



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 05:52 PM UTC

PDB ID : 4Q40 / pdb_00004q40
Title : Crystal structure of Schistosoma mansoni arginase in complex with L-valine
Authors : Hai, Y.; Edwards, J.E.; Van Zandt, M.C.; Hoffmann, K.F.; Christianson, D.W.
Deposited on : 2014-04-12
Resolution : 1.83 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

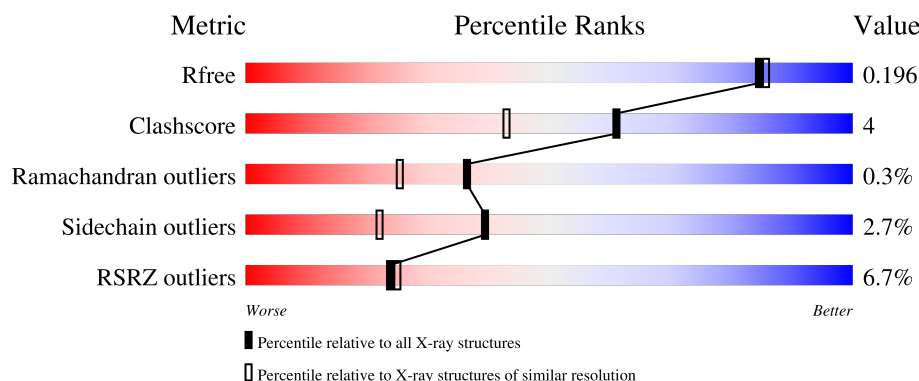
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 $\leq 5\%$. 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	385	
1	B	385	
1	C	385	
1	D	385	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11397 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	1	0
			2574	1621	450	487	16			
1	B	335	Total	C	N	O	S	0	1	0
			2574	1621	450	487	16			
1	C	335	Total	C	N	O	S	0	1	0
			2574	1621	450	487	16			
1	D	331	Total	C	N	O	S	0	0	0
			2539	1601	443	480	15			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q6WVP6
A	-19	GLY	-	expression tag	UNP Q6WVP6
A	-18	SER	-	expression tag	UNP Q6WVP6
A	-17	SER	-	expression tag	UNP Q6WVP6
A	-16	HIS	-	expression tag	UNP Q6WVP6
A	-15	HIS	-	expression tag	UNP Q6WVP6
A	-14	HIS	-	expression tag	UNP Q6WVP6
A	-13	HIS	-	expression tag	UNP Q6WVP6
A	-12	HIS	-	expression tag	UNP Q6WVP6
A	-11	HIS	-	expression tag	UNP Q6WVP6
A	-10	SER	-	expression tag	UNP Q6WVP6
A	-9	SER	-	expression tag	UNP Q6WVP6
A	-8	GLY	-	expression tag	UNP Q6WVP6
A	-7	LEU	-	expression tag	UNP Q6WVP6
A	-6	VAL	-	expression tag	UNP Q6WVP6
A	-5	PRO	-	expression tag	UNP Q6WVP6
A	-4	ARG	-	expression tag	UNP Q6WVP6
A	-3	GLY	-	expression tag	UNP Q6WVP6
A	-2	SER	-	expression tag	UNP Q6WVP6
A	-1	HIS	-	expression tag	UNP Q6WVP6
A	0	MET	-	expression tag	UNP Q6WVP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP Q6WVP6
B	-19	GLY	-	expression tag	UNP Q6WVP6
B	-18	SER	-	expression tag	UNP Q6WVP6
B	-17	SER	-	expression tag	UNP Q6WVP6
B	-16	HIS	-	expression tag	UNP Q6WVP6
B	-15	HIS	-	expression tag	UNP Q6WVP6
B	-14	HIS	-	expression tag	UNP Q6WVP6
B	-13	HIS	-	expression tag	UNP Q6WVP6
B	-12	HIS	-	expression tag	UNP Q6WVP6
B	-11	HIS	-	expression tag	UNP Q6WVP6
B	-10	SER	-	expression tag	UNP Q6WVP6
B	-9	SER	-	expression tag	UNP Q6WVP6
B	-8	GLY	-	expression tag	UNP Q6WVP6
B	-7	LEU	-	expression tag	UNP Q6WVP6
B	-6	VAL	-	expression tag	UNP Q6WVP6
B	-5	PRO	-	expression tag	UNP Q6WVP6
B	-4	ARG	-	expression tag	UNP Q6WVP6
B	-3	GLY	-	expression tag	UNP Q6WVP6
B	-2	SER	-	expression tag	UNP Q6WVP6
B	-1	HIS	-	expression tag	UNP Q6WVP6
B	0	MET	-	expression tag	UNP Q6WVP6
C	-20	MET	-	expression tag	UNP Q6WVP6
C	-19	GLY	-	expression tag	UNP Q6WVP6
C	-18	SER	-	expression tag	UNP Q6WVP6
C	-17	SER	-	expression tag	UNP Q6WVP6
C	-16	HIS	-	expression tag	UNP Q6WVP6
C	-15	HIS	-	expression tag	UNP Q6WVP6
C	-14	HIS	-	expression tag	UNP Q6WVP6
C	-13	HIS	-	expression tag	UNP Q6WVP6
C	-12	HIS	-	expression tag	UNP Q6WVP6
C	-11	HIS	-	expression tag	UNP Q6WVP6
C	-10	SER	-	expression tag	UNP Q6WVP6
C	-9	SER	-	expression tag	UNP Q6WVP6
C	-8	GLY	-	expression tag	UNP Q6WVP6
C	-7	LEU	-	expression tag	UNP Q6WVP6
C	-6	VAL	-	expression tag	UNP Q6WVP6
C	-5	PRO	-	expression tag	UNP Q6WVP6
C	-4	ARG	-	expression tag	UNP Q6WVP6
C	-3	GLY	-	expression tag	UNP Q6WVP6
C	-2	SER	-	expression tag	UNP Q6WVP6
C	-1	HIS	-	expression tag	UNP Q6WVP6
C	0	MET	-	expression tag	UNP Q6WVP6

