



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:03 PM GMT

PDB ID : 4GYR
Title : Granulibacter bethesdensis allophanate hydrolase apo
Authors : Lin, Y.; St Maurice, M.
Deposited on : 2012-09-05
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

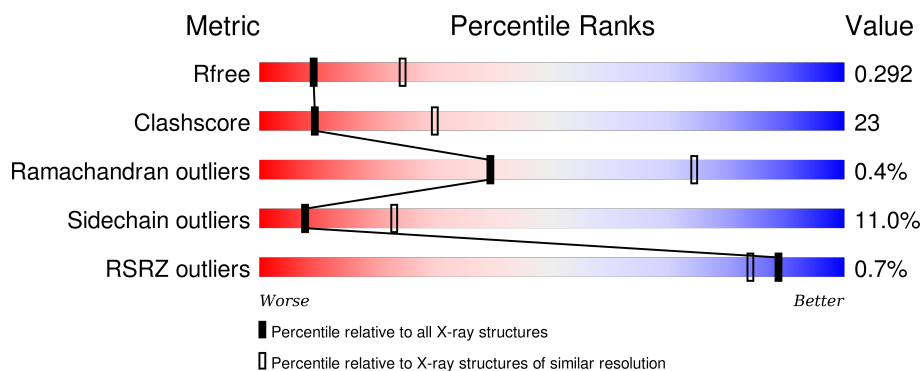
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	621	 46% 24% • 26%
1	B	621	 46% 24% • 26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6930 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 Allophanate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	11	1	0
			3404	2159	583	651	11			
1	B	461	Total	C	N	O	S	9	1	0
			3410	2165	586	648	11			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	EXPRESSION TAG	UNP Q0BRB0
A	-27	GLY	-	EXPRESSION TAG	UNP Q0BRB0
A	-26	SER	-	EXPRESSION TAG	UNP Q0BRB0
A	-25	SER	-	EXPRESSION TAG	UNP Q0BRB0
A	-24	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-23	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-22	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-21	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-20	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-19	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-18	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-17	HIS	-	EXPRESSION TAG	UNP Q0BRB0
A	-16	ASP	-	EXPRESSION TAG	UNP Q0BRB0
A	-15	TYR	-	EXPRESSION TAG	UNP Q0BRB0
A	-14	ASP	-	EXPRESSION TAG	UNP Q0BRB0
A	-13	ILE	-	EXPRESSION TAG	UNP Q0BRB0
A	-12	PRO	-	EXPRESSION TAG	UNP Q0BRB0
A	-11	THR	-	EXPRESSION TAG	UNP Q0BRB0
A	-10	SER	-	EXPRESSION TAG	UNP Q0BRB0
A	-9	GLU	-	EXPRESSION TAG	UNP Q0BRB0
A	-8	ASN	-	EXPRESSION TAG	UNP Q0BRB0
A	-7	LEU	-	EXPRESSION TAG	UNP Q0BRB0
A	-6	TYR	-	EXPRESSION TAG	UNP Q0BRB0
A	-5	PHE	-	EXPRESSION TAG	UNP Q0BRB0
A	-4	GLN	-	EXPRESSION TAG	UNP Q0BRB0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q0BRB0
A	-2	LEU	-	EXPRESSION TAG	UNP Q0BRB0
A	-1	LEU	-	EXPRESSION TAG	UNP Q0BRB0
A	0	GLN	-	EXPRESSION TAG	UNP Q0BRB0
B	-28	MET	-	EXPRESSION TAG	UNP Q0BRB0
B	-27	GLY	-	EXPRESSION TAG	UNP Q0BRB0
B	-26	SER	-	EXPRESSION TAG	UNP Q0BRB0
B	-25	SER	-	EXPRESSION TAG	UNP Q0BRB0
B	-24	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-23	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-22	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-21	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-20	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-19	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-18	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-17	HIS	-	EXPRESSION TAG	UNP Q0BRB0
B	-16	ASP	-	EXPRESSION TAG	UNP Q0BRB0
B	-15	TYR	-	EXPRESSION TAG	UNP Q0BRB0
B	-14	ASP	-	EXPRESSION TAG	UNP Q0BRB0
B	-13	ILE	-	EXPRESSION TAG	UNP Q0BRB0
B	-12	PRO	-	EXPRESSION TAG	UNP Q0BRB0
B	-11	THR	-	EXPRESSION TAG	UNP Q0BRB0
B	-10	SER	-	EXPRESSION TAG	UNP Q0BRB0
B	-9	GLU	-	EXPRESSION TAG	UNP Q0BRB0
B	-8	ASN	-	EXPRESSION TAG	UNP Q0BRB0
B	-7	LEU	-	EXPRESSION TAG	UNP Q0BRB0
B	-6	TYR	-	EXPRESSION TAG	UNP Q0BRB0
B	-5	PHE	-	EXPRESSION TAG	UNP Q0BRB0
B	-4	GLN	-	EXPRESSION TAG	UNP Q0BRB0
B	-3	GLY	-	EXPRESSION TAG	UNP Q0BRB0
B	-2	LEU	-	EXPRESSION TAG	UNP Q0BRB0
B	-1	LEU	-	EXPRESSION TAG	UNP Q0BRB0
B	0	GLN	-	EXPRESSION TAG	UNP Q0BRB0

