Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 02:15 PM EDT

PDB ID	:	4RHJ
Title	:	Crystal structure of wild-type T. brucei arginase-like protein in a reduced form
Authors	:	Hai, Y.; Barrett, M.P.; Christianson, D.W.
Deposited on	:	2014-10-02
Resolution	:	1.80 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
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:

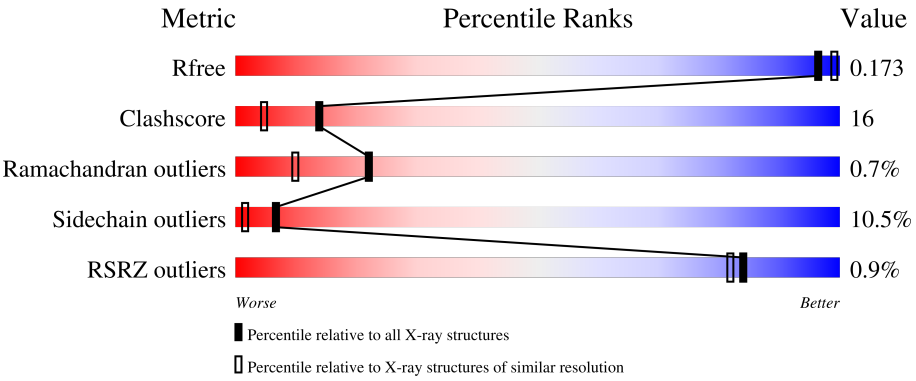
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	351	52% 27% · 18%
1	B	351	51% 28% · 19%
1	C	351	55% 22% 5% 18%
1	D	351	55% 24% · 17%
1	E	351	47% 31% · 18%

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Mol	Chain	Length	Quality of chain
1	F	351	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13644 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	289	Total	C	N	O	S	0	1	0
			2231	1422	380	415	14			
1	B	286	Total	C	N	O	S	0	0	0
			2205	1406	376	409	14			
1	C	287	Total	C	N	O	S	0	1	0
			2211	1410	374	413	14			
1	D	290	Total	C	N	O	S	0	1	0
			2231	1422	379	416	14			
1	E	287	Total	C	N	O	S	0	1	0
			2214	1412	377	411	14			
1	F	288	Total	C	N	O	S	0	2	0
			2228	1421	379	414	14			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q581Y0
A	-18	GLY	-	expression tag	UNP Q581Y0
A	-17	SER	-	expression tag	UNP Q581Y0
A	-16	SER	-	expression tag	UNP Q581Y0
A	-15	HIS	-	expression tag	UNP Q581Y0
A	-14	HIS	-	expression tag	UNP Q581Y0
A	-13	HIS	-	expression tag	UNP Q581Y0
A	-12	HIS	-	expression tag	UNP Q581Y0
A	-11	HIS	-	expression tag	UNP Q581Y0
A	-10	HIS	-	expression tag	UNP Q581Y0
A	-9	SER	-	expression tag	UNP Q581Y0
A	-8	SER	-	expression tag	UNP Q581Y0
A	-7	GLY	-	expression tag	UNP Q581Y0
A	-6	LEU	-	expression tag	UNP Q581Y0
A	-5	VAL	-	expression tag	UNP Q581Y0
A	-4	PRO	-	expression tag	UNP Q581Y0
A	-3	ARG	-	expression tag	UNP Q581Y0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q581Y0
A	-1	SER	-	expression tag	UNP Q581Y0
A	0	HIS	-	expression tag	UNP Q581Y0
B	-19	MET	-	expression tag	UNP Q581Y0
B	-18	GLY	-	expression tag	UNP Q581Y0
B	-17	SER	-	expression tag	UNP Q581Y0
B	-16	SER	-	expression tag	UNP Q581Y0
B	-15	HIS	-	expression tag	UNP Q581Y0
B	-14	HIS	-	expression tag	UNP Q581Y0
B	-13	HIS	-	expression tag	UNP Q581Y0
B	-12	HIS	-	expression tag	UNP Q581Y0
B	-11	HIS	-	expression tag	UNP Q581Y0
B	-10	HIS	-	expression tag	UNP Q581Y0
B	-9	SER	-	expression tag	UNP Q581Y0
B	-8	SER	-	expression tag	UNP Q581Y0
B	-7	GLY	-	expression tag	UNP Q581Y0
B	-6	LEU	-	expression tag	UNP Q581Y0
B	-5	VAL	-	expression tag	UNP Q581Y0
B	-4	PRO	-	expression tag	UNP Q581Y0
B	-3	ARG	-	expression tag	UNP Q581Y0
B	-2	GLY	-	expression tag	UNP Q581Y0
B	-1	SER	-	expression tag	UNP Q581Y0
B	0	HIS	-	expression tag	UNP Q581Y0
C	-19	MET	-	expression tag	UNP Q581Y0
C	-18	GLY	-	expression tag	UNP Q581Y0
C	-17	SER	-	expression tag	UNP Q581Y0
C	-16	SER	-	expression tag	UNP Q581Y0
C	-15	HIS	-	expression tag	UNP Q581Y0
C	-14	HIS	-	expression tag	UNP Q581Y0
C	-13	HIS	-	expression tag	UNP Q581Y0
C	-12	HIS	-	expression tag	UNP Q581Y0
C	-11	HIS	-	expression tag	UNP Q581Y0
C	-10	HIS	-	expression tag	UNP Q581Y0
C	-9	SER	-	expression tag	UNP Q581Y0
C	-8	SER	-	expression tag	UNP Q581Y0
C	-7	GLY	-	expression tag	UNP Q581Y0
C	-6	LEU	-	expression tag	UNP Q581Y0
C	-5	VAL	-	expression tag	UNP Q581Y0
C	-4	PRO	-	expression tag	UNP Q581Y0
C	-3	ARG	-	expression tag	UNP Q581Y0
C	-2	GLY	-	expression tag	UNP Q581Y0
C	-1	SER	-	expression tag	UNP Q581Y0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q581Y0
D	-19	MET	-	expression tag	UNP Q581Y0
D	-18	GLY	-	expression tag	UNP Q581Y0
D	-17	SER	-	expression tag	UNP Q581Y0
D	-16	SER	-	expression tag	UNP Q581Y0
D	-15	HIS	-	expression tag	UNP Q581Y0
D	-14	HIS	-	expression tag	UNP Q581Y0
D	-13	HIS	-	expression tag	UNP Q581Y0
D	-12	HIS	-	expression tag	UNP Q581Y0
D	-11	HIS	-	expression tag	UNP Q581Y0
D	-10	HIS	-	expression tag	UNP Q581Y0
D	-9	SER	-	expression tag	UNP Q581Y0
D	-8	SER	-	expression tag	UNP Q581Y0
D	-7	GLY	-	expression tag	UNP Q581Y0
D	-6	LEU	-	expression tag	UNP Q581Y0
D	-5	VAL	-	expression tag	UNP Q581Y0
D	-4	PRO	-	expression tag	UNP Q581Y0
D	-3	ARG	-	expression tag	UNP Q581Y0
D	-2	GLY	-	expression tag	UNP Q581Y0
D	-1	SER	-	expression tag	UNP Q581Y0
D	0	HIS	-	expression tag	UNP Q581Y0
E	-19	MET	-	expression tag	UNP Q581Y0
E	-18	GLY	-	expression tag	UNP Q581Y0
E	-17	SER	-	expression tag	UNP Q581Y0
E	-16	SER	-	expression tag	UNP Q581Y0
E	-15	HIS	-	expression tag	UNP Q581Y0
E	-14	HIS	-	expression tag	UNP Q581Y0
E	-13	HIS	-	expression tag	UNP Q581Y0
E	-12	HIS	-	expression tag	UNP Q581Y0
E	-11	HIS	-	expression tag	UNP Q581Y0
E	-10	HIS	-	expression tag	UNP Q581Y0
E	-9	SER	-	expression tag	UNP Q581Y0
E	-8	SER	-	expression tag	UNP Q581Y0
E	-7	GLY	-	expression tag	UNP Q581Y0
E	-6	LEU	-	expression tag	UNP Q581Y0
E	-5	VAL	-	expression tag	UNP Q581Y0
E	-4	PRO	-	expression tag	UNP Q581Y0
E	-3	ARG	-	expression tag	UNP Q581Y0
E	-2	GLY	-	expression tag	UNP Q581Y0
E	-1	SER	-	expression tag	UNP Q581Y0
E	0	HIS	-	expression tag	UNP Q581Y0
F	-19	MET	-	expression tag	UNP Q581Y0