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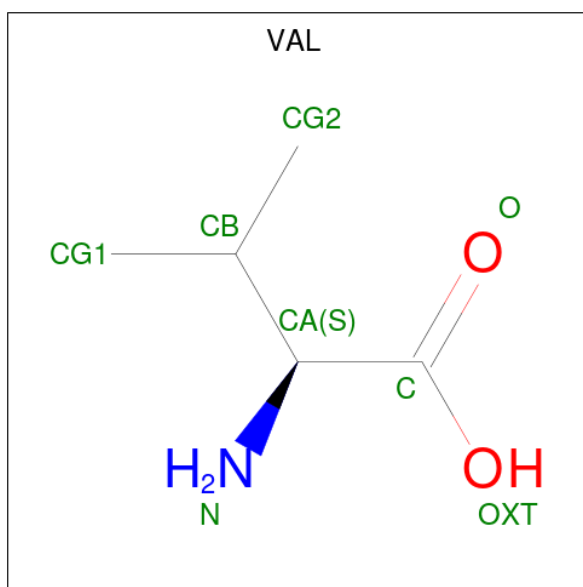
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP Q6WVP6
D	-19	GLY	-	expression tag	UNP Q6WVP6
D	-18	SER	-	expression tag	UNP Q6WVP6
D	-17	SER	-	expression tag	UNP Q6WVP6
D	-16	HIS	-	expression tag	UNP Q6WVP6
D	-15	HIS	-	expression tag	UNP Q6WVP6
D	-14	HIS	-	expression tag	UNP Q6WVP6
D	-13	HIS	-	expression tag	UNP Q6WVP6
D	-12	HIS	-	expression tag	UNP Q6WVP6
D	-11	HIS	-	expression tag	UNP Q6WVP6
D	-10	SER	-	expression tag	UNP Q6WVP6
D	-9	SER	-	expression tag	UNP Q6WVP6
D	-8	GLY	-	expression tag	UNP Q6WVP6
D	-7	LEU	-	expression tag	UNP Q6WVP6
D	-6	VAL	-	expression tag	UNP Q6WVP6
D	-5	PRO	-	expression tag	UNP Q6WVP6
D	-4	ARG	-	expression tag	UNP Q6WVP6
D	-3	GLY	-	expression tag	UNP Q6WVP6
D	-2	SER	-	expression tag	UNP Q6WVP6
D	-1	HIS	-	expression tag	UNP Q6WVP6
D	0	MET	-	expression tag	UNP Q6WVP6

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

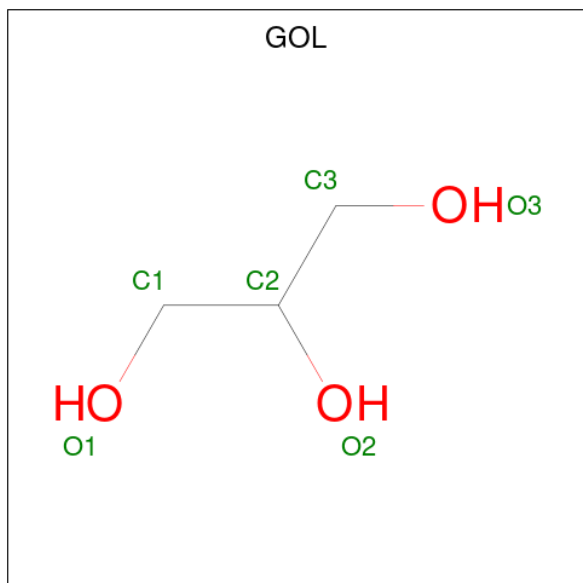
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0

- Molecule 3 is VALINE (CCD ID: VAL) (formula: C₅H₁₁NO₂).