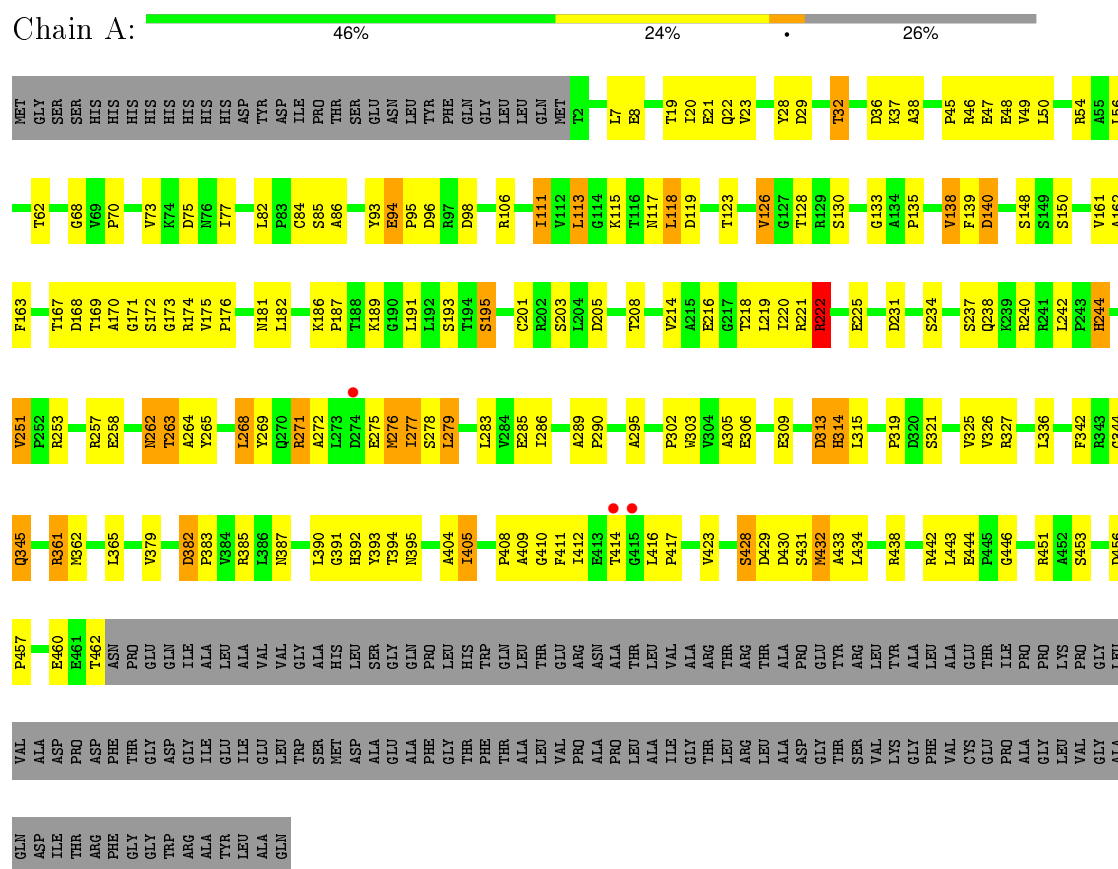
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	65	Total O 65 65	0	0
2	B	51	Total O 51 51	0	0

