



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:19 PM UTC

PDB ID : 3O4H / pdb_00003o4h
Title : Structure and Catalysis of Acylaminoacyl Peptidase
Authors : Harmat, V.; Domokos, K.; Menyhard, D.K.; Pallo, A.; Szeltner, Z.; Szamosi, I.; Beke-Somfai, T.; Naray-Szabo, G.; Polgar, L.
Deposited on : 2010-07-27
Resolution : 1.82 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

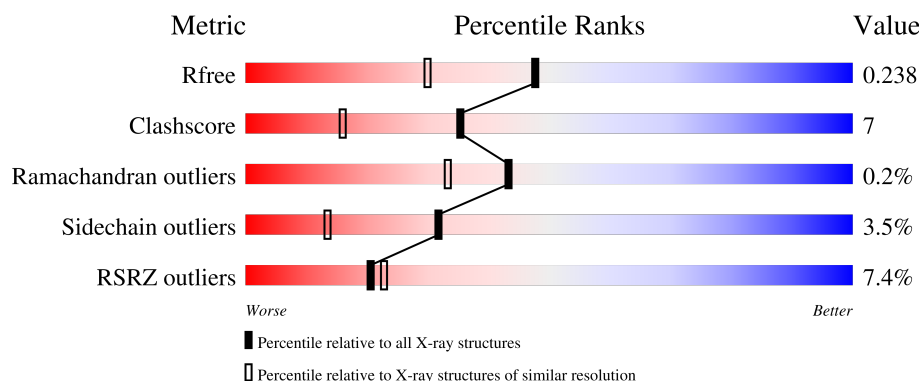
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	582	8% 88% 9% ...
1	B	582	8% 87% 9% ..
1	C	582	12% 86% 11% ..
1	D	582	9% 86% 10% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18167 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.

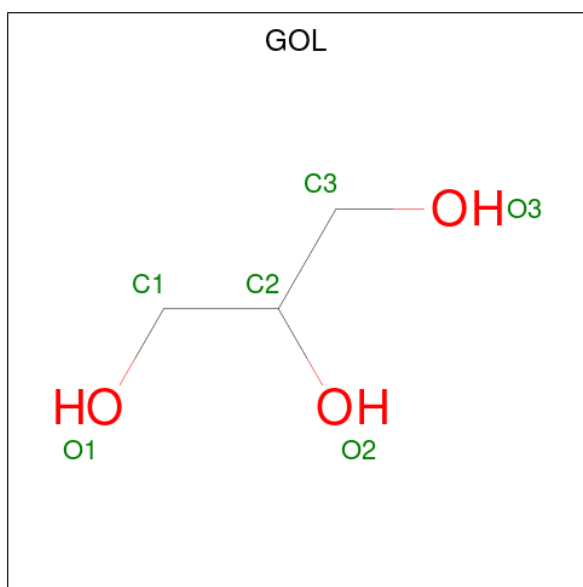
- Molecule 1 is a protein called Acylamino-acid-releasing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	5	0
			4350	2756	760	822	12			
1	B	574	Total	C	N	O	S	0	2	0
			4255	2712	734	797	12			
1	C	577	Total	C	N	O	S	0	5	0
			4309	2743	745	808	13			
1	D	575	Total	C	N	O	S	0	1	0
			4287	2721	747	807	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	524	ALA	ASP	engineered mutation	UNP Q9YBQ2
B	524	ALA	ASP	engineered mutation	UNP Q9YBQ2
C	524	ALA	ASP	engineered mutation	UNP Q9YBQ2
D	524	ALA	ASP	engineered mutation	UNP Q9YBQ2

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			12	6	6		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	313	Total	O	0	0
			313	313		
4	B	216	Total	O	0	0
			216	216		

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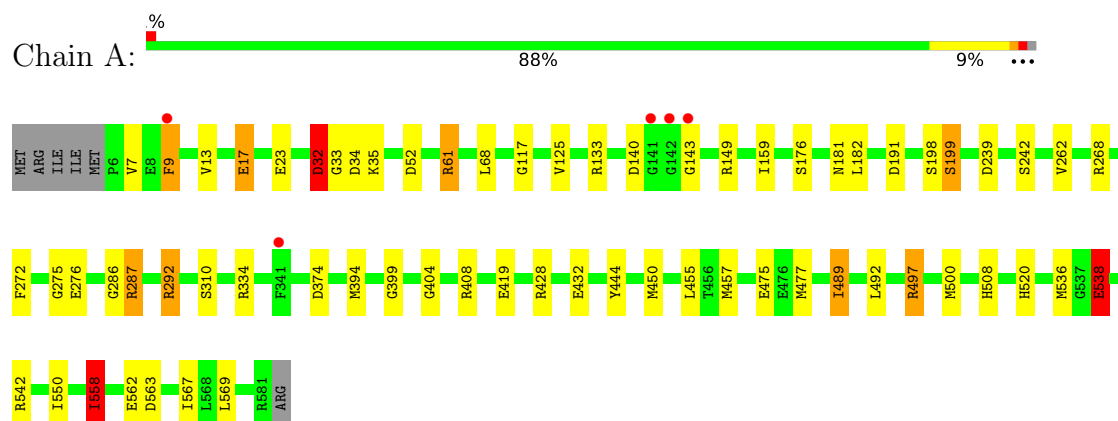
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	205	Total 205	O 205	0	0
4	D	194	Total 194	O 194	0	0

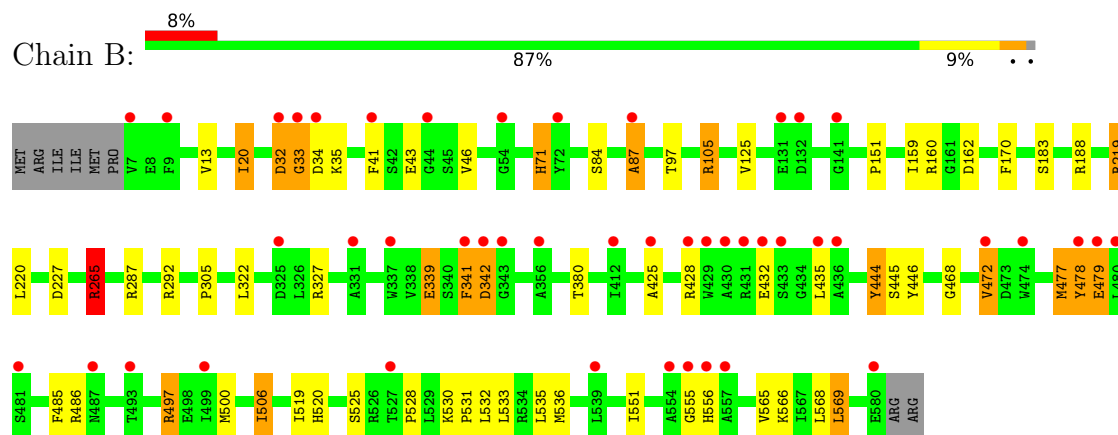
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

