Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2023 – 01:12 PM EDT

PDB ID	:	4Q40
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 (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:

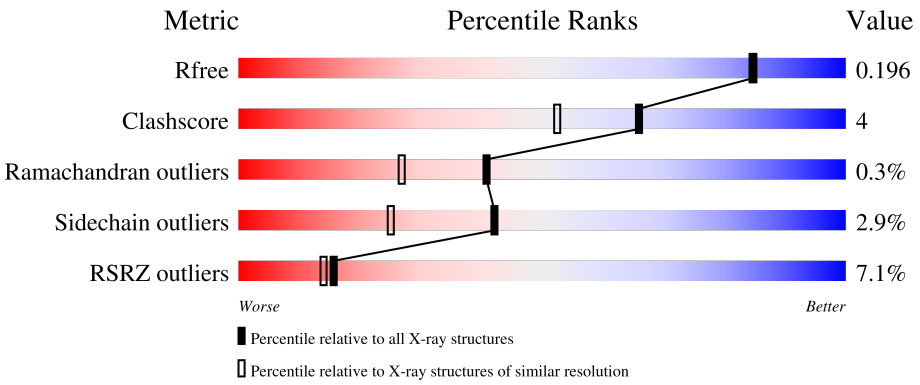
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	385	% 81% 5% 13%
1	B	385	4% 81% 6% 13%
1	C	385	3% 78% 9% • 13%
1	D	385	17% 73% 12% • 14%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	335	2574	1621	450	487	16	0	1	0
1	B	335	2574	1621	450	487	16	0	1	0
1	C	335	2574	1621	450	487	16	0	1	0
1	D	331	2539	1601	443	480	15	0	0	0

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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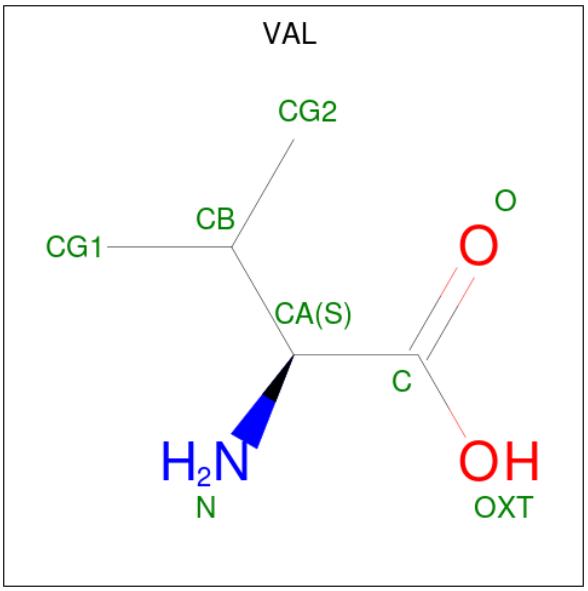
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP Q6WVP6
D	-19	GLY	-	expression tag	UNP Q6WVP6
D	-18	SER	-	expression tag	UNP Q6WVP6
D	-17	SER	-	expression tag	UNP Q6WVP6
D	-16	HIS	-	expression tag	UNP Q6WVP6
D	-15	HIS	-	expression tag	UNP Q6WVP6
D	-14	HIS	-	expression tag	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 (three-letter code: MN) (formula: Mn).

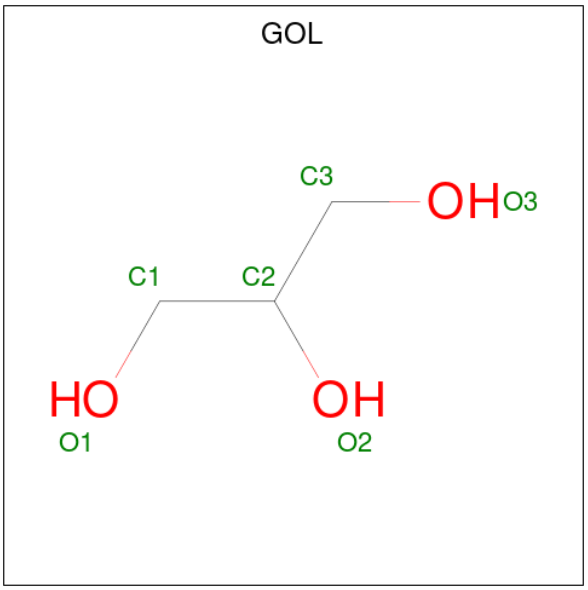
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0