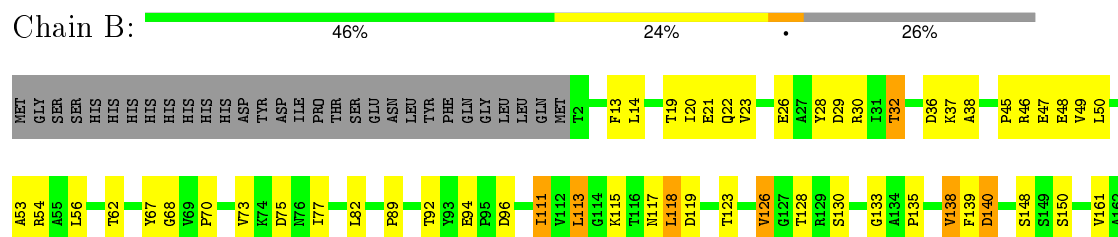
3 Residue-property plots

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: Allophanate hydrolase



• Molecule 1: Allophanate hydrolase



VAL	GLY	ALA	GLN	ASP	ILE	THR	ARG	PHE	GLY	GLY	TRP	ARG	S453	Q345	R253	F163
													GLY	D456	L351	T257
VAL	LEU	VAL	ALA	ASP	THR	PHE	GLY	GLY	ASP	GLY	ILE	ALA	P457	L351	R257	D168
													GLY	T258	T169	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	Q354	T260	T170	F171
													GLY	E261	G261	G171
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	S461	G362	T262	S172
													GLY	T462	T263	G173
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	ASN	L365	T264	R174
													GLY	P379	T265	V175
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	D382	V379	T268	P176
													GLY	ILE	T269	A177
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	P383	D382	T271	F178
													GLY	ILE	T272	A179
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	V384	A272	T273	N180
													GLY	ILE	T274	N181
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	L386	T274	T275	L182
													GLY	ILE	T276	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	N387	E275	T276	K186
													GLY	ILE	T277	P187
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	L390	S278	T278	
													GLY	ILE	T279	L191
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	H392	T280	T281	L192
													GLY	ILE	T282	L193
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	T394	A281	T283	S193
													GLY	ILE	T284	S195
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	N395	L283	T283	
													GLY	ILE	T284	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	A404	T284	T284	C201
													GLY	ILE	T285	S202
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	L405	T285	T286	S203
													GLY	ILE	T286	L204
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	P408	T288	T289	D205
													GLY	ILE	T290	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	A409	T289	T290	
													GLY	ILE	T290	T208
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	G410	T291	T291	V214
													GLY	ILE	T292	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	F411	T292	T292	T218
													GLY	ILE	T293	L219
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	A423	T293	T293	L220
													GLY	ILE	T294	R221
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA		E309	T294	E222
													GLY	ILE	T295	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	S428	D313	T295	E225
													GLY	ILE	T296	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	D429	H314	T296	D231
													GLY	ILE	T297	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	S431	L315	T297	
													GLY	ILE	T298	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	A432	T299	T298	S234
													GLY	ILE	T299	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	L434	D320	T299	S237
													GLY	ILE	T300	Q238
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	R438	T301	T300	R239
													GLY	ILE	T302	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	L443	T303	T301	R240
													GLY	ILE	T304	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	E444	T304	T302	S237
													GLY	ILE	T305	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	P445	T305	T303	Q238
													GLY	ILE	T306	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	G446	T306	T304	R240
													GLY	ILE	T307	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	P400	T307	T305	S237
													GLY	ILE	T308	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	R451	T308	T306	R239
													GLY	ILE	T309	
VAL	THR	ARG	PHE	GLY	GLY	TRP	GLY	GLY	ASP	GLY	ILE	ALA	L453	T309	T307	R240
													GLY	ILE	T310	

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	78.09 Å 78.09 Å 397.54 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.05 – 2.80 40.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.05-2.80) 99.9 (40.05-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.99 (at 2.81 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.256 , 0.307 0.243 , 0.292	Depositor DCC
R_{free} test set	2025 reflections (6.05%)	DCC
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 33510 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6930	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	1/3478 (0.0%)	0.52	3/4752 (0.1%)
1	B	0.31	1/3484 (0.0%)	0.52	2/4757 (0.0%)
All	All	0.32	2/6962 (0.0%)	0.52	5/9509 (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
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	GLU	CD-OE1	-8.74	1.16	1.25
1	A	460	GLU	CD-OE1	-8.44	1.16	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	A	222	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	460	GLU	CG-CD-OE1	-5.73	106.84	118.30
1	B	460	GLU	CG-CD-OE1	-5.68	106.94	118.30
1	A	460	GLU	CG-CD-OE2	5.02	128.33	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	ASN	Peptide
1	B	262	ASN	Peptide

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	3404	0	3333	157	0
1	B	3410	0	3347	149	1
2	A	65	0	0	23	1
2	B	51	0	0	10	0
All	All	6930	0	6680	305	1

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 23.