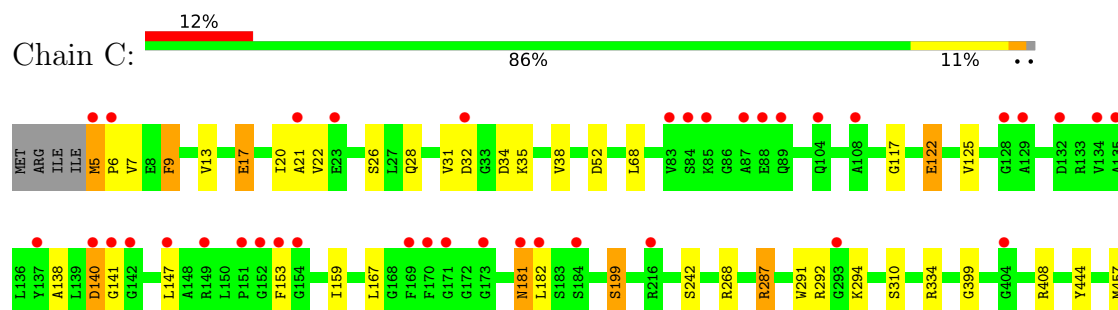
• Molecule 1: Acylamino-acid-releasing enzyme

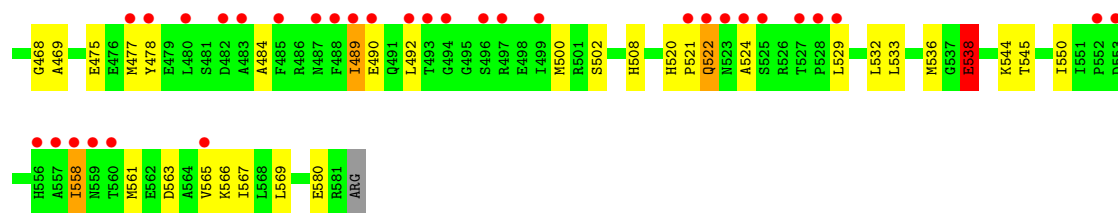


• Molecule 1: Acylamino-acid-releasing enzyme

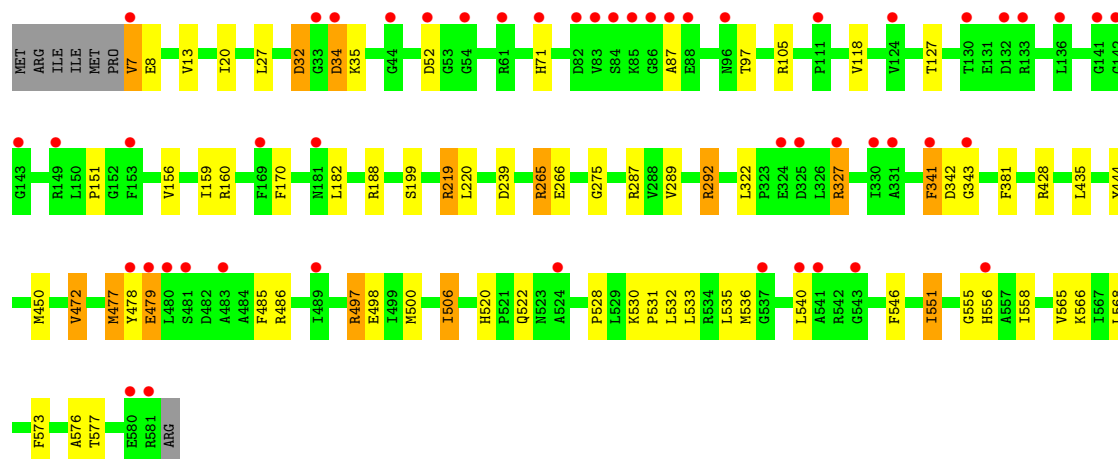
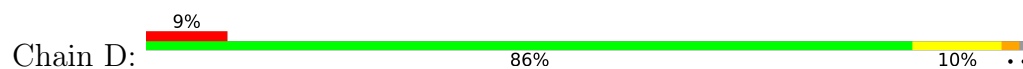


• Molecule 1: Acylamino-acid-releasing enzyme





● Molecule 1: Acylamino-acid-releasing enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.41Å 97.98Å 98.80Å 105.69° 103.52° 100.36°	Depositor
Resolution (Å)	24.62 – 1.82 24.62 – 1.82	Depositor EDS
% Data completeness (in resolution range)	95.3 (24.62-1.82) 95.2 (24.62-1.82)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.203 , 0.234 0.208 , 0.238	Depositor DCC
R_{free} test set	10894 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18167	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.05	18/4457 (0.4%)	1.02	15/6050 (0.2%)
1	B	1.12	26/4354 (0.6%)	1.06	15/5917 (0.3%)
1	C	1.01	16/4410 (0.4%)	1.01	19/5994 (0.3%)
1	D	1.07	17/4382 (0.4%)	1.08	14/5953 (0.2%)
All	All	1.06	77/17603 (0.4%)	1.04	63/23914 (0.3%)

