1:B:101:HIS:CD2	1:B:276:MET:HG3	2.52	0.43
1:A:19:GLN:CB	1:A:20:PRO:HD2	2.43	0.43
1:A:148:LEU:HB3	1:A:169:ILE:CD1	2.47	0.43
1:B:118:LEU:O	1:B:118:LEU:HD12	2.19	0.43
1:B:55:PHE:HA	1:B:79:GLN:HE22	1.83	0.43
1:B:159:VAL:O	1:B:160:PRO:C	2.57	0.43
1:A:261:THR:HG21	1:A:299:ILE:HG23	1.98	0.43
1:B:152:LEU:HG	1:B:193:LEU:HD21	2.00	0.43
1:B:21:ARG:NH1	1:B:245:GLY:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:CB	1:B:280:PRO:HG2	2.49	0.43
1:B:274:ASP:HB3	1:B:276:MET:SD	2.59	0.43
1:B:30:VAL:HA	1:B:33:LYS:HG3	2.01	0.43
1:B:237:ASP:HA	1:B:238:PRO:HD3	1.91	0.43
1:B:12:GLY:O	1:B:53:LEU:HG	2.18	0.43
1:B:61:ASP:OD2	1:B:69:ASN:HA	2.19	0.43
1:B:167:PRO:HG3	3:B:373:HOH:O	2.18	0.42
1:B:118:LEU:HD12	1:B:118:LEU:C	2.40	0.42
1:A:87:VAL:O	1:A:90:ASN:HB2	2.19	0.42
1:A:208:ILE:HD11	1:A:260:ILE:HD11	1.97	0.42
1:A:15:PHE:HE2	1:A:73:VAL:HG22	1.85	0.42
1:B:6:ARG:HA	1:B:6:ARG:HD3	1.65	0.42
1:B:258:LEU:HD12	1:B:308:ARG:HD3	2.01	0.42
1:B:259:TYR:CE2	1:B:263:GLU:HG3	2.54	0.42
1:A:253:THR:CG2	1:A:254:TYR:N	2.82	0.42
1:B:190:LEU:N	1:B:190:LEU:HD23	2.35	0.42
1:A:124:ASP:OD1	1:A:125:ALA:N	2.52	0.42
1:B:133:LEU:CD1	1:B:157:PRO:HD3	2.49	0.42
1:A:237:ASP:HA	1:A:238:PRO:HD3	1.91	0.42
1:A:175:VAL:HG11	1:A:215:THR:HG22	2.00	0.42
1:A:10:ILE:HD13	1:A:95:LEU:HB3	2.02	0.42
1:B:30:VAL:O	1:B:33:LYS:HG3	2.20	0.42
1:A:67:VAL:HG21	1:A:132:PRO:HB3	2.01	0.42
1:B:48:LYS:O	1:B:50:TYR:CD1	2.73	0.42
1:B:17:LYS:HD2	1:B:72:SER:HB3	2.02	0.42
1:A:198:PHE:CE1	1:A:215:THR:HG22	2.55	0.42
1:B:111:HIS:C	1:B:111:HIS:CD2	2.93	0.42
1:B:236:LEU:HD11	1:B:299:ILE:CD1	2.49	0.42
1:B:17:LYS:NZ	1:B:57:ASP:OD2	2.54	0.41
1:B:176:TYR:CE2	1:B:195:ILE:HG21	2.54	0.41
1:A:11:ILE:HD13	1:A:50:TYR:HB2	2.01	0.41
1:B:56:ALA:HB2	3:B:410:HOH:O	2.20	0.41
1:B:30:VAL:HG12	1:B:293:VAL:HG21	2.01	0.41
1:B:26:GLU:CD	1:B:280:PRO:HG2	2.41	0.41
1:A:83:LYS:CD	1:A:83:LYS:N	2.84	0.41
1:A:225:ARG:HG3	1:A:225:ARG:H	1.73	0.41
1:B:48:LYS:O	1:B:50:TYR:CE1	2.74	0.41
1:B:10:ILE:HD13	1:B:95:LEU:HD13	1.98	0.41
1:B:58:ILE:HA	1:B:59:PRO:HD2	1.83	0.41
1:A:71:ARG:O	1:A:75:LYS:HB2	2.20	0.41
1:B:231:PHE:CZ	1:B:299:ILE:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PRO:HG2	1:B:21:ARG:HE	1.86	0.41