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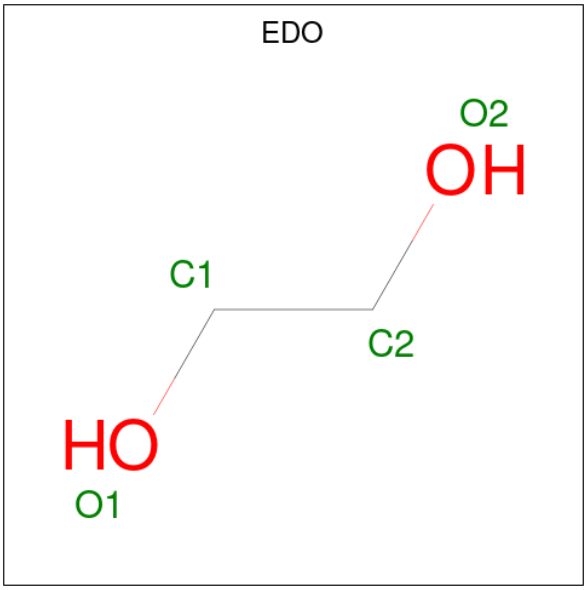
Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP Q581Y0
F	-17	SER	-	expression tag	UNP Q581Y0
F	-16	SER	-	expression tag	UNP Q581Y0
F	-15	HIS	-	expression tag	UNP Q581Y0
F	-14	HIS	-	expression tag	UNP Q581Y0
F	-13	HIS	-	expression tag	UNP Q581Y0
F	-12	HIS	-	expression tag	UNP Q581Y0
F	-11	HIS	-	expression tag	UNP Q581Y0
F	-10	HIS	-	expression tag	UNP Q581Y0
F	-9	SER	-	expression tag	UNP Q581Y0
F	-8	SER	-	expression tag	UNP Q581Y0
F	-7	GLY	-	expression tag	UNP Q581Y0
F	-6	LEU	-	expression tag	UNP Q581Y0
F	-5	VAL	-	expression tag	UNP Q581Y0
F	-4	PRO	-	expression tag	UNP Q581Y0
F	-3	ARG	-	expression tag	UNP Q581Y0
F	-2	GLY	-	expression tag	UNP Q581Y0
F	-1	SER	-	expression tag	UNP Q581Y0
F	0	HIS	-	expression tag	UNP Q581Y0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

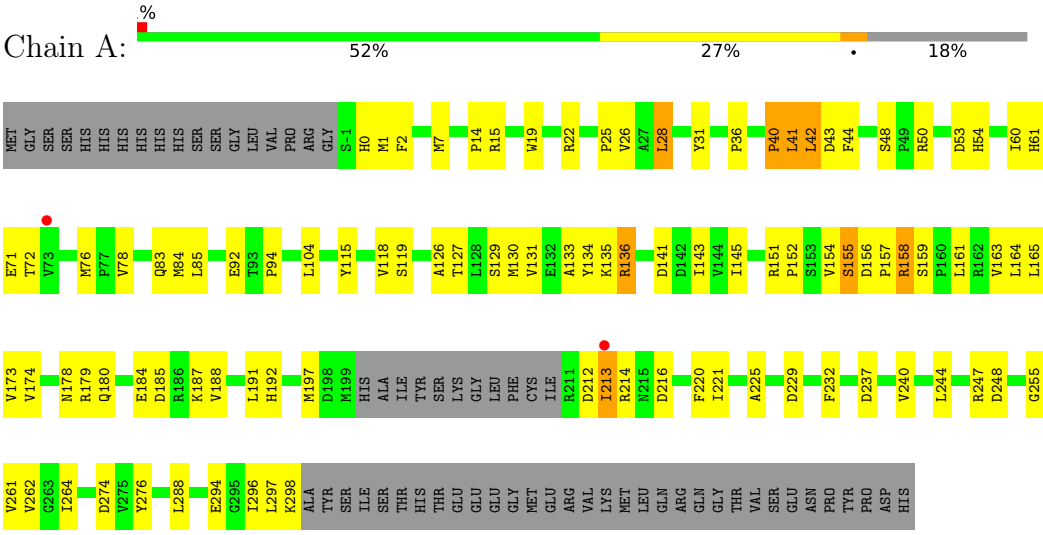
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	43	Total O 43 43	0	0
3	B	52	Total O 52 52	0	0
3	C	60	Total O 61 61	0	1
3	D	54	Total O 55 55	0	1
3	E	51	Total O 52 52	0	1
3	F	44	Total O 45 45	0	1

3 Residue-property plots

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.

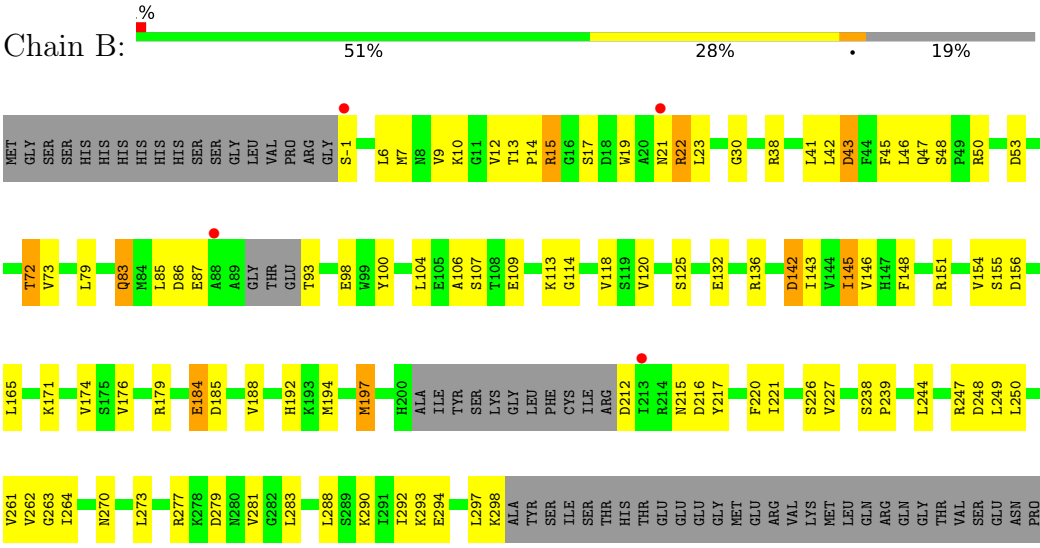
• Molecule 1: Arginase

Chain A:



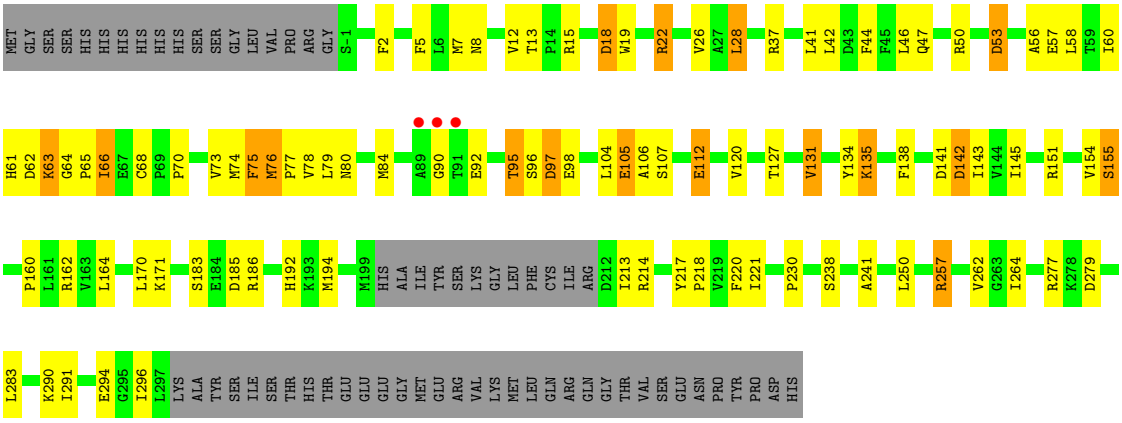
• Molecule 1: Arginase

Chain B:



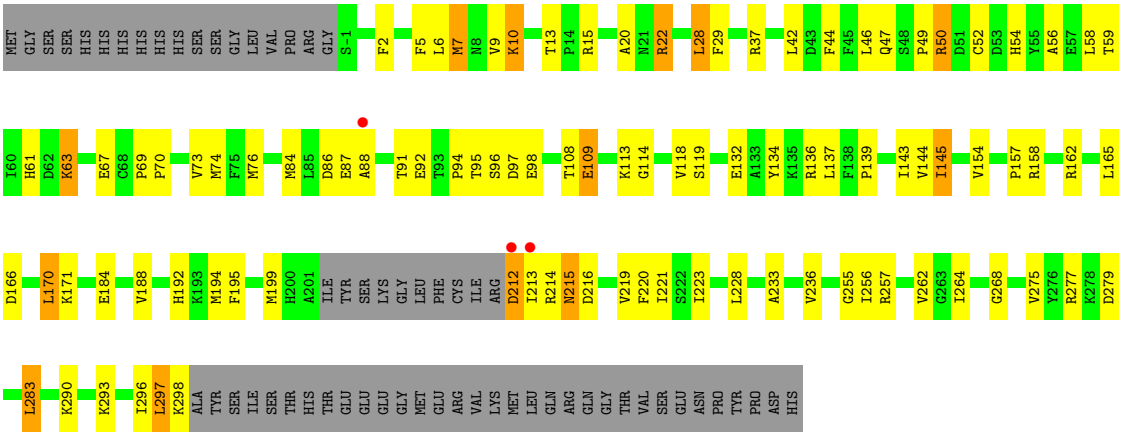
• Molecule 1: Arginase

Chain C:



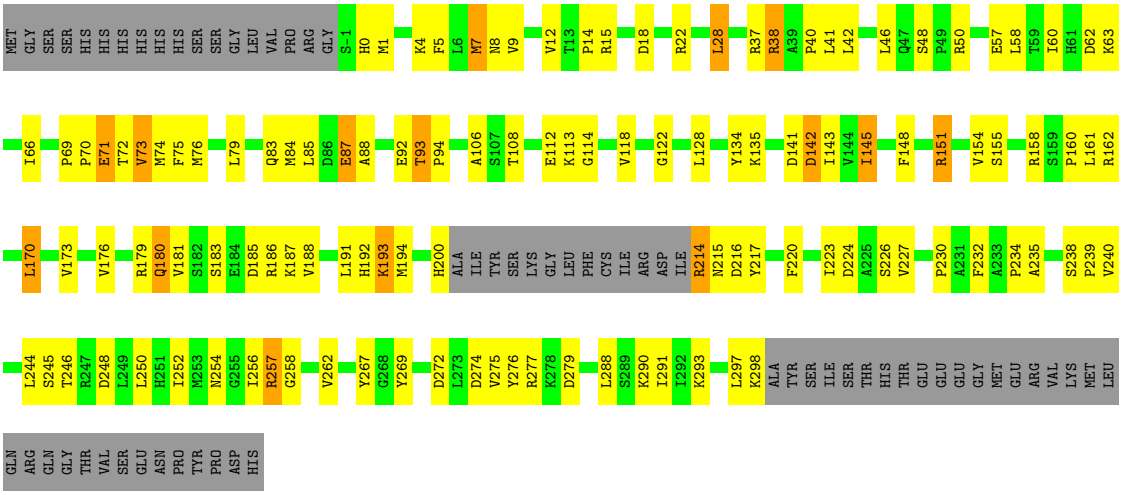
• Molecule 1: Arginase

Chain D:



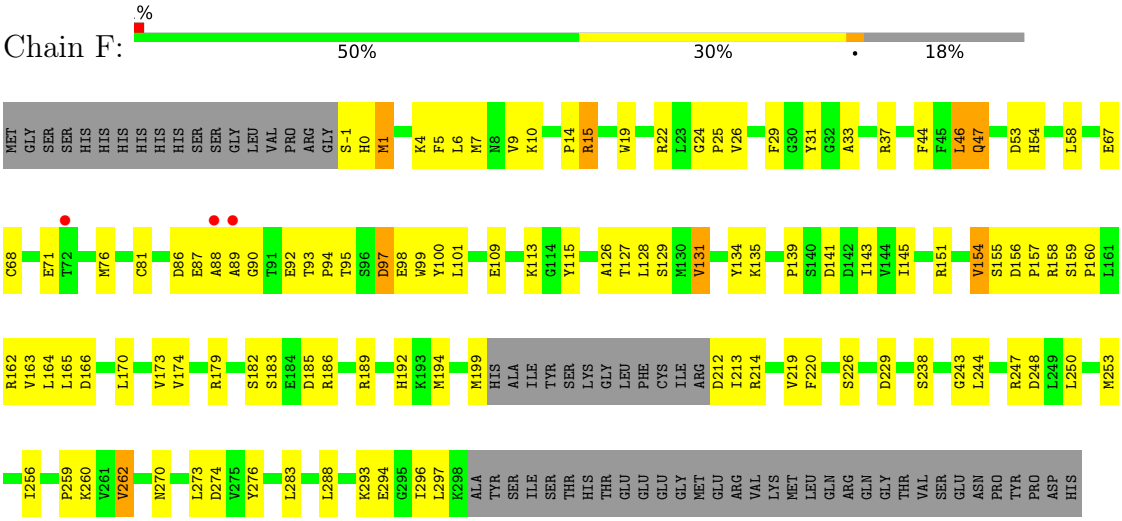
• Molecule 1: Arginase

Chain E:



• Molecule 1: Arginase

Chain F:


%
50%
30%
18%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY S-1 H0 M1 K4 F5 L6 M7 N8 V9 K10 P14 R15 W19 R22 L23 G24 P25 V26 F29 G30 Y31 G32 A33 R37 F44 F45 L46 Q47 D53 H54 L58 E67
C68 E71 T72 M76 C81 D86 E87 A88 A89 G90 T91 E92 T93 P94 T95 S96 D97 E98 W99 Y100 L101 E109 K113 G114 Y115 A126 T127 L128 S129 M130 V131 Y134 K135 P139 S140 D141 D142 I143 V144 I145 R151 V154 S155 D156 P157 R158 S159 P160 L161
R162 V163 L164 L165 D166 L170 V173 V174 R179 S182 S183 E184 D185 R186 R189 H192 K193 M194 M199 HIS ALA ILE TYR SER LYS GLY LEU PHE CYS ILE ARG D212 I213 R214 V219 F220 S226 D229 S238 G243 L244 R247 D248 L249 L250 M253
I256 P259 K260 V261 V262 N270 L273 D274 V275 Y276 L283 L288 K293 E294 G295 I296 L297 K298 ALA TYR SER ILE SER THR HIS THR GLU GLU GLU GLY MET GLU ARG VAL LYS MET LEU GLN ARG GLN GLY THR VAL SER GLU ASN PRO TYR PRO ASP HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	139.24Å 139.24Å 90.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.23 – 1.80 42.23 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.23-1.80) 100.0 (42.23-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.196 , 0.234 0.154 , 0.173	Depositor DCC
R_{free} test set	9089 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l 0.459 for h,-h-k,-l 0.458 for -k,-h,-l	Xtriage
Reported twinning fraction	0.490 for h,-h-k,-l	Depositor
Outliers	0 of 181427 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13644	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.88% 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

5.1 Standard geometry

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

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	0.42	0/2284	0.59	0/3096
1	B	0.42	0/2255	0.59	0/3056
1	C	0.46	0/2264	0.60	0/3071
1	D	0.46	0/2285	0.59	0/3100
1	E	0.41	0/2268	0.59	0/3075
1	F	0.39	0/2284	0.58	0/3096
All	All	0.43	0/13640	0.59	0/18494

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

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	2231	0	2246	79	0
1	B	2205	0	2212	63	0
1	C	2211	0	2220	64	0
1	D	2231	0	2234	70	0
1	E	2214	0	2225	78	0
1	F	2228	0	2246	70	0
2	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	12	0	18	1	0
3	A	43	0	0	3	0
3	B	52	0	0	5	0
3	C	61	0	0	2	0
3	D	55	0	0	1	0
3	E	52	0	0	4	0
3	F	45	0	0	8	0
All	All	13644	0	13407	422	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 16.

