



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:40 AM UTC

PDB ID : 4RHJ / pdb_00004rhj
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

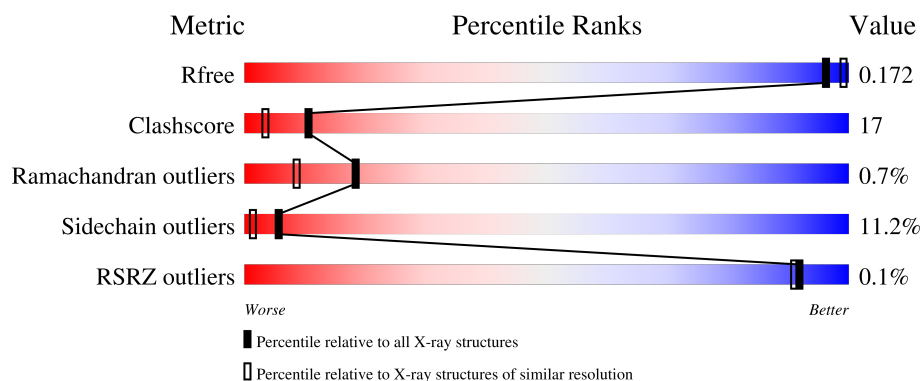
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

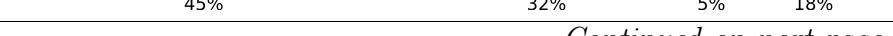
The reported resolution of this entry is 1.80 Å.

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 $\leq 5\%$. 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	351	
1	B	351	
1	C	351	
1	D	351	
1	E	351	

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Mol	Chain	Length	Quality of chain
1	F	351	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (47%), yellow (31%), orange (1%), and grey (18%). The percentages are labeled below the bar.

2 Entry composition

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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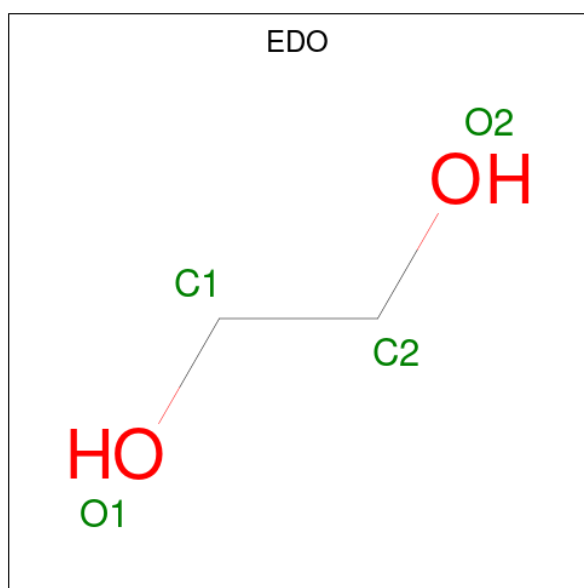
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q581Y0
D	-19	MET	-	expression tag	UNP Q581Y0
D	-18	GLY	-	expression tag	UNP Q581Y0
D	-17	SER	-	expression tag	UNP Q581Y0
D	-16	SER	-	expression tag	UNP Q581Y0
D	-15	HIS	-	expression tag	UNP Q581Y0
D	-14	HIS	-	expression tag	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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