All (305) 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:411:PHE:CE1	1:B:417:PRO:HB3	1.64	1.32
1:B:411:PHE:CE2	1:B:451:ARG:HD2	1.73	1.24
1:A:411:PHE:CE2	1:A:451:ARG:HD2	1.74	1.21
1:B:411:PHE:HE2	1:B:451:ARG:CD	1.54	1.20
1:A:218:THR:CG2	1:A:222:ARG:HH12	1.57	1.17
1:B:218:THR:CG2	1:B:222:ARG:HH12	1.57	1.16
1:A:218:THR:HG22	1:A:222:ARG:NH1	1.63	1.14
1:B:411:PHE:HD1	1:B:417:PRO:HA	1.17	1.09
1:A:411:PHE:CE1	1:A:417:PRO:HB3	1.87	1.09
1:B:411:PHE:HE2	1:B:451:ARG:HD2	0.92	1.08
1:B:218:THR:HG22	1:B:222:ARG:NH1	1.69	1.05
1:B:411:PHE:HE1	1:B:417:PRO:CB	1.69	1.03
1:A:218:THR:HG22	1:A:222:ARG:HH12	1.15	0.98
1:A:411:PHE:HE2	1:A:451:ARG:HD2	1.17	0.98
1:A:75:ASP:O	2:A:619:HOH:O	1.84	0.94
1:B:411:PHE:CD1	1:B:417:PRO:HA	2.01	0.94
1:B:218:THR:HG22	1:B:222:ARG:HH12	1.25	0.93
1:B:244:HIS:CD2	1:B:434:LEU:HD23	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:O	2:A:646:HOH:O	1.88	0.90
1:A:327:ARG:NE	2:A:663:HOH:O	2.06	0.89
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.39	0.88
1:B:411:PHE:CE1	1:B:417:PRO:CB	2.50	0.87
1:A:382:ASP:OD2	1:A:385:ARG:NH1	2.07	0.87
1:A:244:HIS:CD2	1:A:434:LEU:HD23	2.10	0.87
1:B:411:PHE:CE2	1:B:451:ARG:CD	2.46	0.86
1:B:244:HIS:HD2	1:B:434:LEU:HD23	1.42	0.84
1:B:382:ASP:OD2	1:B:385:ARG:NH1	2.11	0.84
1:B:218:THR:CG2	1:B:222:ARG:NH1	2.31	0.84
1:A:410:GLY:O	1:A:411:PHE:HD1	1.63	0.82
1:A:390:LEU:O	2:A:625:HOH:O	1.97	0.82
1:A:138:VAL:HG23	1:A:139:PHE:CE2	2.15	0.82
1:B:411:PHE:HE1	1:B:417:PRO:HB3	0.75	0.81
1:A:138:VAL:HG23	1:A:139:PHE:CD2	2.16	0.80
1:B:169:THR:HG21	1:B:201:CYS:HB2	1.62	0.80
1:A:169:THR:HG21	1:A:201:CYS:HB2	1.62	0.80
1:B:411:PHE:HD2	1:B:451:ARG:CZ	1.94	0.80
1:A:411:PHE:CE2	1:A:451:ARG:CD	2.63	0.79
1:A:140:ASP:OD2	2:A:611:HOH:O	1.99	0.79
1:A:85:SER:N	2:A:619:HOH:O	2.16	0.79
1:A:216:GLU:OE2	2:A:603:HOH:O	1.99	0.78
1:B:138:VAL:HG23	1:B:139:PHE:CE2	2.18	0.78
1:A:218:THR:CG2	1:A:222:ARG:NH1	2.31	0.78
1:B:138:VAL:HG23	1:B:139:PHE:CD2	2.19	0.78
1:A:411:PHE:CD1	1:A:417:PRO:HA	2.19	0.77
1:B:390:LEU:O	2:B:616:HOH:O	2.03	0.77
1:A:313:ASP:N	1:A:313:ASP:OD1	2.17	0.76
1:A:221:ARG:NH1	1:A:225:GLU:OE1	2.18	0.76
1:B:221:ARG:NH1	1:B:225:GLU:OE1	2.19	0.76
1:B:411:PHE:CD2	1:B:451:ARG:CZ	2.69	0.76
1:A:244:HIS:HD2	1:A:434:LEU:HD23	1.51	0.76
1:B:47:GLU:OE2	1:B:54:ARG:NH2	2.18	0.75
1:B:222:ARG:HG3	1:B:222:ARG:HH11	1.50	0.75
1:B:313:ASP:N	1:B:313:ASP:OD1	2.17	0.74
1:A:29:ASP:OD1	1:A:46:ARG:NH2	2.21	0.73
1:A:411:PHE:HE1	1:A:417:PRO:HB3	1.52	0.73
1:A:117:ASN:O	2:A:635:HOH:O	2.07	0.72
1:B:29:ASP:OD1	1:B:46:ARG:NH2	2.21	0.72
1:B:411:PHE:CD1	1:B:417:PRO:CA	2.71	0.72
1:A:244:HIS:HD2	1:A:434:LEU:CD2	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:NH2	1:A:409:ALA:O	2.23	0.71
1:A:47:GLU:HG3	2:A:616:HOH:O	1.90	0.71
1:A:410:GLY:O	1:A:411:PHE:CD1	2.43	0.71
1:B:271:ARG:NH2	1:B:409:ALA:O	2.24	0.70
1:B:148:SER:H	1:B:172:SER:HB3	1.57	0.70
1:A:411:PHE:CE1	1:A:417:PRO:CB	2.70	0.70
1:B:222:ARG:CG	1:B:222:ARG:HH11	2.06	0.69
1:A:148:SER:H	1:A:172:SER:HB3	1.56	0.69
1:B:244:HIS:HD2	1:B:434:LEU:CD2	2.06	0.69
1:A:20:ILE:HG12	1:A:68:GLY:HA3	1.75	0.68
1:A:36:ASP:OD2	2:A:608:HOH:O	2.11	0.68
1:B:20:ILE:HG12	1:B:68:GLY:HA3	1.75	0.67
1:B:262:ASN:ND2	1:B:265:TYR:CG	2.63	0.67
1:A:168:ASP:HB2	1:A:208:THR:HG21	1.77	0.67
1:A:411:PHE:HD2	1:A:451:ARG:NH1	1.93	0.66
1:A:262:ASN:ND2	1:A:265:TYR:CG	2.63	0.66
1:A:309:GLU:OE1	2:A:622:HOH:O	2.14	0.66
1:A:222:ARG:HH11	1:A:222:ARG:CG	2.07	0.66
1:A:218:THR:HG21	1:A:222:ARG:HH12	1.59	0.65
1:B:117:ASN:O	2:B:602:HOH:O	2.14	0.65
1:A:231:ASP:OD2	2:A:631:HOH:O	2.15	0.65
1:A:453:SER:OG	2:A:660:HOH:O	2.13	0.64
1:A:126:VAL:HG11	1:A:379:VAL:HG11	1.80	0.64
1:B:168:ASP:HB2	1:B:208:THR:HG21	1.79	0.64
1:A:411:PHE:CD2	1:A:451:ARG:NH1	2.66	0.63
1:B:411:PHE:CE2	1:B:451:ARG:NE	2.66	0.62
1:A:314:HIS:ND1	2:A:662:HOH:O	2.31	0.62
1:B:126:VAL:HG11	1:B:379:VAL:HG11	1.80	0.62
1:A:244:HIS:CD2	1:A:434:LEU:CD2	2.81	0.62
1:B:13:PHE:HD2	1:B:14:LEU:HD23	1.64	0.62
1:B:218:THR:HG21	1:B:222:ARG:HH12	1.60	0.61
1:B:135:PRO:HG2	1:B:150:SER:HB2	1.82	0.61
1:B:411:PHE:HE2	1:B:451:ARG:NE	1.97	0.61
1:A:411:PHE:HD1	1:A:417:PRO:HA	1.64	0.60
1:B:309:GLU:OE1	2:B:628:HOH:O	2.16	0.60
1:A:56:LEU:HD12	1:A:111:ILE:HD11	1.83	0.60
1:B:56:LEU:HD12	1:B:111:ILE:HD11	1.84	0.60
1:A:135:PRO:HG2	1:A:150:SER:HB2	1.84	0.60
1:B:444:GLU:OE2	1:B:451:ARG:NE	2.32	0.59
1:B:203:SER:OG	1:B:306:GLU:OE1	2.19	0.59