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	C	0	1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	ARG	CZ-NH1	-12.87	1.14	1.32
1	D	265	ARG	CZ-NH1	-12.86	1.14	1.32
1	B	265	ARG	CZ-NH1	-12.39	1.15	1.32
1	B	105	ARG	CZ-NH1	-12.30	1.15	1.32
1	B	339	GLU	C-O	11.77	1.38	1.24
1	C	287	ARG	CZ-NH1	-11.71	1.16	1.32
1	B	160	ARG	CZ-NH1	-11.64	1.16	1.32
1	D	105	ARG	CZ-NH1	-11.54	1.16	1.32
1	A	268	ARG	CZ-NH2	-10.90	1.19	1.33
1	A	292	ARG	CZ-NH2	-10.49	1.19	1.33
1	C	268	ARG	CZ-NH2	-10.42	1.20	1.33
1	B	32[A]	ASP	C-O	-9.91	1.15	1.24
1	B	32[B]	ASP	C-O	-9.91	1.15	1.24
1	D	160	ARG	CZ-NH1	-9.89	1.18	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	ARG	CZ-NH2	-9.75	1.20	1.33
1	A	292	ARG	CZ-NH1	-9.70	1.19	1.32
1	C	292	ARG	CZ-NH2	-9.56	1.21	1.33
1	D	292	ARG	CZ-NH1	-9.38	1.19	1.32
1	D	292	ARG	CZ-NH2	-9.33	1.21	1.33
1	B	485	PHE	CE1-CZ	-9.31	1.10	1.38
1	C	292	ARG	CZ-NH1	-9.25	1.19	1.32
1	A	268	ARG	CZ-NH1	-9.22	1.19	1.32
1	C	268	ARG	CZ-NH1	-8.58	1.20	1.32
1	D	87	ALA	C-O	-8.53	1.13	1.24
1	D	485	PHE	CE1-CZ	-8.44	1.13	1.38
1	A	9	PHE	CE2-CZ	-8.40	1.13	1.38
1	A	444	TYR	CG-CD1	-8.39	1.21	1.39
1	D	485	PHE	CE2-CZ	-8.36	1.13	1.38
1	A	444	TYR	CE2-CZ	-8.29	1.18	1.38
1	D	498	GLU	CD-OE1	8.26	1.41	1.25
1	B	485	PHE	CE2-CZ	-8.15	1.14	1.38
1	B	444	TYR	CE2-CZ	-8.12	1.18	1.38
1	C	9	PHE	CE1-CZ	-8.10	1.14	1.38
1	B	160	ARG	CZ-NH2	-8.10	1.23	1.33
1	B	444	TYR	CG-CD1	-8.00	1.22	1.39
1	D	444	TYR	CG-CD1	-7.96	1.22	1.39
1	D	485	PHE	CG-CD2	-7.85	1.22	1.38
1	A	444	TYR	CE1-CZ	-7.83	1.19	1.38
1	C	9	PHE	CE2-CZ	-7.79	1.15	1.38
1	C	9	PHE	CG-CD2	-7.76	1.22	1.38
1	D	485	PHE	CG-CD1	-7.75	1.22	1.38
1	B	444	TYR	CE1-CZ	-7.72	1.19	1.38
1	B	292	ARG	CZ-NH1	-7.71	1.22	1.32
1	C	9	PHE	CG-CD1	-7.69	1.22	1.38
1	A	444	TYR	CG-CD2	-7.65	1.23	1.39
1	B	444	TYR	CG-CD2	-7.63	1.23	1.39
1	C	444	TYR	CE2-CZ	-7.61	1.20	1.38
1	A	9	PHE	CE1-CZ	-7.60	1.15	1.38
1	C	444	TYR	CE1-CZ	-7.59	1.20	1.38
1	D	444	TYR	CG-CD2	-7.55	1.23	1.39
1	A	17	GLU	CB-CG	-7.51	1.29	1.52
1	C	444	TYR	CG-CD2	-7.41	1.23	1.39
1	B	485	PHE	CG-CD2	-7.34	1.23	1.38
1	C	444	TYR	CG-CD1	-7.31	1.24	1.39
1	A	9	PHE	CG-CD1	-7.28	1.23	1.38
1	C	17	GLU	CB-CG	-7.26	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455	LEU	CG-CD1	-7.19	1.28	1.52
1	B	87	ALA	C-O	-7.15	1.15	1.23
1	D	444	TYR	CE1-CZ	-7.05	1.21	1.38
1	D	160	ARG	CZ-NH2	-7.05	1.24	1.33
1	D	32	ASP	C-O	-6.93	1.12	1.24
1	A	9	PHE	CG-CD2	-6.86	1.24	1.38
1	C	32	ASP	C-O	-6.80	1.15	1.23
1	D	444	TYR	CE2-CZ	-6.66	1.22	1.38
1	B	305	PRO	CA-C	6.62	1.55	1.51
1	A	32[A]	ASP	C-O	-6.49	1.15	1.24
1	A	32[B]	ASP	C-O	-6.49	1.15	1.24
1	B	485	PHE	CG-CD1	-6.40	1.25	1.38
1	B	71	HIS	CA-C	-6.22	1.44	1.52
1	A	140	ASP	CB-CG	-6.21	1.36	1.52
1	C	22	VAL	CA-CB	5.81	1.60	1.54
1	B	33	GLY	C-O	-5.77	1.16	1.23
1	B	220	LEU	CG-CD1	-5.28	1.35	1.52
1	B	32[A]	ASP	C-N	-5.20	1.25	1.33
1	B	32[B]	ASP	C-N	-5.20	1.25	1.33
1	B	341	PHE	C-O	-5.13	1.17	1.24
1	B	227	ASP	N-CA	5.08	1.51	1.46

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	ARG	NE-CZ-NH2	16.79	134.31	119.20
1	D	265	ARG	NE-CZ-NH2	16.60	134.14	119.20
1	B	265	ARG	NE-CZ-NH1	-15.35	106.15	121.50
1	C	287	ARG	NE-CZ-NH2	15.11	132.79	119.20
1	D	265	ARG	NE-CZ-NH1	-14.11	107.39	121.50
1	D	105	ARG	NE-CZ-NH2	13.95	131.75	119.20
1	A	287	ARG	NE-CZ-NH2	13.47	131.32	119.20
1	B	105	ARG	NE-CZ-NH2	13.37	131.23	119.20
1	A	292	ARG	NH1-CZ-NH2	-12.48	103.08	119.30
1	C	292	ARG	NH1-CZ-NH2	-12.45	103.12	119.30
1	C	268	ARG	NH1-CZ-NH2	-11.72	104.07	119.30
1	D	87	ALA	N-CA-C	11.38	127.13	112.34
1	C	268	ARG	NE-CZ-NH2	10.88	128.99	119.20
1	A	268	ARG	NH1-CZ-NH2	-10.77	105.30	119.30
1	C	5	MET	CA-C-N	10.65	131.09	119.90
1	C	5	MET	C-N-CA	10.65	131.09	119.90
1	A	292	ARG	NE-CZ-NH2	10.52	128.66	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASP	N-CA-CB	-10.45	94.70	111.62
1	C	292	ARG	NE-CZ-NH2	10.40	128.56	119.20
1	D	292	ARG	NH1-CZ-NH2	-9.55	106.88	119.30
1	D	160	ARG	NE-CZ-NH2	9.34	127.61	119.20
1	D	292	ARG	NE-CZ-NH2	9.13	127.42	119.20
1	B	292	ARG	NH1-CZ-NH2	-8.93	107.70	119.30
1	D	160	ARG	NH1-CZ-NH2	-8.10	108.78	119.30
1	A	268	ARG	NE-CZ-NH2	8.01	126.41	119.20
1	B	160	ARG	NH1-CZ-NH2	-7.95	108.96	119.30
1	C	17	GLU	CB-CA-C	-7.34	98.61	110.79
1	C	287	ARG	NE-CZ-NH1	-7.18	114.32	121.50
1	B	292	ARG	NE-CZ-NH1	7.08	128.58	121.50
1	A	558	ILE	CB-CA-C	-6.87	102.22	111.15
1	C	122	GLU	CG-CD-OE2	-6.79	102.78	118.40
1	A	538	GLU	CA-CB-CG	6.71	127.53	114.10
1	A	287	ARG	CG-CD-NE	6.60	126.52	112.00
1	A	268	ARG	NE-CZ-NH1	6.58	128.07	121.50
1	C	292	ARG	NE-CZ-NH1	6.54	128.04	121.50
1	B	105	ARG	NH1-CZ-NH2	-6.53	110.81	119.30
1	A	292	ARG	NE-CZ-NH1	6.51	128.01	121.50
1	B	322	LEU	CD1-CG-CD2	-6.33	96.87	110.80
1	D	322	LEU	CD1-CG-CD2	-6.30	96.95	110.80
1	D	105	ARG	NH1-CZ-NH2	-6.17	111.28	119.30
1	C	566	LYS	N-CA-C	6.13	118.76	111.71
1	D	551	ILE	CB-CA-C	-6.13	103.97	110.16
1	D	341	PHE	O-C-N	-6.09	115.15	122.65
1	B	435	LEU	CD1-CG-CD2	-5.93	97.76	110.80
1	C	287	ARG	CG-CD-NE	5.92	125.02	112.00
1	A	287	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	B	569	LEU	CA-C-N	-5.78	113.07	119.19
1	B	569	LEU	C-N-CA	-5.78	113.07	119.19
1	D	435	LEU	CD1-CG-CD2	-5.73	98.19	110.80
1	C	21	ALA	N-CA-C	5.73	118.47	111.82
1	C	538	GLU	CA-CB-CG	5.49	125.07	114.10
1	C	268	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	C	287	ARG	NH1-CZ-NH2	-5.39	112.29	119.30
1	A	287	ARG	NH1-CZ-NH2	-5.34	112.35	119.30
1	D	87	ALA	O-C-N	-5.32	115.42	122.33
1	B	160	ARG	CG-CD-NE	-5.28	100.38	112.00
1	B	160	ARG	CD-NE-CZ	5.22	131.70	124.40
1	B	160	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	A	140	ASP	CA-CB-CG	5.08	117.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	GLY	N-CA-C	5.04	117.41	110.56
1	C	32	ASP	CA-C-N	5.02	129.86	120.87
1	C	32	ASP	C-N-CA	5.02	129.86	120.87
1	B	569	LEU	CB-CG-CD1	5.01	125.73	110.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	31	VAL	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	4350	0	4298	48	0
1	B	4255	0	4151	61	0
1	C	4309	0	4209	83	0
1	D	4287	0	4191	69	0
2	A	18	0	24	0	0
2	B	6	0	8	0	0
2	D	12	0	16	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	313	0	0	6	0
4	B	216	0	0	7	0
4	C	205	0	0	7	0
4	D	194	0	0	4	0
All	All	18167	0	16897	254	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 7.