- Molecule 3 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



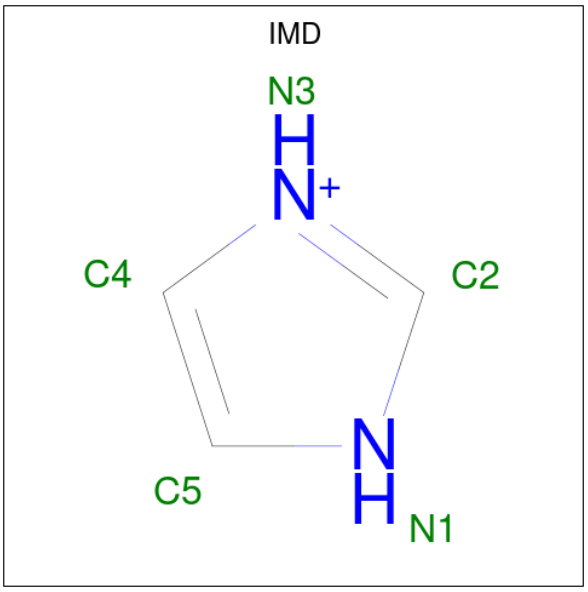
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	8	5	1	2	0	0
3	B	1	8	5	1	2	0	0
3	C	1	8	5	1	2	0	0
3	D	1	8	5	1	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



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

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

- Molecule 6 is water.

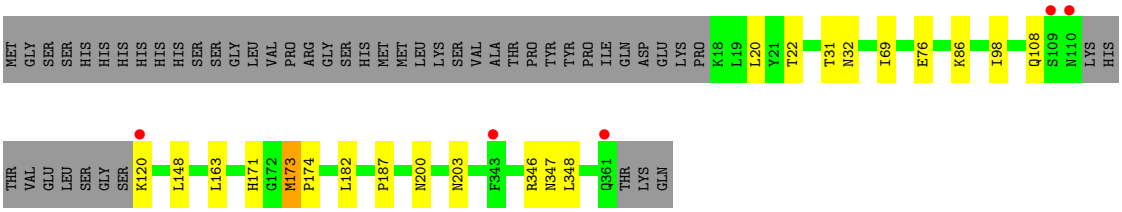
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	324	324	324	0	0
			Total	O		
6	B	315	315	315	0	0
			Total	O		
6	C	245	245	245	0	0
			Total	O		
6	D	135	135	135	0	0

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.

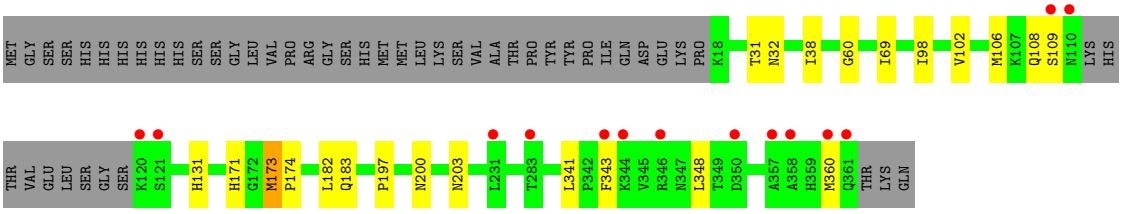
• Molecule 1: Arginase

Chain A:



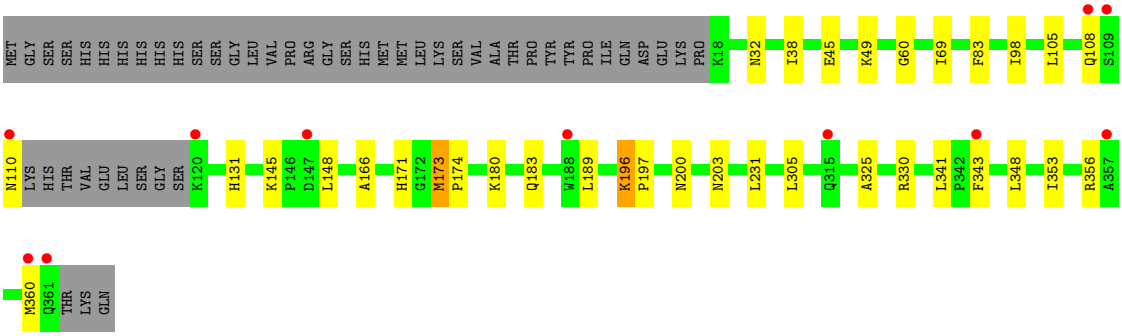
• Molecule 1: Arginase

Chain B:



• Molecule 1: Arginase

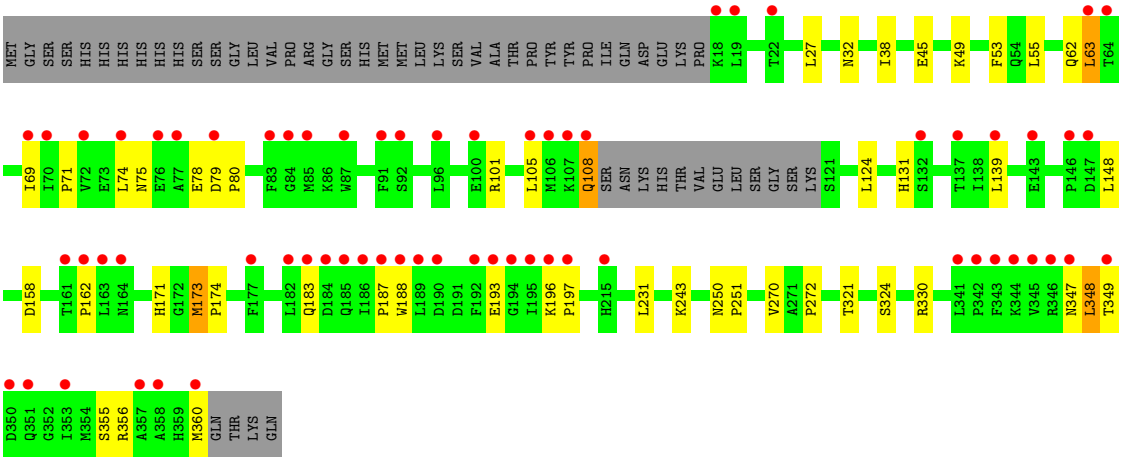
Chain C:



• Molecule 1: Arginase

Chain D:

17%
73%
12%
14%


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET MET LEU LYS SER VAL ALA THR PRO TYR TYR PRO ILE GLN ASP GLU LYS PRO K18 L19 T22 L27 N32 I38 E45 K49 F53 Q54 L55 Q62 L63 T64
I69 I70 P71 V72 E73 L74 N75 E76 A77 E78 D79 P80 F83 G84 M85 K86 W87 F91 S92 L96 E100 R101 L105 M106 K107 Q108 SER ASN LYS HIS THR VAL GLU LEU SER GLY SER LYS S121 L124 H131 S132 T137 I138 L139 E143 P146 D147 L148
D158 T161 P162 L163 N164 H171 G172 M173 P174 F177 L182 Q183 D184 Q185 I186 P187 W188 L189 D190 D191 F192 E193 G194 I195 K196 P197 H215 L231 K243 N250 P251 V270 A271 P272 T321 S324 R330 L341 P342 F343 K344 V345 R346 N347 L348 T349
D350 Q351 G352 I353 M354 S355 R356 A357 A358 H359 M360 GLN THR LYS GLN