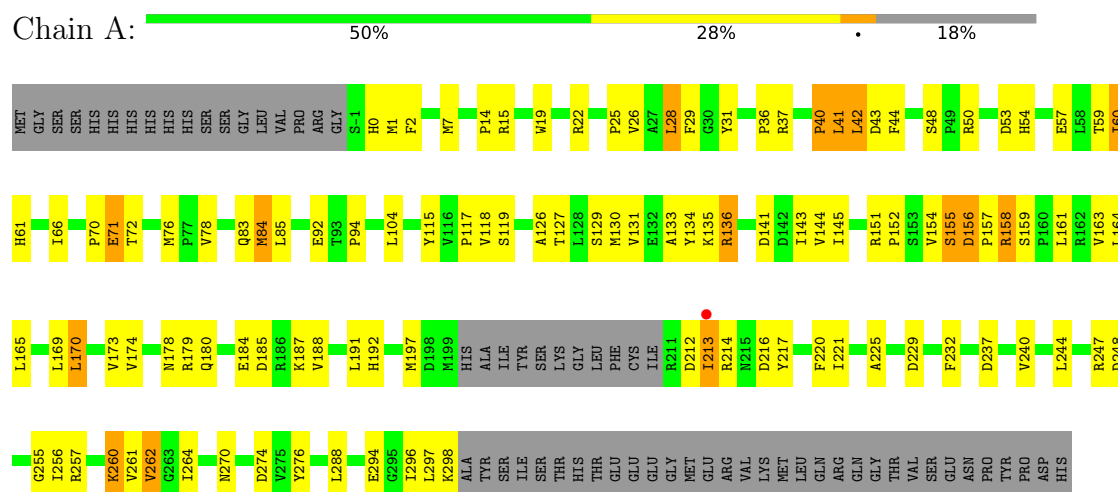
- Molecule 3 is water.