All (254) 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:C:520[A]:HIS:CD2	1:C:521[A]:PRO:HD2	1.52	1.41
1:C:561[B]:MET:HE2	1:C:565:VAL:CG2	1.55	1.37
1:C:520[A]:HIS:CD2	1:C:521[A]:PRO:CD	2.17	1.26
1:C:561[B]:MET:CE	1:C:565:VAL:CG2	2.18	1.21
1:C:561[B]:MET:CE	1:C:565:VAL:HG21	1.69	1.21
1:C:558:ILE:CD1	1:C:567:ILE:CD1	2.23	1.17
1:C:558:ILE:CD1	1:C:567:ILE:HD13	1.75	1.16
1:C:558:ILE:HD13	1:C:567:ILE:HD13	1.26	1.15
1:C:520[A]:HIS:CG	1:C:521[A]:PRO:HD2	1.81	1.15
1:B:477:MET:HE1	1:B:528:PRO:HD2	1.28	1.14
1:A:32[A]:ASP:CG	1:A:33:GLY:H	1.49	1.14
1:C:561[B]:MET:HE2	1:C:565:VAL:HG23	1.28	1.10
1:B:477:MET:HE1	1:B:528:PRO:CD	1.80	1.09
1:C:561[B]:MET:HE1	1:C:565:VAL:HG21	1.30	1.08
1:C:520[A]:HIS:CD2	1:C:521[A]:PRO:HG2	1.90	1.07
1:C:520[A]:HIS:CD2	1:C:521[A]:PRO:CG	2.37	1.06
1:C:558:ILE:HD11	1:C:567:ILE:CD1	1.85	1.06
1:A:558:ILE:CD1	1:A:567:ILE:HD13	1.92	0.98
1:B:477:MET:CE	1:B:528:PRO:HD2	1.97	0.94
1:C:558:ILE:CD1	1:C:567:ILE:HD11	1.95	0.94
1:C:138:ALA:HB2	1:C:147:LEU:HD11	1.47	0.94
1:A:32[B]:ASP:OD2	1:A:33:GLY:N	2.01	0.94
1:C:520[A]:HIS:HD2	1:C:521[A]:PRO:CG	1.78	0.90
1:A:199:SER:N	4:A:840:HOH:O	2.04	0.90
1:B:497:ARG:HG2	1:B:497:ARG:HH11	1.36	0.90
1:D:497:ARG:HG2	1:D:497:ARG:HH11	1.38	0.88
1:A:32[A]:ASP:CG	1:A:33:GLY:N	2.27	0.87
1:C:521[A]:PRO:CB	1:C:524:ALA:HB2	2.05	0.87
1:C:138:ALA:CB	1:C:147:LEU:HD11	2.05	0.86
1:C:520[A]:HIS:HD2	1:C:521[A]:PRO:HG2	1.28	0.86
1:A:558:ILE:HD12	1:A:567:ILE:HD13	1.54	0.86
1:B:478:TYR:HD1	1:B:478:TYR:O	1.62	0.83
1:C:521[A]:PRO:HB2	1:C:524:ALA:H	1.43	0.83
1:A:558:ILE:HD11	1:A:567:ILE:HD13	1.61	0.82
1:B:71:HIS:CE1	4:B:684:HOH:O	2.32	0.81
1:C:521[A]:PRO:HG3	1:C:524:ALA:CB	2.10	0.81
1:D:159:ILE:HD11	1:D:182:LEU:HD22	1.63	0.81
1:C:521[A]:PRO:HB3	1:C:524:ALA:HB2	1.64	0.80
1:C:13:VAL:O	1:C:17:GLU:HG3	1.82	0.79
1:B:71:HIS:HE1	4:B:684:HOH:O	1.65	0.79
1:C:521[A]:PRO:CB	1:C:524:ALA:CB	2.61	0.77
1:D:32:ASP:O	1:D:32:ASP:CG	2.27	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520[A]:HIS:HD2	1:C:521[A]:PRO:CD	1.81	0.77
1:D:551:ILE:CG2	1:D:566:LYS:HE3	2.15	0.76
1:C:521[A]:PRO:CG	1:C:524:ALA:CB	2.64	0.76
1:D:32:ASP:O	1:D:32:ASP:OD2	2.03	0.76
1:B:551:ILE:CG2	1:B:566:LYS:HE3	2.16	0.75
1:C:558:ILE:HD11	1:C:567:ILE:HD11	1.56	0.75
1:D:7:VAL:HG23	1:D:8:GLU:H	1.52	0.74
1:C:138:ALA:HB2	1:C:147:LEU:CD1	2.18	0.73
1:D:478:TYR:CD2	1:D:500:MET:HE1	2.25	0.72
1:C:521[A]:PRO:CG	1:C:524:ALA:HB3	2.19	0.72
1:B:84:SER:HB2	1:B:87:ALA:HB2	1.73	0.71
1:D:533:LEU:HD23	1:D:536:MET:CE	2.21	0.70
1:D:52:ASP:OD1	1:D:292:ARG:NH2	2.22	0.70
1:C:5:MET:N	1:C:6:PRO:HD2	2.07	0.70
1:A:475:GLU:HA	1:A:500:MET:HE2	1.72	0.69
1:B:477:MET:HE1	1:B:528:PRO:CG	2.24	0.68
1:C:477:MET:HE3	1:C:489:ILE:HD11	1.76	0.67
1:D:7:VAL:HG23	1:D:8:GLU:N	2.10	0.67
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.58	0.67
1:B:32[B]:ASP:OD2	1:B:33:GLY:N	2.24	0.66
1:D:34:ASP:N	4:D:715:HOH:O	2.29	0.66
1:A:198:SER:HA	4:A:834:HOH:O	1.95	0.66
1:D:478:TYR:HD1	1:D:478:TYR:O	1.79	0.66
1:D:7:VAL:CG2	1:D:8:GLU:N	2.58	0.65
1:B:533:LEU:HD23	1:B:536:MET:CE	2.25	0.65
1:C:520[A]:HIS:CB	1:C:532:LEU:HD22	2.27	0.65
1:B:32[B]:ASP:OD1	1:B:35:LYS:HD2	1.96	0.64
1:C:457:MET:HE3	4:C:672:HOH:O	1.98	0.63
1:C:521[A]:PRO:CG	1:C:524:ALA:HB2	2.27	0.63
1:D:478:TYR:CE2	1:D:500:MET:HE1	2.35	0.62
1:D:479:GLU:OE2	1:D:497:ARG:NH2	2.31	0.62
1:D:472:VAL:HG13	1:D:506:ILE:HB	1.82	0.62
1:A:199:SER:HB3	4:A:733:HOH:O	2.00	0.61
1:C:521[A]:PRO:HG3	1:C:524:ALA:HB3	1.81	0.61
1:A:9:PHE:CD1	1:B:565:VAL:HG21	2.36	0.60
1:C:26:SER:OG	1:C:28:GLN:NE2	2.34	0.60
1:B:478:TYR:CD1	1:B:478:TYR:C	2.80	0.60
1:C:138:ALA:CB	1:C:147:LEU:CD1	2.76	0.60
1:B:497:ARG:HH11	1:B:497:ARG:CG	2.14	0.60
1:D:497:ARG:HH11	1:D:497:ARG:CG	2.12	0.59
4:C:833:HOH:O	1:D:522:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:TYR:CD1	1:D:486:ARG:HG3	2.37	0.58
1:B:478:TYR:CE1	1:B:486:ARG:CG	2.86	0.58