All (422) 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:165:LEU:HA	1:D:170:LEU:HD11	1.59	0.85
1:C:60:ILE:HG12	1:C:78:VAL:HB	1.61	0.82
1:A:26:VAL:HB	1:A:78:VAL:HG22	1.62	0.81
1:F:58:LEU:HD11	1:F:293:LYS:HG3	1.62	0.80
1:F:-1:SER:OG	1:F:1:MET:SD	2.39	0.79
1:F:-1:SER:HB2	1:F:98:GLU:HB3	1.65	0.79
1:B:22:ARG:HG2	1:B:22:ARG:HH11	1.47	0.79
1:E:71:GLU:HG3	1:E:74:MET:HG3	1.66	0.78
1:F:145[B]:ILE:HG12	1:F:220:PHE:HB3	1.64	0.77
1:A:214:ARG:H	1:A:257:ARG:HG3	1.50	0.75
1:A:118:VAL:HG13	1:A:264:ILE:HB	1.68	0.74
1:A:135:LYS:NZ	1:A:141:ASP:O	2.20	0.74
1:F:135:LYS:NZ	1:F:141:ASP:O	2.21	0.73
1:F:15:ARG:HH22	1:F:22:ARG:H	1.36	0.73
1:F:44:PHE:O	1:F:47:GLN:NE2	2.21	0.73
1:A:14:PRO:HD2	1:E:187:LYS:HD2	1.71	0.72
1:F:157:PRO:HA	1:F:162:ARG:HG2	1.71	0.72
1:C:12:VAL:HG21	1:C:79:LEU:HD21	1.73	0.71
1:F:131:VAL:HG11	1:F:164:LEU:HD11	1.72	0.71
1:B:48:SER:O	1:B:50:ARG:NH1	2.23	0.71
1:C:62:ASP:OD1	1:C:80:ASN:ND2	2.23	0.71
1:B:277:ARG:HE	1:B:281:VAL:HB	1.55	0.70
1:C:50:ARG:HH21	1:C:60:ILE:H	1.36	0.70
1:F:22:ARG:NH1	1:F:68:CYS:SG	2.65	0.70
1:E:277:ARG:NH2	1:E:279:ASP:OD2	2.24	0.70
1:B:53:ASP:OD2	1:B:247:ARG:NH1	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:VAL:O	1:B:162:ARG:NH1	2.24	0.69
1:E:256:ILE:O	1:E:257:ARG:NH1	2.26	0.68
1:E:135:LYS:NZ	1:E:141:ASP:O	2.24	0.68
1:B:83:GLN:NE2	3:B:434:HOH:O	2.27	0.68
1:B:142:ASP:OD1	1:B:142:ASP:N	2.27	0.68
1:F:15:ARG:NH2	1:F:19:TRP:O	2.26	0.68
1:F:253:MET:HA	1:F:256:ILE:HD13	1.75	0.68
1:A:135:LYS:HG2	1:A:169:LEU:HD22	1.76	0.67
1:F:145[B]:ILE:HG13	1:F:170:LEU:HD11	1.76	0.67
1:C:15:ARG:HE	1:C:19:TRP:HB3	1.59	0.67
1:D:15:ARG:HH22	1:D:20:ALA:HA	1.59	0.67
1:A:155:SER:HB2	1:A:184:GLU:HB3	1.77	0.66
1:D:58:LEU:HD23	1:D:76:MET:HE3	1.75	0.66
1:E:58:LEU:HD23	1:E:76:MET:HB2	1.77	0.66
1:B:118:VAL:HG22	1:B:264:ILE:HB	1.78	0.66
1:E:145[B]:ILE:HG12	1:E:220:PHE:HB3	1.77	0.66
1:B:109:GLU:HG3	1:B:113:LYS:HE2	1.79	0.64
1:B:277:ARG:NH2	1:B:279:ASP:OD2	2.30	0.64
1:E:179:ARG:NE	1:E:240:VAL:O	2.26	0.64
1:A:78:VAL:HG21	1:A:296:ILE:HD13	1.80	0.64
1:E:188:VAL:HA	1:E:191:LEU:HB3	1.78	0.64
1:F:243:GLY:N	3:F:409:HOH:O	2.31	0.64
1:F:26:VAL:HG21	1:F:296:ILE:HG23	1.80	0.64
1:A:133:ALA:HA	1:A:136:ARG:HH21	1.63	0.63
1:E:254:ASN:O	1:E:257:ARG:NH2	2.30	0.63
1:A:28:LEU:HD21	1:A:296:ILE:HD11	1.81	0.63
1:C:37:ARG:NH2	1:C:90:GLY:O	2.29	0.62
1:F:250:LEU:HA	1:F:253:MET:HE2	1.81	0.62
1:A:15:ARG:NH2	1:A:22:ARG:O	2.33	0.62
1:A:180:GLN:NE2	3:A:515:HOH:O	2.25	0.62
1:C:22:ARG:NE	1:C:68:CYS:SG	2.68	0.62
1:D:157:PRO:HA	1:D:162:ARG:HG2	1.82	0.61
1:A:40:PRO:O	1:A:42:LEU:N	2.32	0.61
1:E:173:VAL:HB	1:E:194:MET:HG3	1.79	0.61
1:C:13:THR:HG21	1:C:65:PRO:HB3	1.82	0.61
1:D:192:HIS:HB2	1:D:194:MET:HE2	1.82	0.61
1:A:0:HIS:HE1	1:A:92:GLU:HB2	1.64	0.61
1:B:261:VAL:HG13	3:B:437:HOH:O	2.01	0.61
1:B:215:ASN:ND2	1:B:217:TYR:O	2.30	0.61
1:E:50:ARG:HH21	1:E:60:ILE:HG13	1.66	0.61
1:A:212:ASP:HB2	1:A:214:ARG:HG3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ILE:O	1:D:215:ASN:N	2.35	0.60
1:A:127:THR:O	1:A:131:VAL:HG12	2.02	0.60
1:B:184:GLU:O	1:B:188:VAL:HG23	2.01	0.60
1:D:144:VAL:HG12	1:D:171:LYS:HB3	1.84	0.60
1:A:61:HIS:CD2	1:A:66:ILE:HD13	2.37	0.59
1:B:42:LEU:HD23	1:B:83:GLN:HE21	1.66	0.59
1:D:44:PHE:O	1:D:47:GLN:HG3	2.02	0.59
1:F:15:ARG:NH2	1:F:22:ARG:H	2.00	0.59
1:A:151:ARG:NH1	1:A:180:GLN:OE1	2.30	0.59
1:D:59:THR:HB	1:D:61:HIS:HE1	1.67	0.59
1:D:109:GLU:OE2	1:D:113:LYS:NZ	2.28	0.59
1:A:53:ASP:N	1:A:294:GLU:OE2	2.30	0.59
1:A:213:ILE:HG13	1:A:256:ILE:HA	1.84	0.59
1:B:12:VAL:O	1:B:113:LYS:NZ	2.27	0.59
1:A:255:GLY:HA2	1:A:257:ARG:HH22	1.68	0.58
1:D:296:ILE:O	1:D:298:LYS:N	2.36	0.58
1:E:216:ASP:N	3:E:434:HOH:O	2.29	0.58
1:D:290:LYS:HA	3:D:407[A]:HOH:O	2.03	0.58
1:F:4:LYS:NZ	3:F:435:HOH:O	2.25	0.58
1:E:69:PRO:HB2	1:E:73:VAL:O	2.04	0.58
1:B:22:ARG:HG2	1:B:22:ARG:NH1	2.16	0.57
1:B:151:ARG:NH2	1:B:185:ASP:OD2	2.36	0.57
1:F:53:ASP:N	1:F:294:GLU:OE2	2.36	0.57
1:F:71:GLU:OE2	1:F:71:GLU:N	2.34	0.57
1:D:215:ASN:ND2	1:D:257:ARG:O	2.38	0.57
1:A:42:LEU:HD22	1:A:83:GLN:HG2	1.87	0.57
1:A:260:LYS:HE2	1:A:262:VAL:HG12	1.85	0.57
1:C:26:VAL:HG21	1:C:296:ILE:HG23	1.85	0.57
1:A:2:PHE:CZ	1:A:94:PRO:HG2	2.39	0.57
1:E:234:PRO:HG3	1:E:275:VAL:HB	1.86	0.57
1:D:108:THR:OG1	1:D:136:ARG:NH2	2.37	0.57
1:E:244:LEU:HD22	1:E:248:ASP:HB3	1.85	0.57
1:A:152:PRO:HG2	1:A:185:ASP:HB3	1.86	0.56
1:B:179:ARG:NH2	1:B:226:SER:O	2.38	0.56
1:E:154:VAL:O	1:E:162:ARG:NH1	2.37	0.56
1:C:53:ASP:OD1	1:C:290:LYS:NZ	2.30	0.56
1:C:63:LYS:NZ	1:C:64:GLY:O	2.36	0.55
1:F:31:TYR:CD2	1:F:126:ALA:HB2	2.41	0.55
1:A:145[A]:ILE:HD12	1:A:170:LEU:HD21	1.88	0.55
1:A:145[B]:ILE:HD12	1:A:170:LEU:HD21	1.88	0.55
1:B:15:ARG:NH1	1:B:114:GLY:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:HIS:CD2	1:C:66:ILE:HD12	2.41	0.55
1:C:142:ASP:HB2	1:C:217:TYR:CD1	2.41	0.55
1:C:66:ILE:HG21	1:C:77:PRO:HB3	1.89	0.55
1:E:192:HIS:O	1:E:193:LYS:C	2.45	0.55
1:B:72:THR:OG1	1:B:73:VAL:N	2.38	0.55
1:B:270:ASN:HB3	1:B:273:LEU:HD12	1.88	0.55
1:C:57:GLU:O	1:C:76:MET:N	2.40	0.54
1:B:14:PRO:HA	1:B:113:LYS:HB3	1.89	0.54
1:A:152:PRO:HB2	1:A:154:VAL:HG22	1.90	0.54
1:C:15:ARG:NH2	1:C:22:ARG:O	2.40	0.54
1:E:215:ASN:O	1:E:258:GLY:HA2	2.07	0.54
1:B:17:SER:OG	1:D:166:ASP:O	2.20	0.54
1:C:145[B]:ILE:HG12	1:C:220:PHE:HB3	1.89	0.54
1:D:87:GLU:O	1:D:88:ALA:HB3	2.06	0.54
1:B:256:ILE:O	1:B:257:ARG:NH1	2.40	0.54
1:C:142:ASP:HB2	1:C:217:TYR:HD1	1.73	0.54
1:D:137:LEU:O	1:D:139:PRO:HD3	2.08	0.54
1:D:221:ILE:HD12	1:D:256:ILE:HD13	1.89	0.54
1:E:277:ARG:HB2	1:E:279:ASP:OD1	2.08	0.54
1:E:176:VAL:HG11	1:E:252:ILE:HG21	1.89	0.54
1:A:1:MET:HB3	1:A:85:LEU:HD12	1.90	0.54
1:B:45:PHE:HE1	1:B:293:LYS:HG3	1.71	0.54
1:C:53:ASP:N	1:C:294:GLU:OE2	2.27	0.54
1:F:135:LYS:HD3	1:F:139:PRO:HA	1.89	0.54
1:D:70:PRO:HD2	1:D:73:VAL:HG22	1.88	0.54
1:F:154:VAL:O	1:F:162:ARG:NH1	2.36	0.54
1:D:15:ARG:HB3	1:D:114:GLY:HA3	1.90	0.53
1:A:131:VAL:HG23	1:A:143:ILE:HG21	1.90	0.53
1:A:133:ALA:HA	1:A:136:ARG:HE	1.73	0.53
1:A:60:ILE:HD13	1:A:78:VAL:HB	1.91	0.53
1:E:246:THR:O	1:E:250:LEU:HG	2.08	0.53
1:F:15:ARG:NH1	1:F:24:GLY:O	2.41	0.53
1:F:92:GLU:N	1:F:92:GLU:OE1	2.41	0.53
1:D:70:PRO:HD2	1:D:73:VAL:CG2	2.39	0.53
1:E:38:ARG:O	1:E:40:PRO:HD3	2.09	0.53
1:F:244:LEU:HD22	1:F:248:ASP:HB3	1.89	0.53
1:F:15:ARG:NH2	3:F:440:HOH:O	2.41	0.53