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

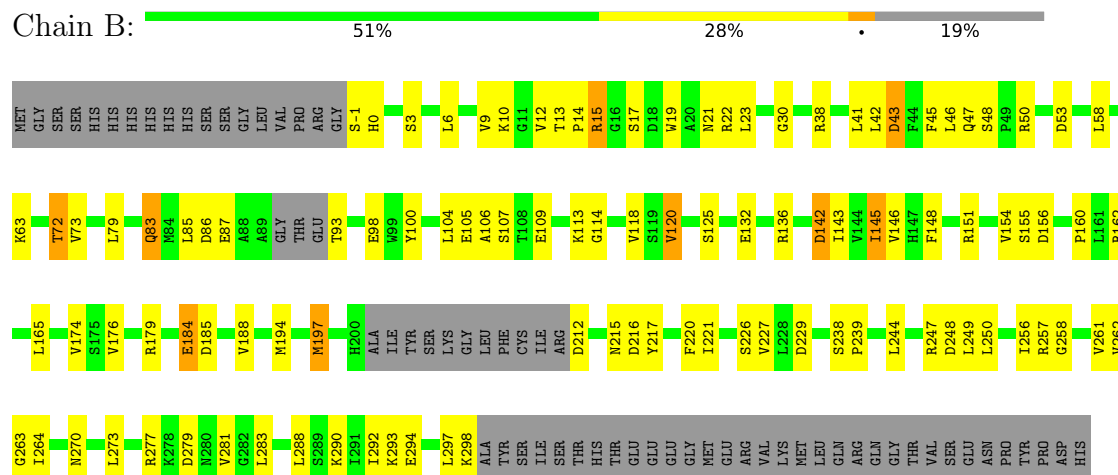
3 Residue-property plots

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

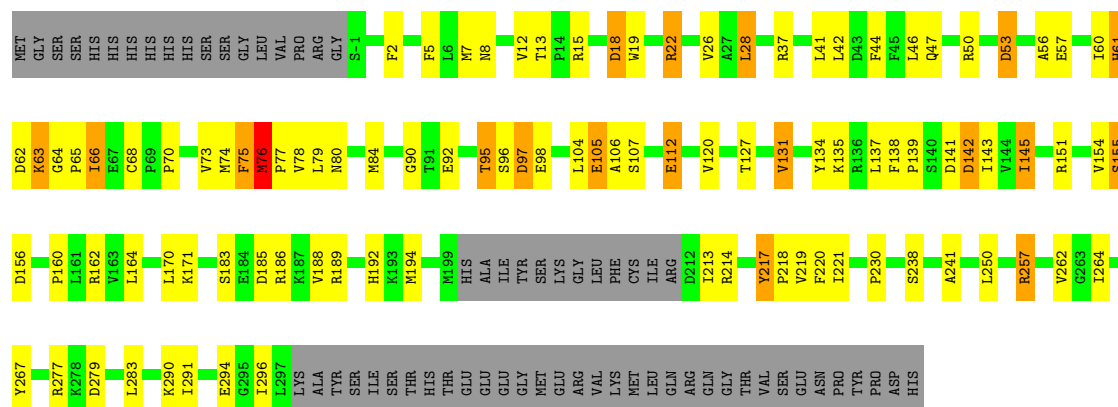


• Molecule 1: Arginase

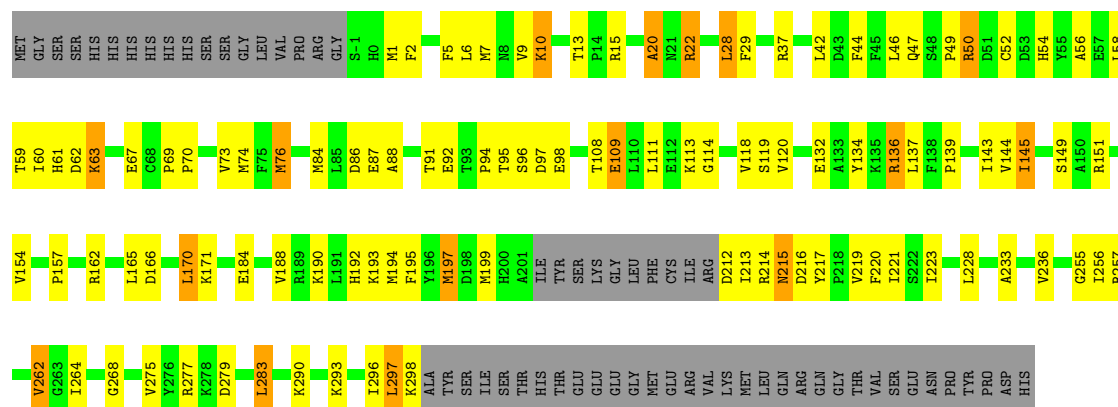


• Molecule 1: Arginase

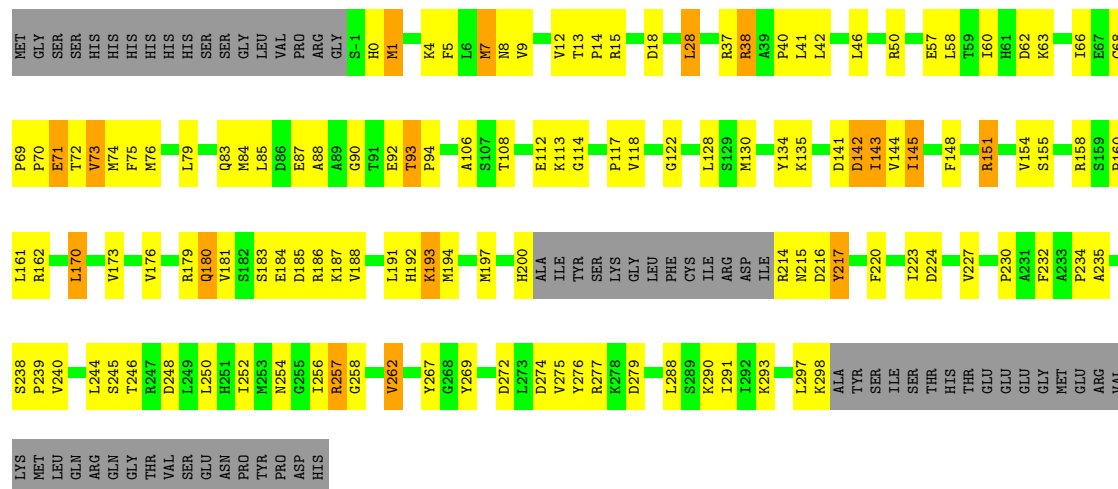




• Molecule 1: Arginase

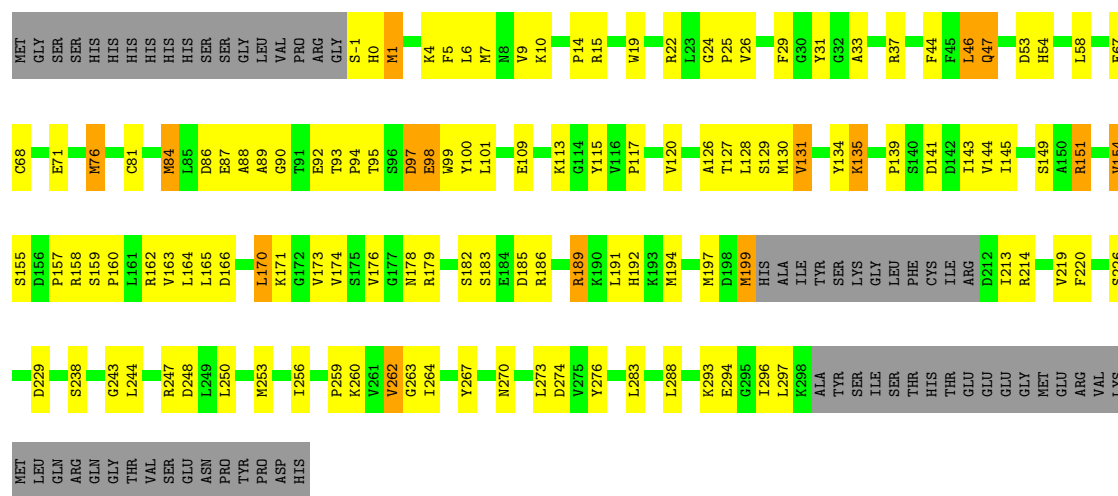


• Molecule 1: Arginase



• Molecule 1: Arginase

Chain F:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 0.172	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)	0.33 , 23.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	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	0.97	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

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	0.58	0/2284	0.95	8/3096 (0.3%)
1	B	0.58	0/2255	0.95	2/3056 (0.1%)
1	C	0.62	0/2264	1.00	8/3071 (0.3%)
1	D	0.64	0/2285	0.95	7/3100 (0.2%)
1	E	0.56	0/2268	0.97	7/3075 (0.2%)
1	F	0.55	0/2284	0.92	4/3096 (0.1%)
All	All	0.59	0/13640	0.96	36/18494 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	20	ALA	N-CA-C	7.30	119.24	111.28
1	F	76	MET	CA-C-N	6.84	127.08	119.90
1	F	76	MET	C-N-CA	6.84	127.08	119.90
1	E	68	CYS	CA-C-N	-6.68	113.50	120.38