1:A:203:SER:OG	1:A:306:GLU:OE1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:OE2	1:A:54:ARG:NH1	2.35	0.59
1:A:442:ARG:NE	2:A:646:HOH:O	2.13	0.59
1:A:162:ALA:O	2:A:602:HOH:O	2.17	0.59
1:B:231:ASP:OD2	2:B:621:HOH:O	2.17	0.58
1:B:221:ARG:NH2	1:B:430:ASP:OD1	2.36	0.58
1:B:21:GLU:OE2	1:B:54:ARG:NH1	2.36	0.58
1:B:36:ASP:OD2	2:B:608:HOH:O	2.17	0.58
1:B:342:PHE:HA	1:B:345:GLN:HG3	1.85	0.58
1:A:119:ASP:HB2	1:A:148:SER:HB2	1.84	0.58
1:B:351:LEU:HA	1:B:354:GLN:HE21	1.69	0.58
1:A:45:PRO:HB2	1:A:48:GLU:HB2	1.86	0.58
1:A:444:GLU:OE2	1:A:451:ARG:NE	2.32	0.57
1:B:181:ASN:OD1	1:B:408:PRO:HB3	2.05	0.57
1:A:221:ARG:NH2	1:A:430:ASP:OD1	2.38	0.57
1:B:45:PRO:HB2	1:B:48:GLU:HB2	1.85	0.57
1:A:244:HIS:ND1	1:A:244:HIS:N	2.53	0.57
1:B:119:ASP:HB2	1:B:148:SER:HB2	1.85	0.57
1:B:277:ILE:HG12	1:B:278:SER:N	2.20	0.57
1:A:279:LEU:HG	1:B:37:LYS:CD	2.34	0.57
1:B:19:THR:N	1:B:22:GLN:OE1	2.38	0.57
1:A:148:SER:H	1:A:172:SER:CB	2.18	0.57
1:A:123:THR:HB	1:A:326:VAL:HG22	1.87	0.56
1:A:181:ASN:OD1	1:A:408:PRO:HB3	2.05	0.56
1:B:148:SER:H	1:B:172:SER:CB	2.18	0.56
1:A:70:PRO:HB2	1:A:113:LEU:HD21	1.87	0.56
1:B:70:PRO:HB2	1:B:113:LEU:HD21	1.87	0.56
1:A:411:PHE:CD2	1:A:451:ARG:CZ	2.89	0.56
1:A:342:PHE:HA	1:A:345:GLN:HG3	1.86	0.56
1:B:244:HIS:CD2	1:B:434:LEU:CD2	2.83	0.56
1:B:28:TYR:O	1:B:32:THR:OG1	2.23	0.55
1:B:231:ASP:HB3	1:B:234:SER:HB2	1.88	0.55
1:B:56:LEU:O	1:B:67:TYR:OH	2.15	0.55
1:A:272:ALA:O	1:A:276:MET:HB2	2.07	0.55
1:A:231:ASP:HB3	1:A:234:SER:HB2	1.87	0.55
1:A:86:ALA:N	2:A:619:HOH:O	2.23	0.55
1:A:262:ASN:ND2	1:A:265:TYR:H	2.04	0.55
1:B:262:ASN:ND2	1:B:265:TYR:H	2.04	0.55
1:B:392:HIS:O	1:B:392:HIS:ND1	2.39	0.55
1:B:26:GLU:OE2	2:B:603:HOH:O	2.18	0.54
1:B:411:PHE:CD2	1:B:451:ARG:NH1	2.75	0.54
1:A:277:ILE:HG12	1:A:278:SER:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ALA:O	1:B:276:MET:HB2	2.07	0.54
1:B:123:THR:HB	1:B:326:VAL:HG22	1.88	0.54
1:A:19:THR:N	1:A:22:GLN:OE1	2.38	0.54
1:B:89:PRO:O	1:B:92:THR:OG1	2.18	0.54
1:B:351:LEU:HD23	1:B:354:GLN:NE2	2.23	0.54
1:A:75:ASP:HA	1:A:115:LYS:HE2	1.91	0.53
1:A:49:VAL:HG11	1:A:113:LEU:HD12	1.90	0.53
1:B:49:VAL:HG11	1:B:113:LEU:HD12	1.91	0.53
1:B:262:ASN:ND2	1:B:265:TYR:CD1	2.77	0.53
1:B:285:GLU:O	1:B:361:ARG:NH2	2.41	0.53
1:B:75:ASP:HA	1:B:115:LYS:HE2	1.91	0.53
1:B:126:VAL:HB	1:B:128:THR:HG23	1.89	0.53
1:A:285:GLU:O	1:A:361:ARG:NH2	2.41	0.53
1:A:126:VAL:HB	1:A:128:THR:HG23	1.91	0.53
1:A:163:PHE:CG	1:A:220:ILE:HD13	2.44	0.53
1:A:28:TYR:O	1:A:32:THR:OG1	2.22	0.53
1:A:325:VAL:HG21	1:A:383:PRO:HB2	1.90	0.52
1:A:262:ASN:ND2	1:A:265:TYR:CD1	2.77	0.52
1:B:163:PHE:CG	1:B:220:ILE:HD13	2.44	0.52
1:A:45:PRO:O	1:A:49:VAL:HG23	2.11	0.52
1:A:412:ILE:HG12	1:A:416:LEU:O	2.10	0.52
1:B:244:HIS:ND1	1:B:244:HIS:N	2.58	0.51
1:B:240:ARG:O	1:B:428:SER:HA	2.11	0.51
1:B:45:PRO:O	1:B:49:VAL:HG23	2.11	0.51
1:A:302:PRO:HA	1:A:336:LEU:HD13	1.93	0.51
1:B:263:THR:OG1	1:B:264:ALA:N	2.44	0.51
1:B:302:PRO:HA	1:B:336:LEU:HD13	1.93	0.51
1:A:20:ILE:HD13	1:A:56:LEU:HB3	1.92	0.50
1:B:412:ILE:HG12	1:B:416:LEU:O	2.11	0.50
1:B:169:THR:OG1	1:B:205:ASP:OD1	2.29	0.50
1:A:73:VAL:HG13	1:A:77:ILE:HB	1.93	0.50
1:A:263:THR:OG1	1:A:264:ALA:N	2.43	0.50
1:B:20:ILE:HD13	1:B:56:LEU:HB3	1.92	0.50
1:B:411:PHE:HD2	1:B:451:ARG:NH1	2.09	0.50
1:B:119:ASP:HB2	1:B:148:SER:CB	2.42	0.49
1:A:414:THR:HG22	2:A:611:HOH:O	2.11	0.49
1:A:119:ASP:HB2	1:A:148:SER:CB	2.42	0.49
1:A:47:GLU:HA	1:A:47:GLU:OE1	2.11	0.49
1:B:289:ALA:N	1:B:290:PRO:HD2	2.27	0.49
1:A:289:ALA:N	1:A:290:PRO:HD2	2.27	0.49
1:B:73:VAL:HG13	1:B:77:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:PHE:CE1	1:B:417:PRO:CA	2.94	0.48
1:B:258:GLU:N	1:B:393:TYR:OH	2.47	0.48
1:A:169:THR:OG1	1:A:205:ASP:OD1	2.29	0.48
1:A:139:PHE:O	1:A:140:ASP:HB2	2.14	0.48
1:B:325:VAL:HG21	1:B:383:PRO:HB2	1.95	0.48
1:A:258:GLU:N	1:A:393:TYR:OH	2.47	0.48
1:A:38:ALA:O	1:A:135:PRO:HG3	2.14	0.48
1:A:73:VAL:CG1	1:A:77:ILE:HB	2.44	0.48
1:A:410:GLY:C	1:A:411:PHE:CD1	2.87	0.47
1:B:38:ALA:O	1:B:135:PRO:HG3	2.15	0.47
1:B:73:VAL:CG1	1:B:77:ILE:HB	2.44	0.47
1:B:170:ALA:O	1:B:174:ARG:NH2	2.47	0.47
1:B:444:GLU:O	1:B:446:GLY:N	2.41	0.47
1:A:391:GLY:HA2	1:A:394:THR:OG1	2.14	0.47
1:A:170:ALA:O	1:A:174:ARG:NH2	2.48	0.47
1:B:139:PHE:O	1:B:140:ASP:HB2	2.13	0.46
1:A:49:VAL:HG11	1:A:113:LEU:CD1	2.45	0.46
1:A:168:ASP:HB2	1:A:208:THR:CG2	2.44	0.46
1:B:49:VAL:HG11	1:B:113:LEU:CD1	2.45	0.46
1:B:193:SER:OG	1:B:195:SER:HB2	2.16	0.46
1:B:391:GLY:HA2	1:B:394:THR:OG1	2.15	0.46
1:A:37:LYS:O	2:A:615:HOH:O	2.21	0.46
