Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 11:54 PM EDT

PDB ID	:	3O4H
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:

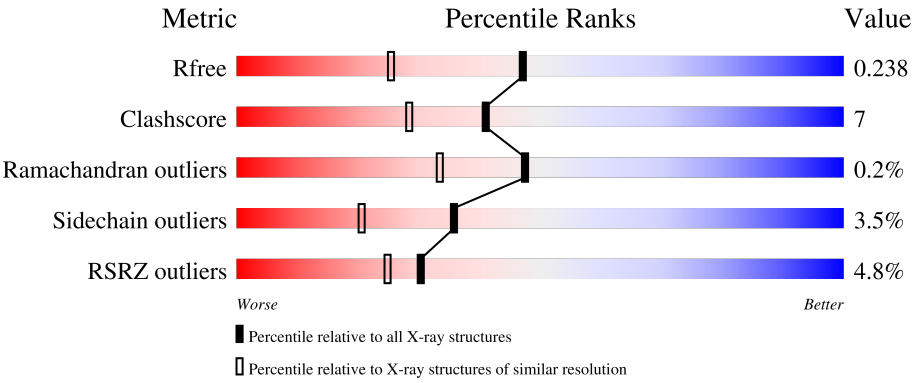
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 1.82 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}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	582	88% 8%
1	B	582	7% 86% 10%
1	C	582	4% 87% 10%
1	D	582	7% 86% 11%

2 Entry composition (i)

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.

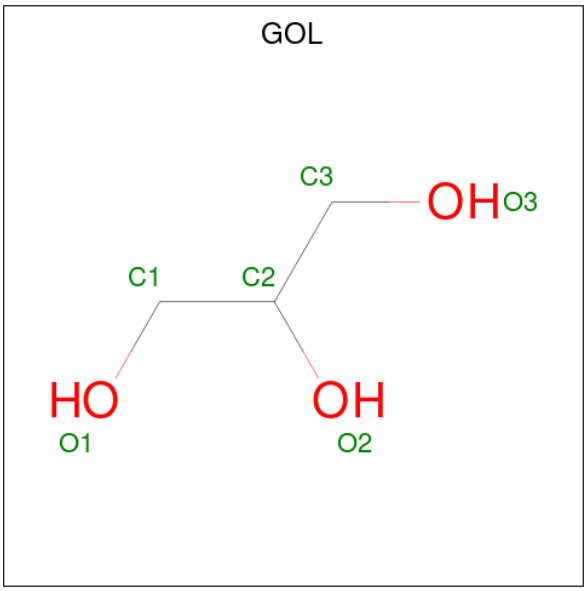
- Molecule 1 is a protein called Acylamino-acid-releasing enzyme.

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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is water.

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

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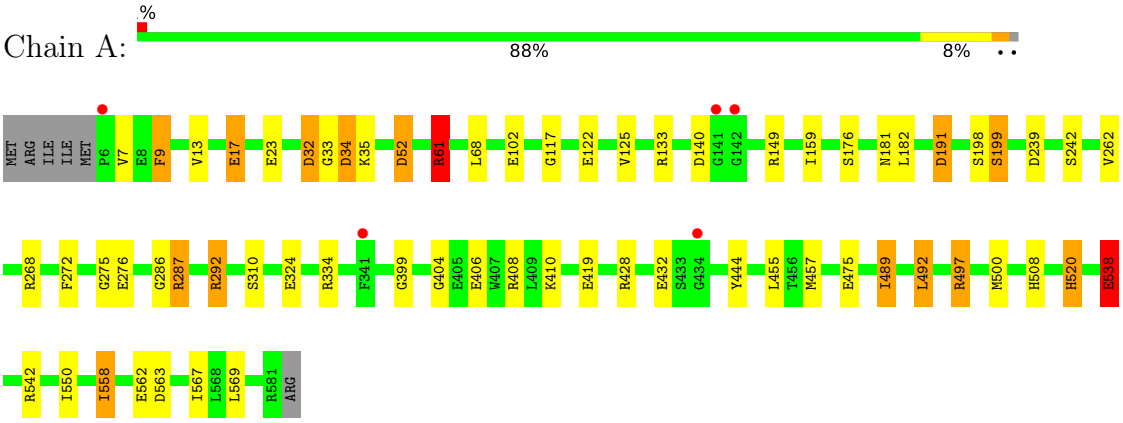
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	205	Total O 205 205	0	0
4	D	194	Total O 194 194	0	0

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.