1	E	68	CYS	C-N-CA	-6.68	113.50	120.38
1	E	217	TYR	CA-C-N	6.54	126.57	119.90
1	E	217	TYR	C-N-CA	6.54	126.57	119.90
1	C	219	VAL	N-CA-C	6.19	116.78	107.75
1	C	156	ASP	CA-C-N	6.17	125.87	119.82
1	C	156	ASP	C-N-CA	6.17	125.87	119.82
1	C	217	TYR	CA-C-N	6.07	126.09	119.90
1	C	217	TYR	C-N-CA	6.07	126.09	119.90
1	A	217	TYR	CA-C-N	5.99	126.34	119.93
1	A	217	TYR	C-N-CA	5.99	126.34	119.93
1	F	98	GLU	N-CA-C	-5.97	106.61	114.31
1	D	62	ASP	N-CA-C	-5.82	106.34	113.50
1	E	143	ILE	N-CA-C	5.82	116.57	108.89
1	D	111	LEU	N-CA-C	5.54	117.13	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	MET	CA-C-N	5.47	126.68	119.84
1	C	76	MET	C-N-CA	5.47	126.68	119.84
1	A	71	GLU	CB-CA-C	-5.42	110.31	116.54
1	D	76	MET	CA-C-N	5.37	126.84	120.23
1	D	76	MET	C-N-CA	5.37	126.84	120.23
1	C	267	TYR	N-CA-C	5.36	116.14	108.74
1	A	156	ASP	CA-C-N	5.35	125.01	119.56
1	A	156	ASP	C-N-CA	5.35	125.01	119.56
1	B	229	ASP	CA-C-N	5.18	124.89	119.82
1	B	229	ASP	C-N-CA	5.18	124.89	119.82
1	F	267	TYR	N-CA-C	5.15	115.85	108.74
1	D	217	TYR	CA-C-N	5.07	125.07	119.90
1	D	217	TYR	C-N-CA	5.07	125.07	119.90
1	A	60	ILE	N-CA-C	5.07	115.15	107.80
1	A	270	ASN	CA-C-N	5.05	125.33	119.47
1	A	270	ASN	C-N-CA	5.05	125.33	119.47
1	E	13	THR	CA-C-N	5.04	125.32	119.92
1	E	13	THR	C-N-CA	5.04	125.32	119.92