1:B:185:GLY:O	1:B:189:ILE:HG12	2.21	0.40
1:B:243:ALA:HB1	1:B:279:ASN:O	2.20	0.40
1:B:26:GLU:HB2	1:B:280:PRO:HG2	2.03	0.40
1:B:5:SER:HB2	1:B:44:GLU:OE2	2.21	0.40
1:B:148:LEU:HB3	1:B:169:ILE:HG12	2.02	0.40
1:B:225:ARG:HB2	1:B:226:PRO:HD2	2.04	0.40
1:A:152:LEU:HD13	1:A:193:LEU:HD21	2.03	0.40
1:B:17:LYS:HG3	3:B:339:HOH:O	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	312/322 (97%)	289 (93%)	20 (6%)	3 (1%)	19 7
1	B	312/322 (97%)	279 (89%)	28 (9%)	5 (2%)	12 3
All	All	624/644 (97%)	568 (91%)	48 (8%)	8 (1%)	15 4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	B	99	GLY
1	A	180	ARG
1	B	143	GLN
1	B	180	ARG
1	B	277	GLU
1	A	143	GLN
1	B	27	GLY

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	263/270 (97%)	249 (95%)	14 (5%)	28 16
1	B	263/270 (97%)	251 (95%)	12 (5%)	33 21
All	All	526/540 (97%)	500 (95%)	26 (5%)	31 18

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	44	GLU
1	A	66	ILE
1	A	77	SER
1	A	118	LEU
1	A	132	PRO
1	A	141	HIS
1	A	152	LEU
1	A	169	ILE
1	A	208	ILE
1	A	225	ARG
1	A	271	SER
1	A	287	GLU
1	A	306	LEU
1	B	33	LYS
1	B	66	ILE
1	B	78	GLU
1	B	129	ILE
1	B	141	HIS
1	B	190	LEU
1	B	219	LEU
1	B	225	ARG
1	B	244	THR
1	B	273	LEU
1	B	278	VAL
1	B	279	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	312	HIS
1	B	65	GLN
1	B	279	ASN
1	B	312	HIS

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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	314/322 (97%)	1.12	46 (14%) 3 3	9, 17, 31, 47	0
1	B	314/322 (97%)	1.54	94 (29%) 1 0	10, 21, 36, 46	0
All	All	628/644 (97%)	1.33	140 (22%) 1 1	9, 19, 34, 47	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	ILE	7.0
1	B	156	ILE	5.7
1	B	62	SER	5.0
1	B	7	THR	5.0
1	B	163	SER	4.9
1	B	57	ASP	4.6
1	A	6	ARG	4.5
1	B	314	PRO	4.4
1	B	66	ILE	4.3
1	A	314	PRO	4.3
1	B	58	ILE	4.2
1	A	163	SER	4.1
1	B	91	GLY	4.0
1	B	50	TYR	4.0
1	B	152	LEU	4.0
1	A	222	ARG	3.8
1	B	8	ILE	3.8
1	B	153	LYS	3.8
1	B	61	ASP	3.7
1	A	8	ILE	3.7
1	B	36	LEU	3.7
1	B	55	PHE	3.7
1	A	63	PRO	3.6
1	B	136	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	158	ASP	3.5
1	B	316	ASP	3.5
1	B	60	ASN	3.5
1	A	224	LYS	3.4