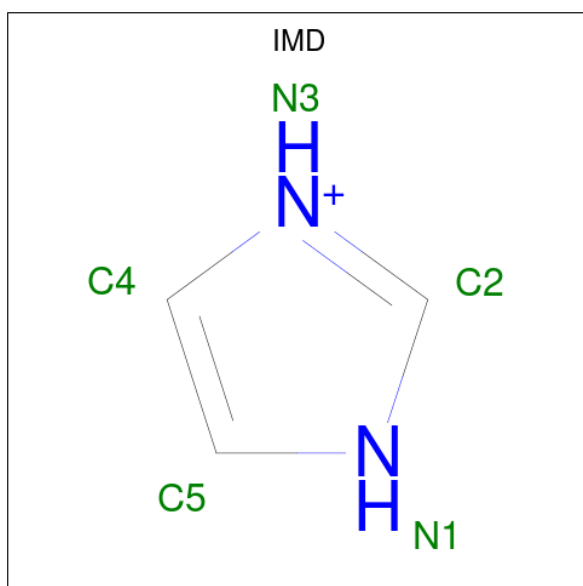
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	5	1	2		
3	B	1	Total	C	N	O	0	0
			8	5	1	2		
3	C	1	Total	C	N	O	0	0
			8	5	1	2		
3	D	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 5 3 2	0	0
5	A	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	N	0	0
			5	3	2		
5	C	1	Total	C	N	0	0
			5	3	2		

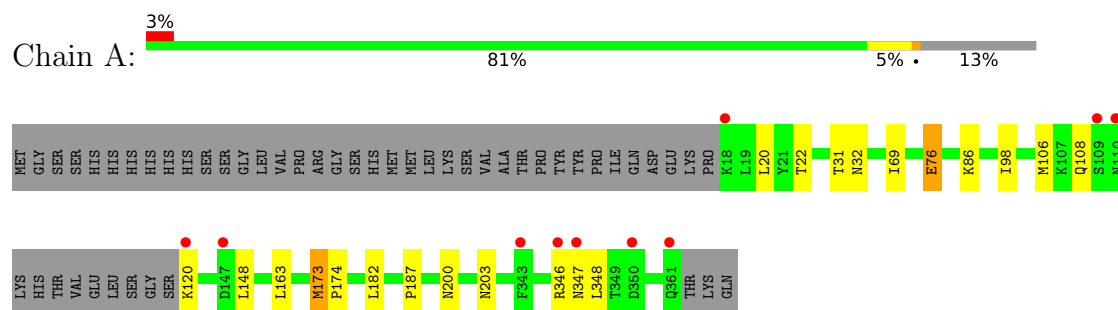
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	324	Total	O	0	0
			324	324		
6	B	315	Total	O	0	0
			315	315		
6	C	245	Total	O	0	0
			245	245		
6	D	135	Total	O	0	0
			135	135		

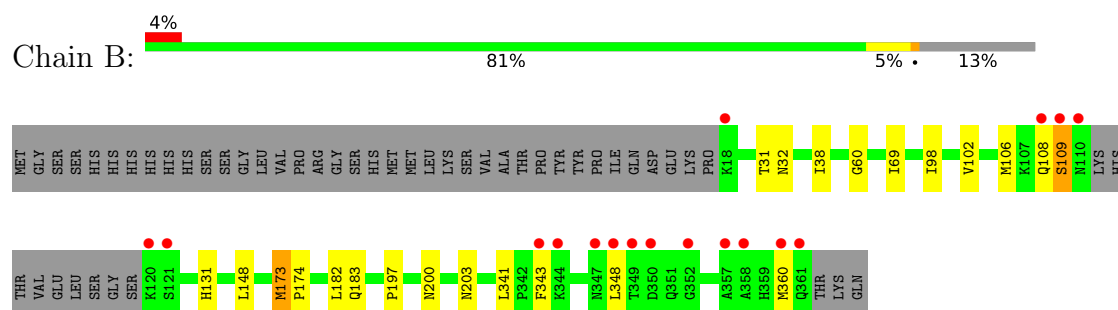
3 Residue-property plots [i](#)

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.