1:C:478:TYR:HD1	1:C:489:ILE:HG21	1.68	0.58
1:D:428:ARG:NH2	4:D:886:HOH:O	2.36	0.58
1:C:475:GLU:HA	1:C:500:MET:HE2	1.84	0.58
1:D:478:TYR:CD1	1:D:478:TYR:C	2.79	0.58
1:A:558:ILE:HD11	1:A:567:ILE:CD1	2.33	0.57
1:C:457:MET:HE1	1:C:508:HIS:CG	2.39	0.57
1:C:5:MET:HA	1:C:580:GLU:OE1	2.04	0.57
1:C:521[A]:PRO:HG3	1:C:524:ALA:HB2	1.81	0.57
1:D:199:SER:HB2	4:D:679:HOH:O	2.04	0.57
1:B:478:TYR:O	1:B:478:TYR:CD1	2.52	0.57
1:B:339:GLU:O	1:B:428:ARG:NH1	2.38	0.57
4:C:694:HOH:O	1:D:546:PHE:CE2	2.52	0.56
1:A:457:MET:HE1	1:A:508:HIS:CG	2.40	0.56
1:D:7:VAL:HG21	1:D:576:ALA:HB1	1.88	0.56
1:B:478:TYR:HD1	1:B:478:TYR:C	2.13	0.56
1:D:551:ILE:HG21	1:D:566:LYS:HE3	1.86	0.56
1:A:558:ILE:CD1	1:A:567:ILE:CD1	2.78	0.56
1:B:478:TYR:CD2	1:B:500:MET:HE1	2.41	0.55
1:A:292:ARG:HH11	1:A:292:ARG:HG2	1.71	0.55
1:D:381:PHE:CZ	1:D:558:ILE:HD12	2.42	0.54
1:A:176:SER:OG	1:A:191:ASP:OD1	2.20	0.54
1:D:478:TYR:O	1:D:478:TYR:CD1	2.59	0.54
1:D:52:ASP:CG	1:D:292:ARG:HH12	2.17	0.53
1:B:425:ALA:HA	1:B:428:ARG:HG2	1.90	0.53
1:D:52:ASP:OD1	1:D:292:ARG:NH1	2.41	0.53
1:D:533:LEU:HD23	1:D:536:MET:HE1	1.90	0.53
1:C:13:VAL:HG21	1:D:13:VAL:HG21	1.92	0.52
1:A:61:ARG:HG2	1:A:61:ARG:NH1	2.23	0.52
1:C:561[B]:MET:HE2	1:C:565:VAL:HG22	1.77	0.52
1:B:551:ILE:HG21	1:B:566:LYS:HE3	1.89	0.52
1:C:520[A]:HIS:O	1:C:550:ILE:HA	2.10	0.52
1:D:573:PHE:O	1:D:577:THR:HG23	2.09	0.52
1:B:497:ARG:HG2	1:B:497:ARG:NH1	2.13	0.52
1:D:478:TYR:CD2	1:D:500:MET:CE	2.91	0.52
1:C:478:TYR:CD1	1:C:489:ILE:HG21	2.45	0.51
1:A:536:MET:HE1	1:A:550:ILE:HD11	1.92	0.51
1:A:562:GLU:HG3	4:A:707:HOH:O	2.11	0.51
1:B:533:LEU:HD23	1:B:536:MET:HE1	1.92	0.51
1:D:32:ASP:HB2	1:D:97:THR:OG1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LYS:HD3	1:C:52:ASP:HB2	1.91	0.51
1:B:20:ILE:CD1	1:B:380:THR:HG21	2.40	0.51
1:C:521[A]:PRO:HB2	1:C:524:ALA:CB	2.41	0.51
1:D:520:HIS:CB	1:D:532:LEU:HD22	2.41	0.51
1:B:520:HIS:CG	1:B:532:LEU:HD22	2.46	0.51
1:D:478:TYR:HD2	1:D:500:MET:SD	2.35	0.50
1:A:32[B]:ASP:OD1	1:A:35:LYS:HG3	2.11	0.50
1:B:20:ILE:HG22	1:B:43:GLU:CG	2.42	0.50
1:C:457:MET:HE1	1:C:508:HIS:CD2	2.46	0.50
1:A:61:ARG:NH1	4:A:732:HOH:O	2.45	0.50
1:C:558:ILE:HD12	1:C:567:ILE:HD11	1.90	0.50
1:D:497:ARG:HG2	1:D:497:ARG:NH1	2.14	0.49
1:B:478:TYR:CE2	1:B:500:MET:HE1	2.47	0.49
1:C:399:GLY:HA2	1:C:408:ARG:O	2.12	0.49
1:D:478:TYR:CE1	1:D:486:ARG:HG3	2.45	0.49
1:C:9:PHE:CD1	1:D:565:VAL:HG21	2.47	0.49
1:B:20:ILE:CG2	1:B:43:GLU:HG2	2.42	0.49
1:C:520[A]:HIS:CG	1:C:532:LEU:HD22	2.48	0.49
1:C:558:ILE:HD13	1:C:567:ILE:CD1	2.04	0.49
1:C:561[B]:MET:CE	1:C:565:VAL:HG23	2.12	0.49
1:B:432:GLU:HA	1:B:432:GLU:OE2	2.12	0.49
1:D:151:PRO:HG2	1:D:170:PHE:CG	2.48	0.49
1:C:125:VAL:HB	1:C:159:ILE:HD11	1.95	0.49
1:A:13:VAL:O	1:A:17:GLU:HG2	2.13	0.49
1:B:151:PRO:HG2	1:B:170:PHE:CG	2.48	0.49
1:B:555:GLY:O	1:B:556:HIS:HD2	1.96	0.49
1:D:219:ARG:CG	1:D:219:ARG:HH11	2.25	0.49
1:B:341:PHE:CG	1:B:342:ASP:N	2.80	0.49
1:A:272:PHE:HA	1:A:276:GLU:O	2.13	0.48
1:A:497:ARG:HB2	1:D:479:GLU:HB3	1.96	0.48
1:A:563:ASP:O	1:A:567:ILE:HG23	2.14	0.48
1:B:32[B]:ASP:HB3	1:B:97:THR:OG1	2.13	0.48
1:A:13:VAL:HG22	1:A:569:LEU:HD21	1.95	0.48
1:A:35:LYS:HD3	1:A:52:ASP:HB2	1.95	0.48
1:C:521[A]:PRO:HB2	1:C:524:ALA:N	2.22	0.48
1:B:479:GLU:OE2	1:B:497:ARG:NH2	2.42	0.48
1:D:520:HIS:CG	1:D:532:LEU:HD22	2.49	0.48
1:B:472:VAL:HG13	1:B:506:ILE:HB	1.96	0.47
1:C:138:ALA:HB3	1:C:147:LEU:HD11	1.92	0.47
1:A:13:VAL:HG21	1:B:13:VAL:HG21	1.96	0.47
1:D:450:MET:HE2	1:D:450:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ARG:HH11	1:B:219:ARG:CG	2.27	0.47
1:C:558:ILE:HG22	1:C:563:ASP:HB2	1.97	0.47
1:D:159:ILE:CD1	1:D:182:LEU:HD22	2.41	0.47
1:D:478:TYR:CE1	1:D:486:ARG:CG	2.97	0.47
1:D:477:MET:HE1	1:D:528:PRO:CD	2.45	0.47
1:A:125:VAL:HB	1:A:159:ILE:HD11	1.97	0.47
1:B:219:ARG:HG3	1:B:219:ARG:NH1	2.29	0.47
1:B:265:ARG:NH2	4:B:705:HOH:O	2.44	0.47
1:D:472:VAL:HG22	1:D:535:LEU:HD22	1.95	0.47