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	82	0
1	B	2205	0	2212	64	0
1	C	2211	0	2220	67	0
1	D	2231	0	2234	74	0
1	E	2214	0	2225	80	0
1	F	2228	0	2246	84	0
2	A	4	0	6	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	449	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 17.

All (449) 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:D:58:LEU:HD23	1:D:76:MET:HE3	1.72	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
1:B:154:VAL:O	1:B:162:ARG:NH1	2.24	0.69
1:F:4:LYS:NZ	3:F:435:HOH:O	2.25	0.68
1:E:256:ILE:O	1:E:257:ARG:NH1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:192:HIS:HB2	1:D:194:MET:HE2	1.77	0.65
1:F:250:LEU:HA	1:F:253:MET:HE2	1.79	0.65
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:F:1:MET:HE1	1:F:92:GLU:HB2	1.80	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: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:A:0:HIS:HE1	1:A:92:GLU:HB2	1.64	0.61
1:B:12:VAL:O	1:B:113:LYS:NZ	2.27	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:A:1:MET:HE2	1:A:37:ARG:HH22	1.64	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:E:192:HIS:O	1:E:193:LYS:C	2.45	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: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: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:E:117:PRO:HB2	1:E:130:MET:HE3	1.87	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: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
1:C:61:HIS:CD2	1:C:66:ILE:HD12	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:ILE:C	1:D:298:LYS:N	2.65	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: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:F:53:ASP:H	1:F:294:GLU:CD	2.15	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:C:104:LEU:O	1:C:107:SER:OG	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LEU:O	1:C:46:LEU:HG	2.08	0.52
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:C:95:THR:OG1	1:C:98:GLU:OE1	2.29	0.51
1:D:296:ILE:C	1:D:298:LYS:H	2.17	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: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: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:D:9:VAL:HG12	1:D:109:GLU:HG2	1.91	0.50
1:D:149:SER:OG	1:D:151:ARG:O	2.25	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:A:260:LYS:HZ1	1:A:261:VAL:C	2.20	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: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:F:31:TYR:HD1	1:F:84:MET:HE3	1.77	0.49
1:C:53:ASP:OD1	1:C:290:LYS:NZ	2.30	0.49
1:C:155:SER:OG	1:C:185:ASP:OD1	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:171:LYS:HD3	1:C:217:TYR:CE1	2.47	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:B:165:LEU:HD13	1:B:194:MET:HE2	1.94	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:D:49:PRO:O	1:D:293:LYS:NZ	2.46	0.48
1:B:148:PHE:HB3	1:B:227:VAL:HG11	1.95	0.48
1:A:117:PRO:HB2	1:A:130:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:PRO:HB2	1:F:130:MET:HE3	1.95	0.47
1:C:19:TRP:HA	1:C:22:ARG:HG3	1.96	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
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:D:1:MET:HE2	1:D:37:ARG:HH22	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:4:LYS:HD3	1:F:86:ASP:OD1	2.15	0.46
1:F:219:VAL:C	1:F:262:VAL:HG13	2.40	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:B:197:MET:HE3	1:B:197:MET:HB2	1.87	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:C:188:VAL:HG12	1:C:194:MET:HE1	1.97	0.45
1:E:297:LEU:CD1	1:E:298:LYS:HG3	2.47	0.45
1:A:174:VAL:CG1	1:A:197:MET:HE1	2.47	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:A:29:PHE:CE2	1:A:84:MET:HE3	2.52	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:C:135:LYS:HA	1:C:135:LYS:HD3	1.72	0.45
1:E:197:MET:HE2	1:E:197:MET:HB3	1.87	0.45
1:B:146:VAL:HG13	1:B:174:VAL:HB	1.99	0.45
1:F:199:MET:HE1	1:F:244:LEU:HD23	2.00	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:E:1:MET:HE2	1:E:1:MET:HB3	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:10:LYS:HZ3	1:F:109:GLU:CD	2.26	0.44
1:F:127:THR:O	1:F:131:VAL:HG12	2.18	0.44
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:F:0:HIS:HE2	1:F:92:GLU:CD	2.25	0.43
1:D:52:CYS:HA	1:D:293:LYS:HE3	1.99	0.43
1:F:1:MET:HB3	1:F:1:MET:HE3	1.81	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:D:76:MET:HE3	1:D:76:MET:HB2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASP:CB	1:A:214:ARG:HG3	2.47	0.42
1:F:1:MET:HE2	1:F:94:PRO:HD3	2.01	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:F:84:MET:HB2	1:F:84:MET:HE2	1.51	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:C:137:LEU:C	1:C:139:PRO:HD3	2.45	0.42
1:D:197:MET:HE3	1:D:197:MET:HB2	1.83	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
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:C:192:HIS:HB2	1:C:194:MET:HE2	2.01	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: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:37:ARG:HH12	1:E:90:GLY:C	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:71:GLU:H	1:F:71:GLU:CD	2.27	0.41
1:F:189:ARG:HA	1:F:194:MET:HE2	2.01	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
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: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:C:2:PHE:CD1	1:C:84:MET:HG2	2.55	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:F:4:LYS:HD3	1:F:86:ASP:CG	2.46	0.41
1:B:109:GLU:O	1:B:113:LYS:HG3	2.21	0.41
1:C:76:MET:HE2	1:C:76:MET:HB2	1.81	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:F:263:GLY:C	1:F:264:ILE:HG13	2.45	0.40
1:A:131:VAL:HG11	1:A:164:LEU:CD1	2.52	0.40
1:C:189:ARG:HA	1:C:194:MET:HE3	2.04	0.40
1:E:37:ARG:HE	1:E:85:LEU:HD21	1.87	0.40
1:F:149:SER:OG	1:F:151:ARG:O	2.29	0.40
1:B:0:HIS:O	1:B:3:SER:OG	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:VAL:HG22	1:F:197:MET:HE2	2.03	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:A:216:ASP:OD1	1:A:216:ASP:N	2.54	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%)	5	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%)	12	4
1	E	284/351 (81%)	264 (93%)	19 (7%)	1 (0%)	30	19
1	F	286/351 (82%)	266 (93%)	18 (6%)	2 (1%)	18	8
All	All	1707/2106 (81%)	1615 (95%)	80 (5%)	12 (1%)	18	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	41	LEU
1	A	237	ASP