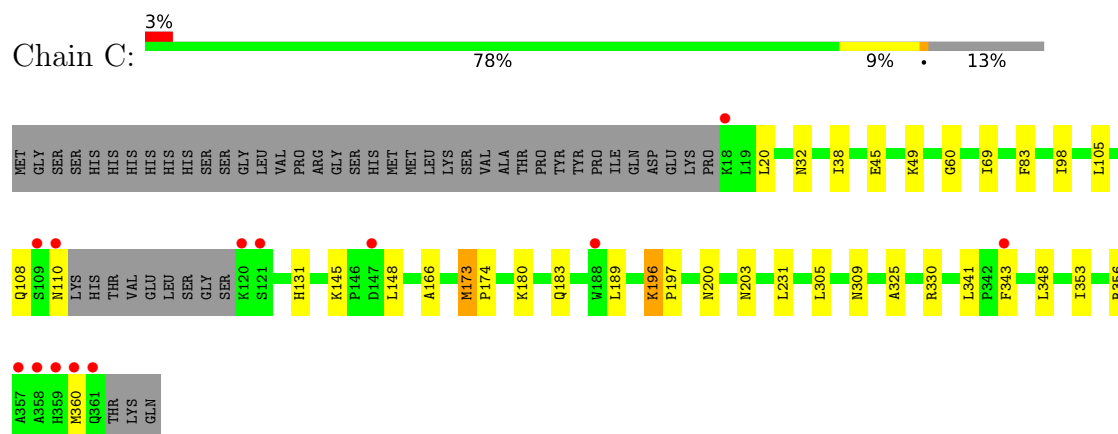
- Molecule 1: Arginase



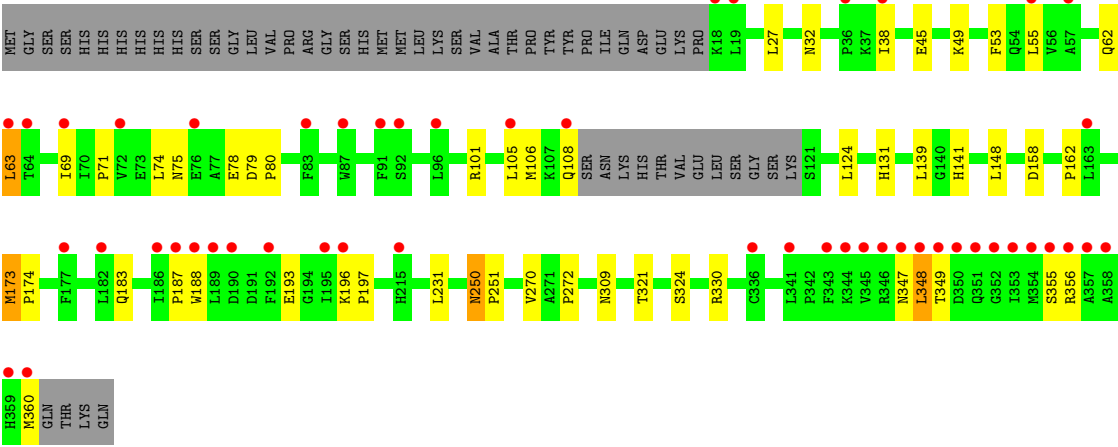
- Molecule 1: Arginase



- Molecule 1: Arginase



- Molecule 1: Arginase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	177.81Å 177.81Å 177.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 1.83 49.31 – 1.83	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.31-1.83) 99.9 (49.31-1.83)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.83Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.174 , 0.195 0.176 , 0.196	Depositor DCC
R_{free} test set	8202 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11397	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IMD, 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	0.50	0/2624	0.75	0/3555
1	B	0.50	0/2624	0.75	0/3555
1	C	0.40	0/2624	0.75	2/3555 (0.1%)
1	D	0.33	0/2586	0.75	4/3505 (0.1%)
All	All	0.44	0/10458	0.75	6/14170 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	309	ASN	CA-C-N	7.58	127.25	119.82
1	D	309	ASN	C-N-CA	7.58	127.25	119.82
1	D	250	ASN	CA-C-N	6.87	127.15	119.32
1	D	250	ASN	C-N-CA	6.87	127.15	119.32
1	C	309	ASN	CA-C-N	5.33	125.04	119.82
1	C	309	ASN	C-N-CA	5.33	125.04	119.82

There are no chirality outliers.

There are no planarity outliers.