1:B:445:SER:OG	1:B:446:TYR:N	2.48	0.46
1:C:13:VAL:HG22	1:C:569:LEU:HD21	1.96	0.46
1:A:133:ARG:HD3	1:A:149:ARG:HD3	1.96	0.46
1:B:520:HIS:CB	1:B:532:LEU:HD22	2.46	0.46
1:B:41:PHE:CD1	1:B:46:VAL:HG22	2.51	0.46
1:B:265:ARG:NE	4:B:705:HOH:O	2.47	0.46
1:B:530:LYS:HB3	1:B:531:PRO:HD3	1.98	0.46
1:C:529[A]:LEU:HD23	1:D:540:LEU:HD13	1.98	0.46
1:A:7:VAL:HG11	1:A:9:PHE:CE2	2.51	0.46
1:B:478:TYR:CD1	1:B:486:ARG:CG	2.99	0.46
1:A:68:LEU:HD22	1:A:117:GLY:HA3	1.97	0.45
1:D:27:LEU:HD21	1:D:289:VAL:HG22	1.98	0.45
1:C:7:VAL:HB	1:C:9:PHE:CE2	2.51	0.45
1:B:265:ARG:CZ	4:B:705:HOH:O	2.64	0.45
1:D:555:GLY:C	1:D:556:HIS:CD2	2.95	0.45
1:C:520[A]:HIS:HB2	1:C:532:LEU:HD22	1.95	0.45
1:C:524:ALA:HB1	4:C:658:HOH:O	2.16	0.45
1:A:538:GLU:OE1	1:A:542:ARG:NE	2.37	0.45
1:A:450:MET:HA	1:A:450:MET:HE2	1.98	0.45
1:B:13:VAL:HG22	1:B:569:LEU:HD21	1.99	0.45
1:D:478:TYR:HD1	1:D:478:TYR:C	2.23	0.44
1:D:341:PHE:O	1:D:343:GLY:N	2.50	0.44
1:B:472:VAL:HG22	1:B:535:LEU:HD22	1.99	0.44
1:D:478:TYR:HD2	1:D:500:MET:CE	2.29	0.44
1:A:374:ASP:CG	1:A:394:MET:HB3	2.42	0.44
1:C:522[B]:GLN:NE2	4:C:694:HOH:O	2.50	0.44
1:D:118:VAL:HG11	1:D:159:ILE:HG22	2.00	0.44
1:B:162:ASP:OD2	1:B:183:SER:OG	2.33	0.44
1:C:538:GLU:OE2	4:C:740:HOH:O	2.21	0.44
1:A:9:PHE:CE1	1:B:565:VAL:HG21	2.53	0.44
1:A:399:GLY:HA2	1:A:408:ARG:O	2.18	0.44
1:B:468:GLY:HA2	1:B:519:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:MET:N	1:C:6:PRO:CD	2.81	0.43
1:B:568:LEU:HD12	1:B:568:LEU:O	2.19	0.43
1:A:239:ASP:HB2	1:A:275:GLY:O	2.18	0.43
1:C:181:ASN:HD22	1:C:181:ASN:HA	1.62	0.43
1:D:219:ARG:CG	1:D:219:ARG:NH1	2.80	0.43
1:B:478:TYR:HD2	1:B:500:MET:CE	2.31	0.43
1:C:20:ILE:CG2	1:C:561[A]:MET:HG3	2.49	0.43
1:C:68:LEU:HD22	1:C:117:GLY:HA3	2.00	0.43
1:C:533:LEU:HD23	1:C:536:MET:CE	2.49	0.43
1:C:468:GLY:O	1:C:469:ALA:C	2.62	0.43
1:B:125:VAL:HB	1:B:159:ILE:HD11	2.02	0.42
1:A:9:PHE:O	1:A:13:VAL:HG23	2.19	0.42
1:C:529[B]:LEU:HD11	1:C:550:ILE:CG2	2.48	0.42
1:A:428[A]:ARG:NH1	1:A:432:GLU:OE1	2.51	0.42
1:B:219:ARG:CG	1:B:219:ARG:NH1	2.81	0.42
1:D:381:PHE:CZ	1:D:558:ILE:CD1	3.03	0.42
1:C:167:LEU:HD11	1:C:199:SER:HA	2.00	0.42
1:D:341:PHE:C	1:D:343:GLY:H	2.28	0.42
1:C:5:MET:O	1:C:580:GLU:CD	2.62	0.42
1:A:497:ARG:HH11	1:A:497:ARG:HD3	1.75	0.42
1:A:520:HIS:O	1:A:550:ILE:HA	2.19	0.42
1:C:291:TRP:O	1:C:294:LYS:HG3	2.20	0.42
1:B:105:ARG:NE	4:B:757:HOH:O	2.41	0.42
1:A:477:MET:HE3	1:A:489:ILE:HD11	2.02	0.42
1:A:428[A]:ARG:CZ	1:A:428[A]:ARG:HB3	2.51	0.41
1:C:544:LYS:O	4:C:833:HOH:O	2.21	0.41
1:D:381:PHE:CD2	1:D:568:LEU:HD13	2.55	0.41
1:D:558:ILE:HD13	1:D:558:ILE:HG21	1.80	0.41
1:A:32[A]:ASP:OD2	1:A:33:GLY:N	2.42	0.41
1:C:489:ILE:HG22	1:C:490:GLU:N	2.35	0.41
1:D:127:THR:HG23	1:D:156:VAL:HG23	2.02	0.41
1:B:444:TYR:HA	1:B:468:GLY:O	2.20	0.41
1:D:239:ASP:HB2	1:D:275:GLY:O	2.21	0.41
1:D:266:GLU:OE1	4:D:629:HOH:O	2.22	0.41
1:C:521[A]:PRO:CB	1:C:524:ALA:HB3	2.45	0.41
1:A:404:GLY:HA2	4:A:690:HOH:O	2.21	0.41
1:C:9:PHE:O	1:C:13:VAL:HG23	2.21	0.41
1:B:432:GLU:HG3	4:B:683:HOH:O	2.21	0.40
1:C:153:PHE:CE1	1:C:484:ALA:HB1	2.56	0.40
1:D:35:LYS:HG2	1:D:52:ASP:HB2	2.03	0.40
1:A:262:VAL:HG21	1:A:286:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ASP:HB2	1:D:97:THR:CB	2.51	0.40
1:D:219:ARG:NH1	1:D:219:ARG:HG3	2.36	0.40
1:C:140:ASP:OD1	1:C:141:GLY:N	2.55	0.40
1:D:327:ARG:NE	1:D:327:ARG:HA	2.37	0.40
1:B:478:TYR:CD2	1:B:500:MET:CE	3.04	0.40
1:D:71:HIS:HE1	1:D:159:ILE:HG23	1.86	0.40
1:D:530:LYS:HB3	1:D:531:PRO:HD3	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	579/582 (100%)	566 (98%)	11 (2%)	2 (0%)	36	26
1	B	574/582 (99%)	554 (96%)	19 (3%)	1 (0%)	43	33
1	C	580/582 (100%)	569 (98%)	11 (2%)	0	100	100
1	D	574/582 (99%)	553 (96%)	19 (3%)	2 (0%)	36	26
All	All	2307/2328 (99%)	2242 (97%)	60 (3%)	5 (0%)	43	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32[A]	ASP
1	A	32[B]	ASP
1	D	34	ASP
1	B	34	ASP
1	D	342	ASP