1:B:271:ARG:O	1:B:275:GLU:HG2	2.16	0.46
1:A:258:GLU:HB3	1:A:392:HIS:NE2	2.31	0.46
1:A:271:ARG:O	1:A:275:GLU:HG2	2.16	0.46
1:A:8:GLU:HG2	2:A:604:HOH:O	2.15	0.46
1:B:222:ARG:HG3	1:B:222:ARG:NH1	2.23	0.46
1:A:411:PHE:CD1	1:A:417:PRO:CA	2.94	0.46
1:B:175:VAL:HB	1:B:176:PRO:HD3	1.98	0.46
1:B:167:THR:O	1:B:172:SER:HB2	2.15	0.45
1:A:193:SER:OG	1:A:195:SER:HB2	2.15	0.45
1:B:113:LEU:HD23	1:B:161:VAL:HG12	1.97	0.45
1:A:138:VAL:CG2	1:A:139:PHE:CE2	2.95	0.45
1:A:167:THR:O	1:A:172:SER:HB2	2.15	0.45
1:A:113:LEU:HD13	1:A:113:LEU:N	2.32	0.45
1:A:242:LEU:O	1:A:244:HIS:CE1	2.69	0.45
1:A:19:THR:O	1:A:23:VAL:HG23	2.17	0.45
1:A:171:GLY:HA2	1:A:174:ARG:NH2	2.32	0.45
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.18	0.45
1:B:434:LEU:HD11	1:B:438:ARG:HE	1.82	0.45
1:A:113:LEU:HD23	1:A:161:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LYS:HE3	1:B:187:PRO:O	2.16	0.45
1:A:315:LEU:O	1:A:319:PRO:HB3	2.17	0.45
1:B:262:ASN:ND2	1:B:265:TYR:CB	2.80	0.45
1:B:113:LEU:HD13	1:B:113:LEU:N	2.32	0.45
1:A:175:VAL:HB	1:A:176:PRO:HD3	1.99	0.45
1:A:442:ARG:NH1	1:A:442:ARG:O	2.49	0.45
1:B:171:GLY:HA2	1:B:174:ARG:NH2	2.32	0.45
1:A:214:VAL:HG11	1:A:433:ALA:O	2.17	0.45
1:A:434:LEU:HD11	1:A:438:ARG:HE	1.82	0.44
1:A:262:ASN:ND2	1:A:265:TYR:CB	2.81	0.44
1:A:444:GLU:O	1:A:446:GLY:N	2.40	0.44
1:B:201:CYS:HA	1:B:306:GLU:HB2	1.99	0.44
1:A:7:LEU:N	2:A:603:HOH:O	2.49	0.44
1:A:186:LYS:HE3	1:A:187:PRO:O	2.17	0.44
1:A:201:CYS:HA	1:A:306:GLU:HB2	1.99	0.44
1:A:456:ASP:HB3	1:A:457:PRO:HA	1.99	0.44
1:B:268:LEU:HA	1:B:268:LEU:HD22	1.66	0.44
1:B:365:LEU:HB3	1:B:423:VAL:HB	2.00	0.44
1:A:362:MET:SD	1:A:365:LEU:HD13	2.58	0.44
1:A:365:LEU:HB3	1:A:423:VAL:HB	2.00	0.44
1:A:409:ALA:HB1	1:A:443:LEU:HD23	2.00	0.44
1:B:302:PRO:HG3	1:B:344:GLY:HA3	2.00	0.44
1:A:240:ARG:O	1:A:428:SER:HA	2.17	0.44
1:A:189:LYS:HG2	2:A:633:HOH:O	2.18	0.44
1:B:456:ASP:HB3	1:B:457:PRO:HA	1.99	0.43
1:B:258:GLU:CG	1:B:260:TYR:CE2	3.01	0.43
1:A:8:GLU:N	2:A:603:HOH:O	2.09	0.43
1:B:303:TRP:C	1:B:305:ALA:H	2.21	0.43
1:B:453:SER:OG	2:B:651:HOH:O	2.21	0.43
1:B:168:ASP:HB2	1:B:208:THR:CG2	2.46	0.43
1:B:362:MET:SD	1:B:365:LEU:HD13	2.58	0.43
1:B:409:ALA:HB1	1:B:443:LEU:HD23	2.01	0.43
1:A:168:ASP:OD2	1:A:173:GLY:N	2.49	0.43
1:A:82:LEU:HD13	1:A:115:LYS:HG2	2.01	0.43
1:A:251:VAL:O	1:A:286:ILE:HG13	2.18	0.43
1:B:258:GLU:HG3	1:B:260:TYR:CE2	2.54	0.43
1:B:428:SER:O	1:B:432:MET:HB2	2.19	0.43
1:B:214:VAL:HG11	1:B:433:ALA:O	2.18	0.43
1:A:303:TRP:C	1:A:305:ALA:H	2.23	0.42
1:B:404:ALA:C	1:B:405:ILE:HG13	2.38	0.42
1:A:404:ALA:C	1:A:405:ILE:HG13	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LEU:O	1:B:319:PRO:HB3	2.20	0.42
1:B:251:VAL:O	1:B:286:ILE:HG13	2.19	0.42
1:A:302:PRO:HG3	1:A:344:GLY:HA3	2.00	0.42
1:A:271:ARG:HE	1:A:271:ARG:HB3	1.39	0.42
1:B:168:ASP:OD2	1:B:173:GLY:N	2.48	0.42
1:B:262:ASN:HD22	1:B:265:TYR:CB	2.33	0.42
1:A:251:VAL:HG12	1:A:269:TYR:OH	2.19	0.42
1:B:253:ARG:O	1:B:257:ARG:HG3	2.20	0.42
1:B:182:LEU:O	1:B:408:PRO:HD3	2.19	0.42
1:B:19:THR:O	1:B:23:VAL:HG23	2.20	0.42
1:A:118:LEU:O	1:A:130:SER:HB2	2.20	0.42
1:A:98:ASP:OD1	1:A:106:ARG:NH1	2.52	0.42
1:B:258:GLU:HG3	1:B:260:TYR:CD2	2.54	0.42
1:A:268:LEU:HD22	1:A:268:LEU:HA	1.70	0.42
1:A:182:LEU:O	1:A:408:PRO:HD3	2.19	0.42
1:B:138:VAL:HG22	1:B:180:ASN:OD1	2.20	0.41
1:B:82:LEU:HD13	1:B:115:LYS:HG2	2.02	0.41
1:A:295:ALA:HB1	1:A:395:ASN:HB2	2.02	0.41
1:B:295:ALA:HB1	1:B:395:ASN:HB2	2.02	0.41
1:A:253:ARG:O	1:A:257:ARG:HG3	2.21	0.41
1:B:20:ILE:HG22	1:B:53:ALA:HB1	2.03	0.41
1:B:411:PHE:CE2	1:B:451:ARG:CZ	3.01	0.41
1:B:258:GLU:HB3	1:B:392:HIS:NE2	2.35	0.41
1:A:94:GLU:HA	1:A:95:PRO:HD2	1.85	0.41
1:A:262:ASN:HD22	1:A:265:TYR:CB	2.33	0.41
1:A:428:SER:O	1:A:432:MET:HB2	2.20	0.41
1:B:30:ARG:O	2:B:644:HOH:O	2.22	0.41
1:B:118:LEU:O	1:B:130:SER:HB2	2.21	0.41
1:B:409:ALA:HB2	1:B:420:VAL:HG22	2.02	0.41
1:B:262:ASN:HD22	1:B:265:TYR:HB2	1.86	0.41
1:A:411:PHE:HE1	1:A:417:PRO:CB	2.25	0.40
1:A:242:LEU:O	1:A:244:HIS:HE1	2.04	0.40
1:A:277:ILE:C	1:A:279:LEU:H	2.25	0.40
1:B:178:ALA:HA	2:B:617:HOH:O	2.20	0.40
1:A:117:ASN:ND2	1:A:133:GLY:O	2.54	0.40
1:A:262:ASN:HD22	1:A:265:TYR:HB2	1.87	0.40
1:B:386:LEU:HD12	1:B:386:LEU:HA	1.81	0.40
1:B:245:VAL:O	2:B:645:HOH:O	2.22	0.40
1:B:117:ASN:ND2	1:B:133:GLY:O	2.54	0.40
1:A:432:MET:HE3	1:A:432:MET:HB3	1.94	0.40
1:A:84:CYS:HB3	1:A:93:TYR:CE1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:LEU:O	2:A:661:HOH:O[1_565]	2.03	0.17