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	2574	0	2590	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2574	0	2590	11	0
1	C	2574	0	2590	24	0
1	D	2539	0	2553	34	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	8	0	8	0	0
3	B	8	0	8	0	0
3	C	8	0	8	0	0
3	D	8	0	8	0	0
4	A	18	0	24	1	0
4	B	12	0	16	0	0
4	C	12	0	16	1	0
5	A	10	0	10	0	0
5	B	15	0	15	1	0
5	C	10	0	10	3	0
6	A	324	0	0	2	0
6	B	315	0	0	3	0
6	C	245	0	0	2	0
6	D	135	0	0	2	0
All	All	11397	0	10446	87	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 4.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:LEU:HB3	1:D:78:GLU:HG3	1.54	0.90
1:D:69:ILE:HD11	1:D:101:ARG:HG2	1.60	0.84
1:D:270:VAL:HG22	1:D:324:SER:OG	1.84	0.78
1:C:348:LEU:HD11	1:C:353:ILE:HB	1.70	0.73
1:B:109:SER:HB2	6:B:506:HOH:O	1.89	0.72
1:D:173:MET:N	1:D:174:PRO:HD3	2.04	0.71
5:B:408:IMD:H2	6:B:733:HOH:O	1.91	0.71
1:C:69:ILE:HD13	1:C:98:ILE:HA	1.77	0.65
1:D:45:GLU:HG2	1:D:49:LYS:HE2	1.82	0.61
1:C:348:LEU:CD1	1:C:353:ILE:HB	2.30	0.61
1:C:105:LEU:O	1:C:108:GLN:HG2	2.01	0.59
1:D:139:LEU:HD11	1:D:196:LYS:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:GLU:CG	1:D:49:LYS:HE2	2.32	0.59
1:D:75:ASN:OD1	1:D:78:GLU:HG2	2.03	0.58
4:A:406:GOL:O3	5:C:401:IMD:H4	2.04	0.58
1:A:22:THR:HG23	1:A:120:LYS:HD3	1.85	0.58
1:C:38:ILE:HG22	6:C:566:HOH:O	2.05	0.56
1:A:86:LYS:HE2	6:A:519:HOH:O	2.05	0.55
1:A:106:MET:HE1	6:A:562:HOH:O	2.07	0.54
1:D:347:ASN:ND2	1:D:349:THR:H	2.05	0.54
1:D:158:ASP:O	1:D:174:PRO:HD2	2.07	0.54
1:D:173:MET:N	1:D:174:PRO:CD	2.71	0.54
1:B:183:GLN:HG3	1:B:197:PRO:HG2	1.89	0.53
1:D:183:GLN:HG3	1:D:197:PRO:HG2	1.90	0.53
1:C:200:ASN:H	1:C:203:ASN:HD22	1.56	0.53
1:A:76:GLU:H	1:A:76:GLU:CD	2.14	0.53
1:B:200:ASN:H	1:B:203:ASN:HD22	1.56	0.53
1:C:166:ALA:O	5:C:407:IMD:H2	2.08	0.53
1:D:148:LEU:C	1:D:148:LEU:HD12	2.33	0.53
1:C:356:ARG:O	1:C:360:MET:HG2	2.09	0.52
1:A:69:ILE:HD13	1:A:98:ILE:HA	1.90	0.52
1:D:38:ILE:HG22	6:D:503:HOH:O	2.09	0.52
1:C:183:GLN:HG3	1:C:197:PRO:HG2	1.92	0.51
1:C:45:GLU:HG3	1:C:49:LYS:HD3	1.92	0.51
1:C:200:ASN:H	1:C:203:ASN:ND2	2.09	0.51
1:A:148:LEU:C	1:A:148:LEU:HD12	2.35	0.51
1:C:148:LEU:HD12	1:C:148:LEU:C	2.37	0.50
1:D:348:LEU:HD11	1:D:355:SER:HB3	1.93	0.50
1:B:200:ASN:H	1:B:203:ASN:ND2	2.10	0.50
1:D:272:PRO:HD2	1:D:321:THR:OG1	2.13	0.49
1:A:163:LEU:CD2	1:A:187:PRO:HG3	2.43	0.49
1:C:173:MET:N	1:C:174:PRO:CD	2.76	0.49
1:D:250:ASN:N	1:D:251:PRO:HD3	2.27	0.49
1:D:158:ASP:HB3	1:D:174:PRO:HD2	1.95	0.48
1:D:347:ASN:OD1	1:D:349:THR:HB	2.14	0.48
1:C:196:LYS:H	1:C:196:LYS:HD3	1.79	0.48
1:A:347:ASN:HD22	1:A:348:LEU:H	1.62	0.47
1:D:55:LEU:HD13	1:D:330:ARG:HD2	1.96	0.47
1:B:60:GLY:HA3	1:B:343:PHE:CZ	2.50	0.47
1:A:346:ARG:HB3	1:A:346:ARG:NH1	2.31	0.46
1:D:162:PRO:HG2	1:D:187:PRO:HD2	1.98	0.46
1:D:55:LEU:CD1	1:D:330:ARG:HD2	2.46	0.46
1:C:110:ASN:HD21	1:C:145:LYS:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASN:HD22	1:A:348:LEU:N	2.13	0.45
1:B:102:VAL:O	1:B:106:MET:HG2	2.16	0.45
1:D:45:GLU:HG3	6:D:521:HOH:O	2.16	0.45
1:A:347:ASN:ND2	1:A:348:LEU:N	2.65	0.45
1:A:200:ASN:H	1:A:203:ASN:ND2	2.15	0.44
1:B:173:MET:N	1:B:174:PRO:CD	2.80	0.44
1:C:196:LYS:H	1:C:196:LYS:CD	2.30	0.44
1:B:348:LEU:HD23	1:B:348:LEU:HA	1.85	0.44
1:C:60:GLY:HA3	1:C:343:PHE:CZ	2.53	0.43
1:C:348:LEU:HD11	1:C:353:ILE:CB	2.44	0.43
1:D:173:MET:H	1:D:174:PRO:HD3	1.82	0.43
1:A:173:MET:N	1:A:174:PRO:CD	2.81	0.43
1:C:305:LEU:HD21	1:C:325:ALA:HB1	2.00	0.43
1:D:105:LEU:O	1:D:108:GLN:HG2	2.18	0.43
1:C:83:PHE:CE2	1:C:189:LEU:HD21	2.54	0.43
1:A:200:ASN:H	1:A:203:ASN:HD22	1.66	0.43
5:C:407:IMD:H5	6:C:669:HOH:O	2.18	0.43
1:D:69:ILE:HD11	1:D:101:ARG:CG	2.39	0.42
1:D:79:ASP:N	1:D:80:PRO:HD3	2.35	0.42
1:D:106:MET:HE2	1:D:141:HIS:CD2	2.54	0.42
1:D:45:GLU:CD	1:D:49:LYS:HE2	2.45	0.42
1:B:38:ILE:HG22	6:B:537:HOH:O	2.18	0.42
1:B:69:ILE:HD13	1:B:98:ILE:HA	2.02	0.42
1:C:200:ASN:HD22	1:C:203:ASN:HD21	1.68	0.42
1:D:348:LEU:HD12	1:D:348:LEU:C	2.44	0.42
1:D:356:ARG:O	1:D:360:MET:HG2	2.20	0.41
1:D:53:PHE:CD2	1:D:63:LEU:HD13	2.56	0.41
1:D:188:TRP:CH2	1:D:193:GLU:HB2	2.54	0.41
1:C:180:LYS:HD2	1:C:200:ASN:OD1	2.20	0.41
1:D:69:ILE:O	1:D:71:PRO:HD3	2.21	0.41
1:C:38:ILE:HD11	4:C:405:GOL:H31	2.02	0.41
1:A:22:THR:CG2	1:A:120:LYS:HD3	2.50	0.40
1:B:148:LEU:HD12	1:B:148:LEU:C	2.46	0.40
1:C:110:ASN:N	1:C:110:ASN:HD22	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	332/385 (86%)	325 (98%)	6 (2%)	1 (0%)	36	25
1	B	332/385 (86%)	326 (98%)	5 (2%)	1 (0%)	36	25
1	C	332/385 (86%)	322 (97%)	9 (3%)	1 (0%)	36	25
1	D	327/385 (85%)	316 (97%)	10 (3%)	1 (0%)	36	25
All	All	1323/1540 (86%)	1289 (97%)	30 (2%)	4 (0%)	36	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	173	MET
1	A	173	MET
1	B	173	MET
1	C	173	MET