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	450/468 (96%)	434 (96%)	16 (4%)	31	13
1	B	425/468 (91%)	411 (97%)	14 (3%)	33	15
1	C	434/468 (93%)	415 (96%)	19 (4%)	25	9
1	D	434/468 (93%)	421 (97%)	13 (3%)	36	17
All	All	1743/1872 (93%)	1681 (96%)	62 (4%)	32	13

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	34	ASP
1	A	61	ARG
1	A	181	ASN
1	A	182	LEU
1	A	199	SER
1	A	242	SER
1	A	287	ARG
1	A	310	SER
1	A	334	ARG
1	A	419	GLU
1	A	489	ILE
1	A	492	LEU
1	A	497	ARG
1	A	538	GLU
1	A	558	ILE
1	B	20	ILE
1	B	188	ARG
1	B	219	ARG
1	B	265	ARG
1	B	287	ARG
1	B	327	ARG
1	B	342	ASP
1	B	472	VAL

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Mol	Chain	Res	Type
1	B	477	MET
1	B	478	TYR
1	B	479	GLU
1	B	497	ARG
1	B	506	ILE
1	B	525	SER
1	C	34	ASP
1	C	38	VAL
1	C	122	GLU
1	C	140	ASP
1	C	181	ASN
1	C	182	LEU
1	C	199	SER
1	C	242	SER
1	C	287	ARG
1	C	310	SER
1	C	334	ARG
1	C	489	ILE
1	C	492	LEU
1	C	502	SER
1	C	522[A]	GLN
1	C	522[B]	GLN
1	C	538	GLU
1	C	545	THR
1	C	558	ILE
1	D	7	VAL
1	D	20	ILE
1	D	188	ARG
1	D	219	ARG
1	D	220	LEU
1	D	265	ARG
1	D	287	ARG
1	D	327	ARG
1	D	472	VAL
1	D	477	MET
1	D	479	GLU
1	D	497	ARG
1	D	506	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	89	GLN
1	A	104	GLN
1	A	508	HIS
1	B	284	ASN
1	B	556	HIS
1	C	28	GLN
1	C	65	ASN
1	C	181	ASN
1	C	508	HIS
1	C	556	HIS
1	D	28	GLN
1	D	71	HIS
1	D	556	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	D	585	-	5,5,5	0.49	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	583[B]	-	5,5,5	0.65	0	5,5,5	0.61	0
2	GOL	B	584	-	5,5,5	0.45	0	5,5,5	0.70	0
2	GOL	A	583[A]	-	5,5,5	0.61	0	5,5,5	0.56	0
2	GOL	D	584	-	5,5,5	0.62	0	5,5,5	0.94	0
2	GOL	A	584	-	5,5,5	0.34	0	5,5,5	1.36	1 (20%)

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	GOL	D	585	-	-	4/4/4/4	-
2	GOL	A	583[B]	-	-	4/4/4/4	-
2	GOL	B	584	-	-	4/4/4/4	-
2	GOL	A	583[A]	-	-	4/4/4/4	-
2	GOL	D	584	-	-	2/4/4/4	-
2	GOL	A	584	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	584	GOL	O2-C2-C3	2.06	117.72	109.18