1:B:6:LEU:O	1:B:10:LYS:HG2	2.10	0.52
1:F:162:ARG:O	1:F:166:ASP:HB2	2.09	0.52
1:A:244:LEU:HD22	1:A:248:ASP:HB3	1.91	0.52
1:C:42:LEU:O	1:C:46:LEU:HG	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:ARG:NH2	1:D:279:ASP:OD2	2.40	0.52
1:C:127:THR:O	1:C:131:VAL:HG13	2.09	0.52
1:C:18:ASP:HB2	1:C:68:CYS:HB3	1.92	0.52
1:B:100:TYR:OH	1:B:132:GLU:OE1	2.28	0.52
1:F:25:PRO:HG2	1:F:115:TYR:CD2	2.44	0.52
1:C:154:VAL:O	1:C:162:ARG:NH1	2.43	0.52
1:D:28:LEU:HD22	1:D:118:VAL:HB	1.91	0.52
1:A:53:ASP:OD2	1:A:247:ARG:NH1	2.33	0.51
1:D:59:THR:HB	1:D:61:HIS:CE1	2.46	0.51
1:D:67:GLU:O	1:D:69:PRO:HD3	2.11	0.51
1:B:42:LEU:O	1:B:46:LEU:HG	2.10	0.51
1:E:288:LEU:HD23	1:E:291:ILE:HD12	1.93	0.51
1:F:165:LEU:HB2	3:F:434:HOH:O	2.10	0.51
1:E:148:PHE:HB3	1:E:227:VAL:HG21	1.93	0.51
1:F:0:HIS:NE2	1:F:92:GLU:OE2	2.41	0.51
1:D:296:ILE:C	1:D:298:LYS:N	2.65	0.51
1:F:162:ARG:HA	3:F:434:HOH:O	2.10	0.51
1:D:37:ARG:NH1	1:D:91:THR:HA	2.26	0.50
1:D:145[B]:ILE:HG12	1:D:220:PHE:HB3	1.93	0.50
1:F:29:PHE:HB3	1:F:81:CYS:HB2	1.93	0.50
1:A:158:ARG:HH11	1:A:158:ARG:HB3	1.75	0.50
1:D:22:ARG:HH11	1:D:22:ARG:HA	1.75	0.50
1:F:1:MET:HE1	1:F:92:GLU:HB2	1.91	0.50
1:C:257:ARG:HG3	2:C:402:EDO:H22	1.94	0.50
1:D:15:ARG:NH2	1:D:20:ALA:HA	2.26	0.50
1:F:97:ASP:HA	1:F:100:TYR:HB3	1.93	0.50
1:D:134:TYR:CE1	1:D:143:ILE:HD11	2.46	0.50
1:C:95:THR:OG1	1:C:98:GLU:OE1	2.29	0.50
1:D:9:VAL:HG12	1:D:109:GLU:HG2	1.91	0.50
1:A:0:HIS:CE1	1:A:92:GLU:HB2	2.45	0.50
1:A:119:SER:HB3	1:A:130:MET:SD	2.52	0.50
1:C:134:TYR:CE1	1:C:143:ILE:HD11	2.46	0.50
1:F:37:ARG:HH22	1:F:87:GLU:HA	1.77	0.50
1:F:53:ASP:H	1:F:294:GLU:CD	2.15	0.50
1:A:0:HIS:NE2	1:A:1:MET:SD	2.85	0.50
1:F:165:LEU:HD21	1:F:173:VAL:HG23	1.94	0.50
1:E:220:PHE:HD1	1:E:262:VAL:HG22	1.77	0.49
1:C:155:SER:OG	1:C:185:ASP:OD1	2.20	0.49
1:F:194:MET:SD	3:F:422:HOH:O	2.60	0.49
1:A:92:GLU:OE1	1:A:92:GLU:N	2.43	0.49
1:B:215:ASN:HD22	1:B:258:GLY:HA2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LYS:HD3	1:C:217:TYR:CE1	2.47	0.49
1:B:192:HIS:HB2	1:B:194:MET:HE2	1.94	0.49
1:C:104:LEU:O	1:C:107:SER:OG	2.25	0.49
1:B:244:LEU:HD22	1:B:248:ASP:HB3	1.95	0.49
1:E:14:PRO:HA	1:E:113:LYS:HB3	1.93	0.49
1:F:145[A]:ILE:CG2	1:F:173:VAL:HG22	2.42	0.49
1:A:71:GLU:N	3:A:539:HOH:O	2.38	0.49
1:C:183:SER:OG	1:C:186:ARG:NH2	2.46	0.49
1:D:236:VAL:HG12	1:D:268:GLY:O	2.13	0.49
1:D:215:ASN:H	1:D:215:ASN:HD22	1.61	0.49
1:C:214:ARG:NH2	3:C:559:HOH:O	2.46	0.49
1:D:5:PHE:CG	1:D:84:MET:HA	2.48	0.48
1:D:6:LEU:O	1:D:10:LYS:HD3	2.13	0.48
1:E:87:GLU:OE1	1:E:88:ALA:N	2.46	0.48
1:C:41:LEU:HD23	1:C:120:VAL:HG13	1.95	0.48
1:C:50:ARG:NH2	1:C:60:ILE:H	2.07	0.48
1:D:275:VAL:HG12	1:D:283:LEU:HD22	1.93	0.48
1:A:26:VAL:HG21	1:A:296:ILE:HG23	1.94	0.48
1:B:148:PHE:HB3	1:B:227:VAL:HG11	1.95	0.48
1:C:142:ASP:HB3	1:C:171:LYS:HD2	1.95	0.48
1:D:2:PHE:CD1	1:D:84:MET:HG2	2.49	0.48
1:E:232:PHE:CE1	1:E:245:SER:HA	2.48	0.48
1:F:9:VAL:HG12	1:F:109:GLU:HG2	1.95	0.48
1:E:122:GLY:O	1:E:267:TYR:HB2	2.13	0.48
1:D:94:PRO:HA	1:D:98:GLU:OE2	2.13	0.48
1:B:58:LEU:HD11	1:B:293:LYS:HG2	1.95	0.47
1:D:10:LYS:O	1:D:113:LYS:NZ	2.47	0.47
1:E:70:PRO:O	1:E:72:THR:N	2.47	0.47
1:E:148:PHE:HB2	1:E:223:ILE:HG23	1.95	0.47
1:E:297:LEU:HG	1:E:298:LYS:HG3	1.95	0.47
1:F:88:ALA:O	1:F:90:GLY:N	2.45	0.47
1:B:15:ARG:HD2	1:B:114:GLY:HA3	1.97	0.47
1:A:25:PRO:HG2	1:A:115:TYR:CD2	2.50	0.47
1:C:56:ALA:HA	1:C:74:MET:HB3	1.95	0.47
1:D:63:LYS:H	1:D:63:LYS:HD3	1.78	0.47
1:E:5:PHE:CG	1:E:84:MET:HA	2.49	0.47
1:E:38:ARG:NH2	3:E:444:HOH:O	2.46	0.47
1:C:19:TRP:HA	1:C:22:ARG:HG3	1.96	0.47
1:D:296:ILE:C	1:D:298:LYS:H	2.17	0.47
1:E:151:ARG:HH22	1:E:238:SER:HB2	1.80	0.47
1:E:155:SER:HB3	1:E:185:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:HIS:CD2	1:A:66:ILE:HG21	2.50	0.47
1:A:221:ILE:HB	1:A:264:ILE:HG12	1.97	0.47
1:B:294:GLU:O	1:B:297:LEU:HB3	2.14	0.47
1:C:5:PHE:CG	1:C:84:MET:HA	2.50	0.47
1:C:28:LEU:HD13	1:C:78:VAL:HG13	1.97	0.47
1:E:8:ASN:O	1:E:12:VAL:HG23	2.15	0.47
1:F:155:SER:HB2	1:F:185:ASP:OD1	2.15	0.47
1:C:143:ILE:HD12	1:C:218:PRO:HB2	1.96	0.47
1:D:50:ARG:CZ	1:D:50:ARG:HB3	2.44	0.47
1:E:230:PRO:HG3	1:E:239:PRO:HB3	1.96	0.47
1:F:179:ARG:NH2	1:F:226:SER:O	2.48	0.47
1:F:229:ASP:HA	3:F:409:HOH:O	2.15	0.47
1:B:176:VAL:HG22	1:B:197:MET:SD	2.55	0.47
1:E:4:LYS:HA	1:E:7:MET:HB3	1.97	0.47
1:E:142:ASP:O	1:E:217:TYR:HB3	2.15	0.47
1:F:134:TYR:CD1	1:F:143:ILE:HD11	2.50	0.47
1:B:125:SER:HA	1:B:160:PRO:HB3	1.97	0.47
1:D:76:MET:SD	1:D:297:LEU:HD12	2.55	0.47
1:E:108:THR:O	1:E:112:GLU:HG3	2.15	0.47
1:A:240:VAL:HG22	3:A:514:HOH:O	2.14	0.46
1:B:6:LEU:HD21	1:B:106:ALA:HB2	1.96	0.46
1:E:158:ARG:HA	1:E:158:ARG:HD3	1.68	0.46
1:A:156:ASP:HA	1:A:157:PRO:HD2	1.78	0.46
1:D:54:HIS:O	1:D:56:ALA:N	2.46	0.46
1:D:143:ILE:HD12	1:D:262:VAL:HG11	1.96	0.46
1:E:274:ASP:HB3	1:E:276:TYR:CE2	2.50	0.46
1:A:225:ALA:HB2	1:A:288:LEU:HD11	1.97	0.46
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.80	0.46
1:B:10:LYS:HA	1:B:109:GLU:HG2	1.98	0.46
1:C:138:PHE:HB3	1:C:141:ASP:OD1	2.15	0.46
1:D:256:ILE:O	1:D:257:ARG:NH1	2.48	0.46
1:D:42:LEU:O	1:D:46:LEU:HG	2.15	0.46
1:E:41:LEU:HB2	1:E:269:TYR:CE2	2.51	0.46
1:B:43:ASP:OD2	1:B:43:ASP:N	2.32	0.46
1:C:19:TRP:HE3	1:C:22:ARG:HB2	1.81	0.46
1:C:28:LEU:HD22	1:C:78:VAL:HG11	1.98	0.46
1:C:44:PHE:O	1:C:47:GLN:HG2	2.16	0.46
1:C:61:HIS:CG	1:C:66:ILE:HD12	2.51	0.46
1:F:6:LEU:O	1:F:10:LYS:HD3	2.16	0.46
1:D:95:THR:OG1	1:D:98:GLU:HG3	2.15	0.46
1:E:37:ARG:NE	1:E:85:LEU:HD21	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:LYS:HD3	1:F:86:ASP:OD1	2.15	0.46
1:A:229:ASP:HB3	1:A:232:PHE:HD1	1.79	0.46
1:D:7:MET:SD	1:D:7:MET:N	2.89	0.46
1:A:221:ILE:O	1:A:264:ILE:HA	2.16	0.45
1:B:22:ARG:NH1	1:B:22:ARG:CG	2.77	0.45
1:F:162:ARG:HD2	3:F:434:HOH:O	2.16	0.45
1:A:212:ASP:HB2	1:A:214:ARG:CZ	2.46	0.45
1:E:297:LEU:CD1	1:E:298:LYS:HG3	2.47	0.45
1:A:260:LYS:HZ1	1:A:261:VAL:C	2.20	0.45
1:E:181:VAL:HG12	1:E:186:ARG:HG3	1.99	0.45
1:E:214:ARG:NH2	3:E:410:HOH:O	2.36	0.45
1:F:270:ASN:HB3	1:F:273:LEU:HD12	1.99	0.45
1:D:212:ASP:HA	1:D:255:GLY:O	2.16	0.45
1:B:176:VAL:HA	1:B:197:MET:HG3	1.97	0.45
1:B:250:LEU:HD22	1:B:294:GLU:HG3	1.99	0.45
1:C:134:TYR:HE1	1:C:143:ILE:HD11	1.81	0.45
1:A:174:VAL:CG1	1:A:197:MET:HE1	2.47	0.45
1:C:135:LYS:HA	1:C:135:LYS:HD3	1.72	0.45
1:B:146:VAL:HG13	1:B:174:VAL:HB	1.99	0.45