5.3.2 Protein sidechains

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	283/327 (86%)	277 (98%)	6 (2%)	47	30
1	B	283/327 (86%)	275 (97%)	8 (3%)	38	20
1	C	283/327 (86%)	276 (98%)	7 (2%)	42	24
1	D	278/327 (85%)	270 (97%)	8 (3%)	37	20
All	All	1127/1308 (86%)	1098 (97%)	29 (3%)	39	23

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	31	THR
1	A	32	ASN
1	A	76	GLU
1	A	108	GLN
1	A	182	LEU
1	B	31	THR
1	B	32	ASN
1	B	108	GLN
1	B	109	SER
1	B	131	HIS
1	B	182	LEU
1	B	341	LEU
1	B	360	MET
1	C	20	LEU
1	C	32	ASN
1	C	131	HIS
1	C	196	LYS
1	C	231	LEU
1	C	330	ARG
1	C	341	LEU
1	D	27	LEU
1	D	32	ASN
1	D	62	GLN
1	D	63	LEU
1	D	124	LEU
1	D	131	HIS
1	D	231	LEU
1	D	348	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	108	GLN
1	A	110	ASN
1	A	203	ASN
1	A	347	ASN
1	A	351	GLN
1	B	81	GLN
1	B	108	GLN

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Mol	Chain	Res	Type
1	B	110	ASN
1	B	200	ASN
1	B	203	ASN
1	B	361	GLN
1	C	25	ASN
1	C	62	GLN
1	C	81	GLN
1	C	110	ASN
1	C	203	ASN
1	C	359	HIS
1	D	62	GLN
1	D	81	GLN
1	D	203	ASN
1	D	223	HIS
1	D	335	HIS
1	D	347	ASN
1	D	359	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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
4	GOL	B	404	-	5,5,5	0.43	0	5,5,5	0.50	0
4	GOL	A	405	-	5,5,5	0.27	0	5,5,5	0.38	0
5	IMD	C	407	-	5,5,5	0.69	0	5,5,5	0.37	0
4	GOL	A	406	-	5,5,5	0.47	0	5,5,5	0.27	0
5	IMD	B	407	-	5,5,5	0.64	0	5,5,5	0.42	0
5	IMD	C	401	-	5,5,5	0.64	0	5,5,5	0.43	0
4	GOL	C	405	-	5,5,5	0.38	0	5,5,5	0.50	0
5	IMD	B	406	-	5,5,5	0.66	0	5,5,5	0.38	0
3	VAL	D	403	-	6,7,7	0.90	1 (16%)	8,9,9	1.23	2 (25%)
3	VAL	C	404	-	6,7,7	0.88	1 (16%)	8,9,9	1.31	2 (25%)
5	IMD	A	408	-	5,5,5	0.68	0	5,5,5	0.42	0
4	GOL	A	404	-	5,5,5	0.35	0	5,5,5	0.68	0
4	GOL	B	405	-	5,5,5	0.20	0	5,5,5	0.57	0
4	GOL	C	406	-	5,5,5	0.33	0	5,5,5	0.36	0
5	IMD	A	407	-	5,5,5	0.68	0	5,5,5	0.44	0
3	VAL	B	403	-	6,7,7	0.98	1 (16%)	8,9,9	1.36	2 (25%)
5	IMD	B	408	-	5,5,5	0.66	0	5,5,5	0.53	0
3	VAL	A	403	-	6,7,7	0.94	1 (16%)	8,9,9	1.27	1 (12%)