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	460/621 (74%)	429 (93%)	29 (6%)	2 (0%)	39 74
1	B	460/621 (74%)	428 (93%)	30 (6%)	2 (0%)	39 74
All	All	920/1242 (74%)	857 (93%)	59 (6%)	4 (0%)	39 74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	THR
1	B	263	THR
1	A	140	ASP
1	B	140	ASP

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	340/482 (70%)	303 (89%)	37 (11%)	8 23
1	B	340/482 (70%)	302 (89%)	38 (11%)	7 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	680/964 (70%)	605 (89%)	75 (11%)	8 23

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	50	LEU
1	A	62	THR
1	A	94	GLU
1	A	96	ASP
1	A	111	ILE
1	A	113	LEU
1	A	118	LEU
1	A	126	VAL
1	A	138	VAL
1	A	191	LEU
1	A	195	SER
1	A	219	LEU
1	A	222	ARG
1	A	237	SER
1	A	238	GLN
1	A	244	HIS
1	A	251	VAL
1	A	268	LEU
1	A	271	ARG
1	A	276	MET
1	A	277	ILE
1	A	279	LEU
1	A	283	LEU
1	A	313	ASP
1	A	314	HIS
1	A	321	SER
1	A	345	GLN
1	A	361	ARG
1	A	382	ASP
1	A	387	ASN
1	A	405	ILE
1	A	428	SER
1	A	429	ASP
1	A	431	SER
1	A	432	MET
1	A	462	THR