1:C:192:HIS:HB2	1:C:194:MET:HE2	1.98	0.45
1:B:-1:SER:HB2	1:B:98:GLU:OE1	2.16	0.44
1:B:227:VAL:HG22	1:B:244:LEU:HD12	1.99	0.44
1:E:42:LEU:O	1:E:46:LEU:HG	2.17	0.44
1:D:154:VAL:HB	1:D:188:VAL:HG11	1.98	0.44
1:B:263:GLY:O	3:B:437:HOH:O	2.21	0.44
1:E:28:LEU:HG	1:E:118:VAL:HG12	1.99	0.44
1:A:31:TYR:CE2	1:A:126:ALA:HB2	2.53	0.44
1:A:260:LYS:NZ	1:A:261:VAL:O	2.44	0.44
1:B:6:LEU:HA	1:B:6:LEU:HD23	1.61	0.44
1:B:45:PHE:CE1	1:B:293:LYS:HG3	2.52	0.44
1:E:134:TYR:HD1	1:E:143:ILE:HD11	1.83	0.44
1:F:165:LEU:HB3	1:F:192:HIS:CD2	2.53	0.44
1:B:145:ILE:HB	1:B:220:PHE:HB3	2.00	0.44
1:F:159:SER:O	1:F:163:VAL:HG23	2.18	0.44
1:A:145[A]:ILE:HG12	1:A:220:PHE:HB3	2.00	0.44
1:B:288:LEU:O	1:B:292:ILE:HG13	2.18	0.44
1:C:143:ILE:CD1	1:C:218:PRO:HB2	2.48	0.44
1:C:277:ARG:HB2	1:C:279:ASP:OD1	2.18	0.44
1:E:50:ARG:NH2	1:E:60:ILE:HG13	2.31	0.44
1:E:244:LEU:HD11	1:E:252:ILE:HD12	2.00	0.44
1:F:127:THR:O	1:F:131:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:PRO:O	3:B:447:HOH:O	2.21	0.44
1:D:132:GLU:O	1:D:136:ARG:HB2	2.18	0.44
1:E:145[A]:ILE:HD13	1:E:161:LEU:HD13	1.99	0.44
1:E:235:ALA:HB2	1:E:274:ASP:HA	2.00	0.44
1:E:18:ASP:OD1	1:E:18:ASP:N	2.41	0.43
1:F:46:LEU:HD22	1:F:46:LEU:HA	1.73	0.43
1:E:145[A]:ILE:HG23	1:E:173:VAL:HA	2.00	0.43
1:D:49:PRO:O	1:D:293:LYS:NZ	2.46	0.43
1:D:52:CYS:HA	1:D:293:LYS:HE3	1.99	0.43
1:F:14:PRO:HA	1:F:113:LYS:HB3	2.01	0.43
1:A:104:LEU:HG	1:A:136:ARG:NH2	2.34	0.43
1:B:104:LEU:HD11	1:B:136:ARG:NH1	2.33	0.43
1:E:128:LEU:HB2	1:E:160:PRO:HB3	2.01	0.43
1:F:93:THR:HA	1:F:94:PRO:HD2	1.88	0.43
1:D:9:VAL:CG1	1:D:109:GLU:HG2	2.49	0.43
1:E:224:ASP:HB2	1:E:267:TYR:CZ	2.53	0.43
1:F:128:LEU:HB2	1:F:160:PRO:HB3	2.00	0.43
1:A:15:ARG:HE	1:A:19:TRP:CB	2.31	0.43
1:C:221:ILE:HB	1:C:264:ILE:HG12	2.00	0.43
1:E:70:PRO:O	1:E:73:VAL:N	2.52	0.43
1:A:133:ALA:HA	1:A:136:ARG:NH2	2.32	0.43
1:E:257:ARG:NH2	1:E:298:LYS:HD3	2.34	0.43
1:A:145[B]:ILE:HG12	1:A:220:PHE:HB3	2.00	0.43
1:A:170:LEU:HD12	1:A:170:LEU:HA	1.82	0.43
1:D:56:ALA:HA	1:D:74:MET:HB3	2.01	0.43
1:E:290:LYS:HD2	1:E:293:LYS:CE	2.48	0.43
1:F:143:ILE:O	1:F:170:LEU:HD13	2.19	0.43
1:F:31:TYR:CE2	1:F:33:ALA:HB3	2.54	0.42
1:A:212:ASP:CB	1:A:214:ARG:HG3	2.47	0.42
1:A:214:ARG:H	1:A:257:ARG:CG	2.24	0.42
1:D:118:VAL:HG22	1:D:264:ILE:HB	2.01	0.42
1:E:12:VAL:HG21	1:E:79:LEU:HD21	2.01	0.42
1:E:161:LEU:HD21	1:E:173:VAL:HG11	2.00	0.42
1:D:184:GLU:O	1:D:188:VAL:HG23	2.18	0.42
1:D:228:LEU:HB2	1:D:233:ALA:HB3	2.01	0.42
1:A:152:PRO:HG2	1:A:185:ASP:CB	2.49	0.42
1:B:15:ARG:HH21	1:B:19:TRP:HB3	1.85	0.42
1:C:250:LEU:CD2	1:C:291:ILE:HD13	2.50	0.42
1:E:15:ARG:CZ	1:E:114:GLY:HA3	2.50	0.42
1:F:58:LEU:HD23	1:F:76:MET:HB2	2.01	0.42
1:A:50:ARG:NH2	1:A:60:ILE:HG13	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ILE:HD12	1:D:256:ILE:HA	2.00	0.42
1:F:54:HIS:ND1	1:F:297:LEU:HD21	2.35	0.42
1:A:179:ARG:HG3	1:A:240:VAL:HG11	2.01	0.42
1:B:41:LEU:HD23	1:B:120:VAL:HG13	2.01	0.42
1:C:15:ARG:NE	1:C:19:TRP:HB3	2.31	0.42
1:C:142:ASP:OD1	1:C:142:ASP:N	2.51	0.42
1:D:165:LEU:HB3	1:D:192:HIS:CD2	2.55	0.42
1:E:38:ARG:NH2	1:E:272:ASP:OD1	2.53	0.42
1:E:73:VAL:HG12	1:E:75:PHE:HE2	1.85	0.42
1:A:134:TYR:CD1	1:A:143:ILE:HD11	2.54	0.42
1:D:63:LYS:HD3	1:D:63:LYS:N	2.34	0.42
1:D:277:ARG:HB2	1:D:279:ASP:OD1	2.20	0.42
1:E:191:LEU:C	1:E:192:HIS:HD1	2.23	0.42
1:F:31:TYR:CE2	1:F:126:ALA:HB2	2.55	0.42
1:F:174:VAL:HG21	1:F:213:ILE:HG23	2.02	0.42
1:C:70:PRO:O	1:C:73:VAL:HG22	2.19	0.41
1:C:75:PHE:HD1	1:C:75:PHE:HA	1.66	0.41
1:D:165:LEU:HD23	1:D:170:LEU:CD1	2.50	0.41
1:E:106:ALA:HB3	3:E:428:HOH:O	2.20	0.41
1:E:257:ARG:HA	1:E:257:ARG:HD3	1.90	0.41
1:F:94:PRO:HG2	1:F:99:TRP:NE1	2.35	0.41
1:F:274:ASP:HB3	1:F:276:TYR:CE2	2.55	0.41
1:A:127:THR:HA	1:A:220:PHE:CZ	2.55	0.41
1:B:45:PHE:O	1:B:48:SER:HB2	2.21	0.41
1:C:105:GLU:HG3	1:C:106:ALA:N	2.32	0.41
1:E:151:ARG:HD2	1:E:180:GLN:HB3	2.01	0.41
1:F:5:PHE:CE2	1:F:9:VAL:HG21	2.55	0.41
1:A:104:LEU:HG	1:A:136:ARG:HH22	1.85	0.41
1:A:28:LEU:HD22	1:A:118:VAL:HB	2.02	0.41
1:A:159:SER:O	1:A:163:VAL:HG23	2.20	0.41
1:B:53:ASP:OD1	1:B:290:LYS:NZ	2.26	0.41
1:C:53:ASP:OD2	3:C:538:HOH:O	2.21	0.41
1:C:95:THR:HB	1:C:97:ASP:OD2	2.19	0.41
1:B:30:GLY:HA3	1:B:83:GLN:HG3	2.02	0.41
1:C:250:LEU:HD21	1:C:291:ILE:HD13	2.02	0.41
1:E:183:SER:HA	1:E:186:ARG:HD3	2.01	0.41
1:A:44:PHE:O	1:A:48:SER:OG	2.37	0.41
1:B:79:LEU:HD12	1:B:79:LEU:HA	1.84	0.41
1:B:221:ILE:HG13	3:B:437:HOH:O	2.21	0.41
1:D:275:VAL:CG1	1:D:283:LEU:HD22	2.50	0.41
1:F:154:VAL:HG12	1:F:162:ARG:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASP:HB3	1:A:276:TYR:CE2	2.55	0.41
1:C:230:PRO:HD2	1:C:241:ALA:HA	2.03	0.41
1:E:224:ASP:OD2	1:E:226:SER:OG	2.38	0.41
1:F:219:VAL:C	1:F:262:VAL:HG13	2.40	0.41
1:A:165:LEU:HD21	1:A:173:VAL:HG23	2.02	0.41
1:B:148:PHE:CD1	1:B:249:LEU:HD11	2.56	0.41
1:D:91:THR:N	1:D:92:GLU:OE1	2.54	0.41
1:A:41:LEU:HA	1:A:44:PHE:HB3	2.03	0.41
1:A:216:ASP:OD1	1:A:216:ASP:N	2.54	0.41
1:C:2:PHE:CD1	1:C:84:MET:HG2	2.55	0.41
1:C:58:LEU:HD23	1:C:76:MET:HE3	2.03	0.41
1:D:165:LEU:HD23	1:D:170:LEU:HD13	2.02	0.41
1:E:134:TYR:CD1	1:E:143:ILE:HD11	2.56	0.41
1:B:109:GLU:O	1:B:113:LYS:HG3	2.21	0.41
1:E:93:THR:HA	1:E:94:PRO:HD3	1.95	0.41
1:A:152:PRO:HG3	1:A:178:ASN:OD1	2.22	0.40
1:E:145[B]:ILE:HD12	1:E:170:LEU:HD21	2.02	0.40
1:A:131:VAL:HG11	1:A:164:LEU:CD1	2.52	0.40
1:B:165:LEU:HD13	1:B:194:MET:HE1	2.03	0.40
1:E:37:ARG:HE	1:E:85:LEU:HD21	1.87	0.40
1:F:182:SER:O	1:F:186:ARG:HG3	2.21	0.40
1:A:31:TYR:CD2	1:A:126:ALA:HB2	2.56	0.40
1:C:112:GLU:HA	1:C:112:GLU:OE2	2.22	0.40
1:C:160:PRO:O	1:C:164:LEU:HG	2.21	0.40
1:D:29:PHE:CZ	1:D:119:SER:HB2	2.56	0.40
1:D:213:ILE:O	1:D:215:ASN:ND2	2.55	0.40
1:F:10:LYS:HD2	1:F:109:GLU:HG2	2.04	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	286/351 (82%)	266 (93%)	14 (5%)	6 (2%)	7 1
1	B	280/351 (80%)	272 (97%)	8 (3%)	0	100 100
1	C	284/351 (81%)	272 (96%)	12 (4%)	0	100 100
1	D	287/351 (82%)	275 (96%)	9 (3%)	3 (1%)	15 5
1	E	284/351 (81%)	264 (93%)	19 (7%)	1 (0%)	34 21
1	F	286/351 (82%)	266 (93%)	18 (6%)	2 (1%)	22 10
All	All	1707/2106 (81%)	1615 (95%)	80 (5%)	12 (1%)	22 10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	41	LEU
1	A	237	ASP
1	D	214	ARG
1	D	297	LEU
1	D	199	MET
1	F	89	ALA
1	A	70	PRO
1	A	297	LEU
1	E	71	GLU
1	A	36	PRO
1	F	259	PRO