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
4	GOL	B	404	-	-	2/4/4/4	-
4	GOL	A	405	-	-	0/4/4/4	-
5	IMD	C	407	-	-	-	0/1/1/1
4	GOL	A	406	-	-	4/4/4/4	-
5	IMD	B	407	-	-	-	0/1/1/1
5	IMD	C	401	-	-	-	0/1/1/1
4	GOL	C	405	-	-	2/4/4/4	-
5	IMD	B	406	-	-	-	0/1/1/1
3	VAL	D	403	-	-	4/8/8/8	-
3	VAL	C	404	-	-	1/8/8/8	-
5	IMD	A	408	-	-	-	0/1/1/1
4	GOL	A	404	-	-	1/4/4/4	-
4	GOL	B	405	-	-	2/4/4/4	-
4	GOL	C	406	-	-	3/4/4/4	-
5	IMD	A	407	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VAL	B	403	-	-	2/8/8/8	-
5	IMD	B	408	-	-	-	0/1/1/1
3	VAL	A	403	-	-	1/8/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	VAL	OXT-C	-2.09	1.24	1.30
3	A	403	VAL	OXT-C	-2.09	1.24	1.30
3	D	403	VAL	OXT-C	-2.04	1.24	1.30
3	C	404	VAL	OXT-C	-2.00	1.24	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	VAL	OXT-C-O	-3.06	117.13	124.08
3	C	404	VAL	OXT-C-O	-2.70	117.96	124.08
3	B	403	VAL	OXT-C-O	-2.66	118.05	124.08
3	D	403	VAL	OXT-C-O	-2.63	118.12	124.08
3	B	403	VAL	OXT-C-CA	2.53	122.88	114.15
3	C	404	VAL	OXT-C-CA	2.39	122.39	114.15
3	D	403	VAL	OXT-C-CA	2.18	121.65	114.15

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	406	GOL	O1-C1-C2-C3
4	B	404	GOL	O1-C1-C2-C3
4	C	405	GOL	O1-C1-C2-C3
4	C	406	GOL	O1-C1-C2-C3
4	C	406	GOL	O1-C1-C2-O2
4	A	406	GOL	C1-C2-C3-O3
4	A	406	GOL	O1-C1-C2-O2
4	A	406	GOL	O2-C2-C3-O3
4	C	405	GOL	O1-C1-C2-O2
4	B	404	GOL	O1-C1-C2-O2
4	B	405	GOL	O1-C1-C2-O2
4	A	404	GOL	O1-C1-C2-O2
3	D	403	VAL	N-CA-CB-CG1
3	D	403	VAL	N-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
3	A	403	VAL	C-CA-CB-CG2
3	B	403	VAL	C-CA-CB-CG2
3	C	404	VAL	C-CA-CB-CG2
3	D	403	VAL	C-CA-CB-CG2
4	B	405	GOL	O1-C1-C2-C3
4	C	406	GOL	C1-C2-C3-O3
3	B	403	VAL	N-CA-CB-CG1
3	D	403	VAL	C-CA-CB-CG1

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	407	IMD	2	0
4	A	406	GOL	1	0
5	C	401	IMD	1	0
4	C	405	GOL	1	0
5	B	408	IMD	1	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