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Mol	Chain	Res	Type
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 ⓘ

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%)	222 (90%)	25 (10%)	7	2
1	B	244/300 (81%)	213 (87%)	31 (13%)	4	1
1	C	245/300 (82%)	216 (88%)	29 (12%)	5	1
1	D	246/300 (82%)	220 (89%)	26 (11%)	6	1
1	E	245/300 (82%)	219 (89%)	26 (11%)	6	1
1	F	247/300 (82%)	215 (87%)	32 (13%)	4	1
All	All	1474/1800 (82%)	1305 (88%)	169 (12%)	6	1

All (169) 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	57	GLU
1	A	59	THR
1	A	72	THR
1	A	76	MET

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Mol	Chain	Res	Type
1	A	84	MET
1	A	129	SER
1	A	136	ARG
1	A	144	VAL
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	262	VAL
1	A	298	LYS
1	B	9	VAL
1	B	13	THR
1	B	15	ARG
1	B	21	ASN
1	B	23	LEU
1	B	38	ARG
1	B	43	ASP
1	B	47	GLN
1	B	63	LYS
1	B	72	THR
1	B	83	GLN
1	B	85	LEU
1	B	86	ASP
1	B	87	GLU
1	B	93	THR
1	B	105	GLU
1	B	107	SER
1	B	120	VAL
1	B	142	ASP
1	B	143	ILE
1	B	145	ILE
1	B	155	SER
1	B	156	ASP
1	B	184	GLU
1	B	197	MET
1	B	212	ASP