4 Data and refinement statistics (i)

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 49.32 – 1.83	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.31-1.83) 99.9 (49.32-1.83)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 1.83Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.174 , 0.195 0.177 , 0.196	Depositor DCC
R_{free} test set	8202 reflections (5.02%)	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 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[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)

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

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	0.39	0/2624	0.54	0/3555
1	B	0.40	0/2624	0.56	0/3555
1	C	0.32	0/2624	0.49	0/3555
1	D	0.28	0/2586	0.45	0/3505
All	All	0.35	0/10458	0.51	0/14170

There are no bond length outliers.

There are no bond angle outliers.

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	14	0
1	B	2574	0	2590	10	0
1	C	2574	0	2590	24	0
1	D	2539	0	2553	32	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	83	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 (83) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:270:VAL:HG22	1:D:324:SER:HG	1.77	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:148:LEU:C	1:D:148:LEU:HD12	2.33	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:76:GLU:H	1:A:76:GLU:CD	2.14	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:148:LEU:C	1:A:148:LEU:HD12	2.35	0.46
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:148:LEU:HD12	1:C:148:LEU:C	2.37	0.46
1:C:110:ASN:HD21	1:C:145:LYS:HE3	1.81	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:110:ASN:N	1:C:110:ASN:HD22	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	332/385 (86%)	325 (98%)	6 (2%)	1 (0%)	41 27
1	B	332/385 (86%)	326 (98%)	5 (2%)	1 (0%)	41 27
1	C	332/385 (86%)	322 (97%)	9 (3%)	1 (0%)	41 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	327/385 (85%)	316 (97%)	10 (3%)	1 (0%)	41	27
All	All	1323/1540 (86%)	1289 (97%)	30 (2%)	4 (0%)	41	27

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 (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	283/327 (86%)	277 (98%)	6 (2%)	53	38
1	B	283/327 (86%)	275 (97%)	8 (3%)	43	26
1	C	283/327 (86%)	276 (98%)	7 (2%)	47	31
1	D	278/327 (85%)	267 (96%)	11 (4%)	31	14
All	All	1127/1308 (86%)	1095 (97%)	32 (3%)	42	26

All (32) 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	108	GLN
1	A	171	HIS
1	A	182	LEU
1	B	31	THR
1	B	32	ASN
1	B	108	GLN
1	B	131	HIS

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Mol	Chain	Res	Type
1	B	171	HIS
1	B	182	LEU
1	B	341	LEU
1	B	360	MET
1	C	32	ASN
1	C	131	HIS
1	C	171	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	108	GLN
1	D	124	LEU
1	D	131	HIS
1	D	171	HIS
1	D	231	LEU
1	D	243	LYS
1	D	348	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	110	ASN
1	A	203	ASN
1	A	347	ASN
1	B	81	GLN
1	B	108	GLN
1	B	110	ASN
1	B	203	ASN
1	B	361	GLN
1	C	62	GLN
1	C	81	GLN
1	C	110	ASN
1	C	203	ASN
1	C	351	GLN
1	C	359	HIS
1	D	62	GLN

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Mol	Chain	Res	Type
1	D	81	GLN
1	D	203	ASN
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 monosaccharides 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	$\#\|Z\| > 2$
5	IMD	A	408	-	3,5,5	0.42	0	4,5,5	0.59	0
5	IMD	B	407	-	3,5,5	0.38	0	4,5,5	0.59	0
4	GOL	A	406	-	5,5,5	0.46	0	5,5,5	0.26	0
4	GOL	C	405	-	5,5,5	0.37	0	5,5,5	0.46	0
4	GOL	B	404	-	5,5,5	0.42	0	5,5,5	0.47	0
5	IMD	C	401	-	3,5,5	0.38	0	4,5,5	0.52	0
4	GOL	A	404	-	5,5,5	0.35	0	5,5,5	0.64	0
4	GOL	C	406	-	5,5,5	0.33	0	5,5,5	0.33	0
5	IMD	C	407	-	3,5,5	0.44	0	4,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	VAL	C	404	-	5,7,7	0.92	0	7,9,9	1.37	2 (28%)
4	GOL	B	405	-	5,5,5	0.20	0	5,5,5	0.53	0
5	IMD	A	407	-	3,5,5	0.42	0	4,5,5	0.56	0
5	IMD	B	406	-	3,5,5	0.39	0	4,5,5	0.51	0
3	VAL	D	403	-	5,7,7	0.94	0	7,9,9	1.29	2 (28%)
4	GOL	A	405	-	5,5,5	0.27	0	5,5,5	0.35	0
5	IMD	B	408	-	3,5,5	0.36	0	4,5,5	0.67	0
3	VAL	A	403	-	5,7,7	0.96	1 (20%)	7,9,9	1.33	1 (14%)
3	VAL	B	403	-	5,7,7	1.01	1 (20%)	7,9,9	1.42	2 (28%)