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, 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	335/385 (87%)	-0.32	10 (2%) 52 57	11, 19, 39, 63	1 (0%)
1	B	335/385 (87%)	-0.29	17 (5%) 33 35	10, 18, 43, 73	1 (0%)
1	C	335/385 (87%)	0.15	13 (3%) 43 46	20, 28, 46, 74	1 (0%)
1	D	331/385 (85%)	1.31	50 (15%) 5 6	25, 39, 58, 74	17 (5%)
All	All	1336/1540 (86%)	0.21	90 (6%) 24 25	10, 26, 52, 74	20 (1%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	349	THR	14.0
1	D	360	MET	12.7
1	D	348	LEU	12.0
1	D	351	GLN	11.4
1	D	350	ASP	10.9
1	D	353	ILE	8.4
1	D	345	VAL	7.6
1	D	352	GLY	7.2
1	D	354	MET	6.8
1	D	358	ALA	6.6
1	D	357	ALA	6.3
1	D	347	ASN	6.0
1	D	344	LYS	6.0
1	D	359	HIS	5.9
1	B	109	SER	5.6
1	D	346	ARG	5.4
1	D	355	SER	5.3
1	A	110	ASN	5.2
1	A	109	SER	5.2
1	A	343	PHE	4.9
1	B	343	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	356	ARG	4.5
1	D	343	PHE	4.3
1	B	121	SER	4.3
1	B	110	ASN	4.0
1	B	120	LYS	4.0
1	C	357	ALA	3.6
1	D	186	ILE	3.4
1	C	110	ASN	3.4
1	D	18	LYS	3.3
1	D	188	TRP	3.2
1	A	120	LYS	3.2
1	C	18	LYS	3.1
1	B	358	ALA	3.1
1	D	163	LEU	3.1
1	D	177	PHE	3.0
1	A	361	GLN	3.0
1	A	18	LYS	2.9
1	B	18	LYS	2.9
1	D	19	LEU	2.9
1	D	83	PHE	2.8
1	C	361	GLN	2.7
1	D	76	GLU	2.7
1	D	192	PHE	2.7
1	D	189	LEU	2.7
1	C	120	LYS	2.7
1	C	358	ALA	2.6
1	D	96	LEU	2.6
1	A	147	ASP	2.6
1	C	359	HIS	2.6
1	D	341	LEU	2.6
1	D	108	GLN	2.5
1	B	348	LEU	2.4
1	B	361	GLN	2.4
1	D	38	ILE	2.4
1	D	215	HIS	2.4
1	A	350	ASP	2.4
1	D	196	LYS	2.4
1	C	343	PHE	2.4
1	D	187	PRO	2.4
1	D	190	ASP	2.3
1	D	63	LEU	2.3
1	C	121	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	55	LEU	2.3
1	D	182	LEU	2.3
1	B	357	ALA	2.3
1	B	352	GLY	2.2
1	B	347	ASN	2.2
1	D	36	PRO	2.2
1	C	188	TRP	2.2
1	D	91	PHE	2.2
1	A	347	ASN	2.2
1	C	360	MET	2.2
1	D	72	VAL	2.2
1	B	350	ASP	2.2
1	D	57	ALA	2.2
1	C	109	SER	2.2
1	D	69	ILE	2.1
1	C	147	ASP	2.1
1	D	92	SER	2.1
1	B	360	MET	2.1
1	A	346	ARG	2.1
1	B	344	LYS	2.1
1	D	336	CYS	2.1
1	D	195	ILE	2.1
1	D	64	THR	2.1
1	D	87	TRP	2.1
1	B	349	THR	2.0
1	B	108	GLN	2.0
1	D	105	LEU	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 oligosaccharides 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. The B-factors column lists the minimum,

median, 95th 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	B-factors(Å ²)	Q<0.9
5	IMD	A	408	5/5	0.61	0.22	38,39,40,42	5
5	IMD	B	408	5/5	0.65	0.22	24,24,29,31	5
5	IMD	C	401	5/5	0.74	0.29	23,26,28,28	5
5	IMD	C	407	5/5	0.79	0.18	37,37,39,41	5
4	GOL	A	406	6/6	0.83	0.19	28,29,30,33	6
3	VAL	D	403	8/8	0.84	0.14	38,41,45,46	0
5	IMD	B	407	5/5	0.85	0.15	26,28,31,33	5
5	IMD	A	407	5/5	0.87	0.15	29,31,35,35	5
4	GOL	B	404	6/6	0.87	0.11	23,33,37,39	0
4	GOL	B	405	6/6	0.88	0.14	19,31,38,42	0
4	GOL	C	405	6/6	0.88	0.12	36,40,41,49	0
4	GOL	A	404	6/6	0.89	0.11	26,33,34,43	0
4	GOL	C	406	6/6	0.89	0.12	27,37,46,47	0
4	GOL	A	405	6/6	0.90	0.13	23,33,39,40	0
5	IMD	B	406	5/5	0.90	0.17	26,31,34,37	5
3	VAL	C	404	8/8	0.91	0.10	22,27,29,30	0
3	VAL	A	403	8/8	0.96	0.07	18,20,24,26	0
3	VAL	B	403	8/8	0.96	0.08	16,19,21,25	0
2	MN	D	401	1/1	0.98	0.07	31,31,31,31	0
2	MN	A	401	1/1	0.99	0.03	14,14,14,14	0
2	MN	D	402	1/1	0.99	0.08	30,30,30,30	0
2	MN	A	402	1/1	1.00	0.02	13,13,13,13	0
2	MN	B	401	1/1	1.00	0.02	14,14,14,14	0
2	MN	B	402	1/1	1.00	0.04	13,13,13,13	0
2	MN	C	402	1/1	1.00	0.03	22,22,22,22	0
2	MN	C	403	1/1	1.00	0.03	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.