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	583[A]	GOL	O1-C1-C2-O2
2	A	583[A]	GOL	O2-C2-C3-O3
2	A	583[B]	GOL	O1-C1-C2-O2
2	A	583[B]	GOL	O1-C1-C2-C3
2	B	584	GOL	O1-C1-C2-C3
2	B	584	GOL	C1-C2-C3-O3
2	D	584	GOL	O1-C1-C2-O2
2	D	584	GOL	O1-C1-C2-C3
2	D	585	GOL	O1-C1-C2-O2
2	D	585	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	D	585	GOL	C1-C2-C3-O3
2	A	583[A]	GOL	O1-C1-C2-C3
2	A	583[A]	GOL	C1-C2-C3-O3
2	A	583[B]	GOL	C1-C2-C3-O3
2	A	584	GOL	O1-C1-C2-C3
2	B	584	GOL	O1-C1-C2-O2
2	B	584	GOL	O2-C2-C3-O3
2	D	585	GOL	O2-C2-C3-O3
2	A	583[B]	GOL	O2-C2-C3-O3
2	A	584	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	576/582 (98%)	0.17	5 (0%) 81 85	19, 38, 51, 63	5 (0%)
1	B	574/582 (98%)	0.62	46 (8%) 18 20	25, 44, 66, 91	2 (0%)
1	C	577/582 (99%)	0.64	70 (12%) 8 9	21, 45, 68, 87	5 (0%)
1	D	575/582 (98%)	0.65	50 (8%) 16 18	19, 46, 71, 84	1 (0%)
All	All	2302/2328 (98%)	0.52	171 (7%) 20 23	19, 42, 66, 91	13 (0%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	33	GLY	6.3
1	B	341	PHE	5.9
1	C	141	GLY	5.8
1	C	524	ALA	5.4
1	D	341	PHE	5.3
1	A	142	GLY	5.1
1	B	556	HIS	4.5
1	D	132	ASP	4.4
1	D	44	GLY	4.3
1	C	558	ILE	4.3
1	D	331	ALA	4.3
1	C	556	HIS	4.2
1	B	132	ASP	4.2
1	C	552	PRO	4.1
1	D	141	GLY	4.1
1	C	480	LEU	4.1
1	C	142	GLY	3.9
1	B	7	VAL	3.9
1	C	147	LEU	3.8
1	D	540	LEU	3.8
1	D	96	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	432	GLU	3.7
1	B	44	GLY	3.6
1	D	83	VAL	3.6
1	B	54	GLY	3.6
1	C	488	PHE	3.6
1	B	478	TYR	3.5
1	B	33	GLY	3.5
1	C	485	PHE	3.5
1	B	343	GLY	3.4
1	B	431	ARG	3.4
1	B	481	SER	3.4
1	B	141	GLY	3.3
1	C	83	VAL	3.3
1	C	529[A]	LEU	3.3
1	D	84	SER	3.2
1	B	342	ASP	3.2
1	C	523	ASN	3.2
1	C	560	THR	3.2
1	B	356	ALA	3.1
1	C	522[A]	GLN	3.1
1	B	555	GLY	3.1
1	D	88	GLU	3.1
1	C	5	MET	3.1
1	B	429	TRP	3.1
1	C	171	GLY	3.1
1	D	7	VAL	3.1
1	A	341	PHE	3.1
1	C	169	PHE	3.1
1	D	537	GLY	3.1
1	C	153	PHE	3.0
1	C	104	GLN	3.0
1	D	86	GLY	2.9
1	B	480	LEU	2.9
1	C	85	LYS	2.9
1	D	325	ASP	2.9
1	C	483	ALA	2.9
1	A	141	GLY	2.9
1	C	6	PRO	2.8
1	D	556	HIS	2.8
1	B	87	ALA	2.8
1	D	541	ALA	2.8
1	B	32[A]	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	131	GLU	2.8
1	D	543	GLY	2.7
1	C	140	ASP	2.7
1	C	182	LEU	2.7
1	B	337	TRP	2.7
1	D	169	PHE	2.7
1	C	88	GLU	2.7
1	D	330	ILE	2.7
1	C	87	ALA	2.6
1	C	557	ALA	2.6
1	C	32	ASP	2.6
1	B	499	ILE	2.6
1	D	61	ARG	2.6
1	D	581	ARG	2.6
1	C	170	PHE	2.6
1	B	34	ASP	2.6
1	C	108	ALA	2.6
1	D	87	ALA	2.6
1	C	181	ASN	2.6
1	C	553	ASP	2.5
1	A	143	GLY	2.5
1	C	135	ALA	2.5
1	B	9	PHE	2.5
1	D	85	LYS	2.5
1	C	496	SER	2.5
1	D	481	SER	2.5
1	D	483	ALA	2.5
1	D	478	TYR	2.5
1	B	433	SER	2.5
1	C	84	SER	2.5
1	C	154	GLY	2.4
1	C	23	GLU	2.4
1	B	436	ALA	2.4
1	C	151	PRO	2.4
1	C	565	VAL	2.4
1	C	128	GLY	2.4
1	C	559	ASN	2.4
1	D	479	GLU	2.4
1	B	325	ASP	2.4
1	B	425	ALA	2.4
1	B	430	ALA	2.4
1	C	21	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	129	ALA	2.4
1	C	521[A]	PRO	2.4
1	B	487	ASN	2.4
1	D	136	LEU	2.4
1	B	479	GLU	2.4
1	C	490	GLU	2.4
1	C	152	GLY	2.4
1	D	54	GLY	2.4
1	D	52	ASP	2.3
1	C	137	TYR	2.3
1	C	184	SER	2.3
1	D	324	GLU	2.3
1	B	435	LEU	2.3
1	B	539	LEU	2.3
1	B	72	TYR	2.3
1	D	181	ASN	2.3
1	D	143	GLY	2.3
1	D	133	ARG	2.3
1	A	9	PHE	2.3
1	B	557	ALA	2.3
1	C	173	GLY	2.3
1	C	489	ILE	2.3
1	D	489	ILE	2.3
1	D	124	VAL	2.3
1	D	480	LEU	2.3
1	C	494	GLY	2.2
1	D	149	ARG	2.2
1	C	492	LEU	2.2
1	D	580	GLU	2.2
1	D	34	ASP	2.2
1	C	499	ILE	2.2
1	D	71	HIS	2.2
1	C	497	ARG	2.2
1	C	89	GLN	2.2
1	B	41	PHE	2.2
1	C	478	TYR	2.2
1	B	474	TRP	2.2
1	B	428	ARG	2.2
1	D	327	ARG	2.2
1	C	132	ASP	2.2
1	C	482	ASP	2.2
1	B	331	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	149	ARG	2.2
1	C	477	MET	2.1
1	B	472	VAL	2.1
1	B	493	THR	2.1
1	C	493	THR	2.1
1	C	527	THR	2.1
1	C	525	SER	2.1
1	C	404	GLY	2.1
1	B	412	ILE	2.1
1	D	82	ASP	2.1
1	C	216	ARG	2.1
1	C	487	ASN	2.1
1	B	527	THR	2.1
1	B	580	GLU	2.1
1	C	293	GLY	2.1
1	D	142	GLY	2.1
1	D	343	GLY	2.1
1	D	524	ALA	2.1
1	D	130	THR	2.0
1	C	528	PRO	2.0
1	B	554	ALA	2.0
1	D	153	PHE	2.0
1	D	111	PRO	2.0
1	C	134	VAL	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	GOL	B	584	6/6	0.81	0.13	48,55,57,60	0
2	GOL	A	584	6/6	0.85	0.15	45,57,58,62	0
2	GOL	D	584	6/6	0.85	0.15	36,46,48,53	0
2	GOL	A	583[B]	6/6	0.88	0.12	29,32,34,34	6
2	GOL	A	583[A]	6/6	0.88	0.12	29,31,34,34	6
2	GOL	D	585	6/6	0.88	0.14	34,52,57,59	0
3	NA	D	583	1/1	0.95	0.11	39,39,39,39	0
3	NA	B	583	1/1	0.96	0.08	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.