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Mol	Chain	Res	Type
1	B	32	THR
1	B	50	LEU
1	B	62	THR
1	B	94	GLU
1	B	96	ASP
1	B	111	ILE
1	B	113	LEU
1	B	118	LEU
1	B	126	VAL
1	B	138	VAL
1	B	191	LEU
1	B	195	SER
1	B	219	LEU
1	B	222	ARG
1	B	237	SER
1	B	238	GLN
1	B	244	HIS
1	B	251	VAL
1	B	268	LEU
1	B	271	ARG
1	B	276	MET
1	B	277	ILE
1	B	279	LEU
1	B	283	LEU
1	B	313	ASP
1	B	314	HIS
1	B	321	SER
1	B	345	GLN
1	B	361	ARG
1	B	382	ASP
1	B	387	ASN
1	B	392	HIS
1	B	405	ILE
1	B	429	ASP
1	B	431	SER
1	B	432	MET
1	B	460	GLU
1	B	462	THR

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	244	HIS
1	A	354	GLN
1	B	244	HIS
1	B	354	GLN
1	B	440	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	461/621 (74%)	-0.31	3 (0%) 89 84	25, 40, 59, 73	9 (1%)
1	B	461/621 (74%)	-0.32	3 (0%) 89 84	25, 41, 59, 74	8 (1%)
All	All	922/1242 (74%)	-0.32	6 (0%) 89 84	25, 40, 59, 74	17 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	ASP	2.9
1	B	244	HIS	2.9
1	B	281	ALA	2.3
1	A	274	ASP	2.1
1	A	414	THR	2.1
1	A	415	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.