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	247/300 (82%)	226 (92%)	21 (8%)	10 3
1	B	244/300 (81%)	211 (86%)	33 (14%)	4 1
1	C	245/300 (82%)	218 (89%)	27 (11%)	6 1
1	D	246/300 (82%)	224 (91%)	22 (9%)	9 2
1	E	245/300 (82%)	218 (89%)	27 (11%)	6 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	247/300 (82%)	220 (89%)	27 (11%)	6 1
All	All	1474/1800 (82%)	1317 (89%)	157 (11%)	7 1

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	A	28	LEU
1	A	42	LEU
1	A	43	ASP
1	A	54	HIS
1	A	72	THR
1	A	76	MET
1	A	84	MET
1	A	129	SER
1	A	136	ARG
1	A	155	SER
1	A	158	ARG
1	A	161	LEU
1	A	170	LEU
1	A	187	LYS
1	A	188	VAL
1	A	191	LEU
1	A	192	HIS
1	A	213	ILE
1	A	260	LYS
1	A	298	LYS
1	B	7	MET
1	B	9	VAL
1	B	13	THR
1	B	15	ARG
1	B	21	ASN
1	B	22	ARG
1	B	23	LEU
1	B	38	ARG
1	B	43	ASP
1	B	47	GLN
1	B	62	ASP
1	B	63	LYS
1	B	72	THR
1	B	83	GLN
1	B	85	LEU