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

All (2) bond length outliers are listed below:

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

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

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	403	VAL	OXT-C-O	-3.07	117.13	124.09
3	C	404	VAL	OXT-C-O	-2.70	117.96	124.09
3	B	403	VAL	OXT-C-O	-2.66	118.05	124.09
3	D	403	VAL	OXT-C-O	-2.63	118.12	124.09
3	B	403	VAL	OXT-C-CA	2.47	122.88	114.22
3	C	404	VAL	OXT-C-CA	2.34	122.39	114.22
3	D	403	VAL	OXT-C-CA	2.12	121.65	114.22

There are no chirality outliers.

All (24) 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
3	D	403	VAL	N-CA-CB-CG1
3	D	403	VAL	N-CA-CB-CG2
4	A	404	GOL	O1-C1-C2-O2
4	B	405	GOL	O1-C1-C2-C3
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	C	406	GOL	C1-C2-C3-O3
4	A	404	GOL	O1-C1-C2-C3
3	B	403	VAL	N-CA-CB-CG1
3	D	403	VAL	C-CA-CB-CG1
3	A	403	VAL	OXT-C-CA-N

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	406	GOL	1	0
4	C	405	GOL	1	0
5	C	401	IMD	1	0
5	C	407	IMD	2	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 (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	335/385 (87%)	-0.03	5 (1%)	73	73	11, 19, 39, 63	0
1	B	335/385 (87%)	0.20	14 (4%)	36	33	10, 18, 43, 73	0
1	C	335/385 (87%)	-0.01	11 (3%)	46	43	20, 28, 46, 74	0
1	D	331/385 (85%)	1.00	65 (19%)	1	1	25, 40, 71, 83	17 (5%)
All	All	1336/1540 (86%)	0.29	95 (7%)	16	14	10, 26, 53, 83	17 (1%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	188	TRP	5.6
1	B	109	SER	5.3
1	C	110	ASN	5.2
1	D	343	PHE	5.0
1	D	190	ASP	4.7
1	D	360	MET	4.7
1	D	192	PHE	4.5
1	D	18	LYS	4.5
1	C	109	SER	4.3
1	D	177	PHE	4.3
1	B	343	PHE	4.2
1	D	189	LEU	4.2
1	D	344	LYS	4.1
1	A	110	ASN	4.1
1	D	345	VAL	4.0
1	B	110	ASN	4.0
1	D	184	ASP	4.0
1	B	358	ALA	3.9
1	D	147	ASP	3.8
1	D	182	LEU	3.8
1	D	186	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	139	LEU	3.7
1	B	361	GLN	3.7
1	D	357	ALA	3.6
1	D	70	ILE	3.6
1	D	350	ASP	3.6
1	C	343	PHE	3.6
1	B	120	LYS	3.5
1	D	346	ARG	3.5
1	D	87	TRP	3.4
1	D	196	LYS	3.4
1	D	96	LEU	3.4
1	B	360	MET	3.4
1	D	84	GLY	3.3
1	D	341	LEU	3.3
1	D	92	SER	3.3
1	D	351	GLN	3.2
1	D	215	HIS	3.1