1	B	286	PRO	3.3
1	B	47	VAL	3.3
1	A	56	ALA	3.2
1	B	90	ASN	3.2
1	B	190	LEU	3.2
1	B	221	GLY	3.2
1	A	140	LEU	3.2
1	B	114	VAL	3.1
1	B	145	VAL	3.1
1	A	156	ILE	3.1
1	B	97	LEU	3.1
1	B	87	VAL	3.1
1	B	164	TRP	3.1
1	A	7	THR	3.0
1	B	273	LEU	3.0
1	B	73	VAL	3.0
1	B	64	PHE	3.0
1	B	44	GLU	3.0
1	B	40	LEU	3.0
1	B	252	LEU	3.0
1	A	233	VAL	2.9
1	A	223	LYS	2.9
1	A	5	SER	2.9
1	B	133	LEU	2.9
1	B	161	GLY	2.9
1	A	153	LYS	2.9
1	B	65	GLN	2.8
1	B	140	LEU	2.8
1	B	193	LEU	2.8
1	B	243	ALA	2.8
1	A	114	VAL	2.8
1	B	236	LEU	2.8
1	A	84	VAL	2.8
1	A	33	LYS	2.8
1	B	48	LYS	2.7
1	B	147	PHE	2.7
1	B	222	ARG	2.7
1	A	87	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	165	VAL	2.7
1	A	179	LEU	2.7
1	B	317	TYR	2.6
1	A	80	LEU	2.6
1	B	315	ILE	2.6
1	B	89	LYS	2.6
1	B	103	LEU	2.6
1	A	11	ILE	2.6
1	B	118	LEU	2.6
1	B	226	PRO	2.6
1	A	47	VAL	2.6
1	A	54	PRO	2.6
1	B	10	ILE	2.5
1	B	291	ARG	2.5
1	B	63	PRO	2.5
1	B	5	SER	2.5
1	A	64	PHE	2.5
1	A	62	SER	2.5
1	B	278	VAL	2.4
1	B	53	LEU	2.4
1	A	154	GLY	2.4
1	A	221	GLY	2.4
1	B	45	CYS	2.4
1	B	167	PRO	2.4
1	B	129	ILE	2.4
1	A	282	LEU	2.4
1	A	290	THR	2.4
1	A	42	GLU	2.3
1	A	55	PHE	2.3
1	B	15	PHE	2.3
1	B	292	THR	2.3
1	B	67	VAL	2.3
1	B	84	VAL	2.3
1	B	289	VAL	2.3
1	B	318	LEU	2.3
1	A	50	TYR	2.3
1	B	37	LEU	2.3
1	B	178	GLY	2.3
1	B	56	ALA	2.3
1	B	59	PRO	2.2
1	B	123	VAL	2.2
1	B	6	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	72	SER	2.2
1	B	297	VAL	2.2
1	B	34	ALA	2.2
1	A	149	LEU	2.2
1	A	18	GLY	2.2
1	A	227	ILE	2.2
1	A	36	LEU	2.2
1	B	24	VAL	2.2
1	B	157	PRO	2.1
1	A	162	PHE	2.1
1	B	162	PHE	2.1
1	B	30	VAL	2.1
1	B	96	VAL	2.1
1	B	134	THR	2.1
1	B	70	PRO	2.1
1	B	98	GLY	2.1
1	B	38	GLU	2.1
1	A	293	VAL	2.1
1	B	29	THR	2.1
1	B	148	LEU	2.1
1	A	92	ARG	2.1
1	B	86	GLU	2.1
1	B	313	LYS	2.0
1	A	53	LEU	2.0
1	A	137	SER	2.0
1	B	80	LEU	2.0
1	B	233	VAL	2.0
1	B	76	ALA	2.0
1	A	210	LYS	2.0
1	B	31	LEU	2.0
1	A	225	ARG	2.0
1	A	278	VAL	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	A	324	1/1	0.98	0.08	-1.97	15,15,15,15	0
2	MN	A	323	1/1	0.99	0.05	-3.06	14,14,14,14	0
2	MN	B	324	1/1	0.96	0.07	-3.63	21,21,21,21	0
2	MN	B	323	1/1	0.99	0.04	-7.39	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.