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Mol	Chain	Res	Type
1	B	86	ASP
1	B	87	GLU
1	B	93	THR
1	B	107	SER
1	B	142	ASP
1	B	143	ILE
1	B	145	ILE
1	B	155	SER
1	B	156	ASP
1	B	171	LYS
1	B	184	GLU
1	B	197	MET
1	B	212	ASP
1	B	216	ASP
1	B	238	SER
1	B	262	VAL
1	B	283	LEU
1	B	298	LYS
1	C	7	MET
1	C	8	ASN
1	C	18	ASP
1	C	22	ARG
1	C	28	LEU
1	C	53	ASP
1	C	63	LYS
1	C	66	ILE
1	C	75	PHE
1	C	76	MET
1	C	92	GLU
1	C	95	THR
1	C	96	SER
1	C	97	ASP
1	C	105	GLU
1	C	112	GLU
1	C	131	VAL
1	C	135	LYS
1	C	142	ASP
1	C	151	ARG
1	C	155	SER
1	C	170	LEU
1	C	213	ILE
1	C	238	SER

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Mol	Chain	Res	Type
1	C	257	ARG
1	C	262	VAL
1	C	283	LEU
1	D	7	MET
1	D	10	LYS
1	D	13	THR
1	D	22	ARG
1	D	28	LEU
1	D	50	ARG
1	D	63	LYS
1	D	86	ASP
1	D	96	SER
1	D	97	ASP
1	D	109	GLU
1	D	145[A]	ILE
1	D	145[B]	ILE
1	D	158	ARG
1	D	170	LEU
1	D	195	PHE
1	D	212	ASP
1	D	215	ASN
1	D	216	ASP
1	D	219	VAL
1	D	223	ILE
1	D	283	LEU
1	E	0	HIS
1	E	1	MET
1	E	7	MET
1	E	9	VAL
1	E	22	ARG
1	E	28	LEU
1	E	38	ARG
1	E	48	SER
1	E	57	GLU
1	E	62	ASP
1	E	63	LYS
1	E	66	ILE
1	E	73	VAL
1	E	83	GLN
1	E	87	GLU
1	E	92	GLU
1	E	93	THR

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Mol	Chain	Res	Type
1	E	142	ASP
1	E	145[A]	ILE
1	E	145[B]	ILE
1	E	151	ARG
1	E	170	LEU
1	E	180	GLN
1	E	193	LYS
1	E	200	HIS
1	E	214	ARG
1	E	257	ARG
1	F	1	MET
1	F	7	MET
1	F	15	ARG
1	F	46	LEU
1	F	47	GLN
1	F	67	GLU
1	F	95	THR
1	F	97	ASP
1	F	101	LEU
1	F	129	SER
1	F	131	VAL
1	F	151	ARG
1	F	154	VAL
1	F	156	ASP
1	F	158	ARG
1	F	183	SER
1	F	189	ARG
1	F	199	MET
1	F	212	ASP
1	F	214[A]	ARG
1	F	214[B]	ARG
1	F	238	SER
1	F	247	ARG
1	F	260	LYS
1	F	262	VAL
1	F	283	LEU
1	F	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	83	GLN

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Mol	Chain	Res	Type
1	D	61	HIS
1	F	47	GLN

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)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	EDO	C	402	-	3,3,3	0.40	0	2,2,2	0.30	0
2	EDO	C	401	-	3,3,3	0.41	0	2,2,2	0.27	0
2	EDO	C	403	-	3,3,3	0.44	0	2,2,2	0.36	0
2	EDO	A	401	-	3,3,3	0.42	0	2,2,2	0.26	0

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
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
2	EDO	C	403	-	-	1/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	403	EDO	O1-C1-C2-O2
2	C	401	EDO	O1-C1-C2-O2
2	A	401	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	402	EDO	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	289/351 (82%)	-0.26	2 (0%) 87 86	12, 24, 47, 64	0
1	B	286/351 (81%)	-0.28	4 (1%) 75 72	10, 22, 42, 68	0
1	C	287/351 (81%)	-0.48	3 (1%) 82 80	9, 21, 40, 57	0
1	D	290/351 (82%)	-0.51	3 (1%) 82 80	8, 21, 40, 63	0
1	E	287/351 (81%)	-0.33	0 100 100	12, 25, 42, 68	0
1	F	288/351 (82%)	-0.36	3 (1%) 82 80	11, 25, 43, 66	0
All	All	1727/2106 (82%)	-0.37	15 (0%) 84 82	8, 23, 43, 68	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	ALA	5.1
1	F	72	THR	4.5
1	A	213	ILE	3.9
1	A	73	VAL	3.2
1	B	213	ILE	3.2
1	F	88	ALA	2.7
1	B	21	ASN	2.6
1	D	88	ALA	2.4
1	F	89	ALA	2.3
1	D	212	ASP	2.3
1	C	91	THR	2.2
1	C	90	GLY	2.2
1	B	-1	SER	2.1
1	C	89	ALA	2.1
1	D	213	ILE	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	C	403	4/4	0.93	0.08	18,18,22,28	0
2	EDO	C	402	4/4	0.95	0.06	17,21,21,27	0
2	EDO	A	401	4/4	0.95	0.09	29,31,35,41	0
2	EDO	C	401	4/4	0.98	0.07	14,15,22,23	0

6.5 Other polymers (i)

There are no such residues in this entry.