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Mol	Chain	Res	Type
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	61	HIS
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	142	ASP
1	C	145[A]	ILE
1	C	145[B]	ILE
1	C	151	ARG
1	C	155	SER
1	C	170	LEU
1	C	213	ILE
1	C	238	SER
1	C	257	ARG
1	C	262	VAL
1	C	283	LEU
1	D	10	LYS
1	D	13	THR
1	D	22	ARG
1	D	28	LEU
1	D	50	ARG
1	D	60	ILE
1	D	63	LYS
1	D	86	ASP

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Mol	Chain	Res	Type
1	D	96	SER
1	D	97	ASP
1	D	109	GLU
1	D	120	VAL
1	D	136	ARG
1	D	145[A]	ILE
1	D	145[B]	ILE
1	D	170	LEU
1	D	190	LYS
1	D	193	LYS
1	D	195	PHE
1	D	197	MET
1	D	215	ASN
1	D	216	ASP
1	D	219	VAL
1	D	223	ILE
1	D	262	VAL
1	D	283	LEU
1	E	0	HIS
1	E	1	MET
1	E	7	MET
1	E	9	VAL
1	E	28	LEU
1	E	38	ARG
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	92	GLU
1	E	93	THR
1	E	142	ASP
1	E	144	VAL
1	E	145[A]	ILE
1	E	145[B]	ILE
1	E	151	ARG
1	E	170	LEU
1	E	180	GLN
1	E	184	GLU
1	E	193	LYS
1	E	200	HIS

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Mol	Chain	Res	Type
1	E	257	ARG
1	E	262	VAL
1	F	1	MET
1	F	7	MET
1	F	46	LEU
1	F	47	GLN
1	F	67	GLU
1	F	84	MET
1	F	95	THR
1	F	97	ASP
1	F	101	LEU
1	F	120	VAL
1	F	129	SER
1	F	131	VAL
1	F	135	LYS
1	F	144	VAL
1	F	151	ARG
1	F	154	VAL
1	F	158	ARG
1	F	170	LEU
1	F	171	LYS
1	F	178	ASN
1	F	183	SER
1	F	189	ARG
1	F	191	LEU
1	F	199	MET
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	83	GLN
1	C	180	GLN
1	C	254	ASN
1	D	61	HIS

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Mol	Chain	Res	Type
1	D	147	HIS
1	D	192	HIS
1	E	251	HIS
1	F	47	GLN
1	F	192	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	401	-	3,3,3	0.39	0	2,2,2	0.31	0
2	EDO	C	401	-	3,3,3	0.38	0	2,2,2	0.32	0
2	EDO	C	402	-	3,3,3	0.37	0	2,2,2	0.34	0
2	EDO	C	403	-	3,3,3	0.41	0	2,2,2	0.38	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	A	401	-	-	1/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	C	403	-	-	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 [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	289/351 (82%)	-0.97	1 (0%) 90 90	12, 24, 47, 64	1 (0%)
1	B	286/351 (81%)	-1.05	0 100 100	10, 22, 42, 68	0
1	C	287/351 (81%)	-1.08	0 100 100	9, 21, 40, 57	1 (0%)
1	D	290/351 (82%)	-1.08	0 100 100	8, 21, 40, 63	1 (0%)
1	E	287/351 (81%)	-0.98	0 100 100	12, 25, 42, 68	1 (0%)
1	F	288/351 (82%)	-0.99	0 100 100	11, 25, 43, 66	2 (0%)
All	All	1727/2106 (82%)	-1.03	1 (0%) 92 91	8, 23, 43, 68	6 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	401	4/4	0.97	0.08	29,31,35,41	0
2	EDO	C	401	4/4	0.99	0.03	14,15,22,23	0
2	EDO	C	402	4/4	0.99	0.04	17,21,21,27	0
2	EDO	C	403	4/4	0.99	0.04	18,18,22,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.