1	C	360	MET	3.1
1	D	163	LEU	3.0
1	D	194	GLY	2.9
1	D	22	THR	2.9
1	A	343	PHE	2.8
1	D	63	LEU	2.8
1	D	193	GLU	2.8
1	D	347	ASN	2.8
1	D	64	THR	2.8
1	D	185	GLN	2.8
1	D	164	ASN	2.8
1	C	120	LYS	2.8
1	D	83	PHE	2.8
1	D	108	GLN	2.8
1	D	91	PHE	2.7
1	D	69	ILE	2.7
1	B	357	ALA	2.7
1	D	100	GLU	2.7
1	C	108	GLN	2.7
1	D	195	ILE	2.6
1	D	358	ALA	2.6
1	D	137	THR	2.6
1	D	161	THR	2.6
1	A	109	SER	2.5
1	D	197	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	361	GLN	2.5
1	D	183	GLN	2.5
1	D	106	MET	2.4
1	D	72	VAL	2.4
1	D	146	PRO	2.4
1	D	187	PRO	2.4
1	D	162	PRO	2.4
1	D	107	LYS	2.4
1	C	361	GLN	2.4
1	C	315	GLN	2.3
1	A	120	LYS	2.3
1	D	76	GLU	2.3
1	B	344	LYS	2.3
1	C	357	ALA	2.3
1	D	105	LEU	2.3
1	C	147	ASP	2.3
1	D	143	GLU	2.2
1	D	342	PRO	2.2
1	C	188	TRP	2.2
1	B	121	SER	2.1
1	D	349	THR	2.1
1	D	79	ASP	2.1
1	D	85	MET	2.1
1	D	353	ILE	2.1
1	B	283	THR	2.1
1	B	346	ARG	2.0
1	D	19	LEU	2.0
1	D	74	LEU	2.0
1	B	350	ASP	2.0
1	D	132	SER	2.0
1	D	77	ALA	2.0
1	B	231	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 monosaccharides 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	0.77	0.34	38,39,40,42	5
5	IMD	C	401	5/5	0.80	0.31	23,26,28,28	5
5	IMD	B	408	5/5	0.81	0.19	24,24,29,31	5
3	VAL	D	403	8/8	0.83	0.13	38,41,45,46	0
5	IMD	C	407	5/5	0.85	0.30	37,37,39,41	5
4	GOL	A	406	6/6	0.86	0.23	28,29,30,33	6
5	IMD	B	407	5/5	0.87	0.19	26,28,31,33	5
4	GOL	B	405	6/6	0.89	0.15	19,31,38,42	0
3	VAL	C	404	8/8	0.89	0.12	22,27,29,30	0
5	IMD	A	407	5/5	0.91	0.14	29,31,35,35	5
4	GOL	A	405	6/6	0.91	0.14	23,33,39,40	0
4	GOL	C	405	6/6	0.92	0.19	36,40,41,49	0
4	GOL	C	406	6/6	0.92	0.14	27,37,46,47	0
4	GOL	B	404	6/6	0.93	0.14	23,33,37,39	0
5	IMD	B	406	5/5	0.93	0.30	26,31,34,37	5
4	GOL	A	404	6/6	0.94	0.10	26,33,34,43	0
3	VAL	A	403	8/8	0.96	0.11	18,20,24,26	0
3	VAL	B	403	8/8	0.96	0.12	16,19,21,25	0
2	MN	D	401	1/1	0.99	0.04	31,31,31,31	0
2	MN	D	402	1/1	0.99	0.04	30,30,30,30	0
2	MN	B	401	1/1	1.00	0.12	14,14,14,14	0
2	MN	B	402	1/1	1.00	0.15	13,13,13,13	0
2	MN	C	402	1/1	1.00	0.07	22,22,22,22	0
2	MN	C	403	1/1	1.00	0.07	22,22,22,22	0
2	MN	A	401	1/1	1.00	0.12	14,14,14,14	0
2	MN	A	402	1/1	1.00	0.12	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.