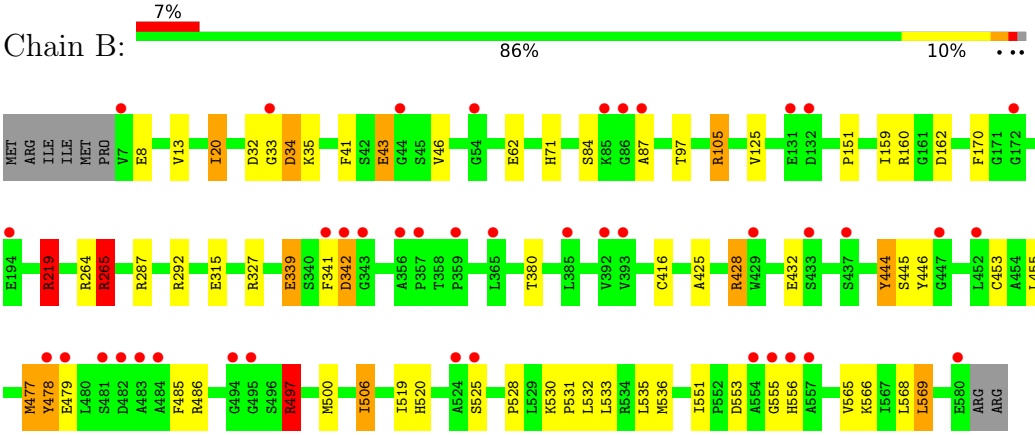
• Molecule 1: Acylamino-acid-releasing enzyme

Chain A:



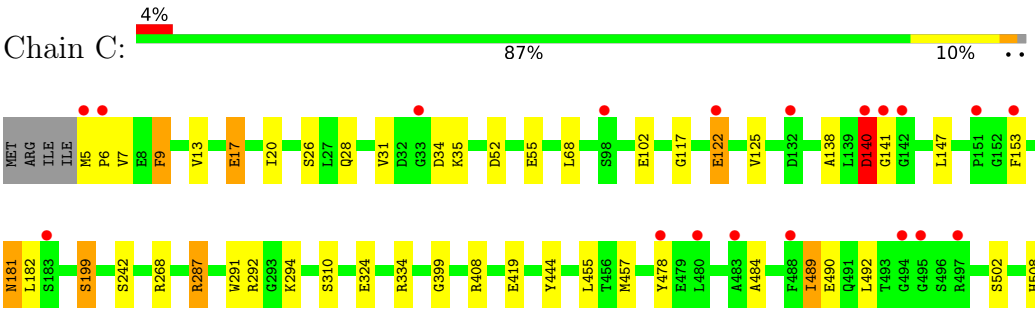
• Molecule 1: Acylamino-acid-releasing enzyme

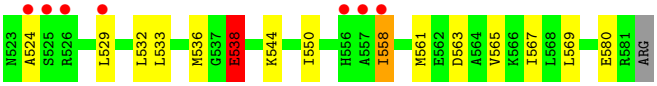
Chain B:



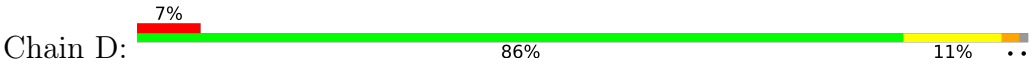
• Molecule 1: Acylamino-acid-releasing enzyme

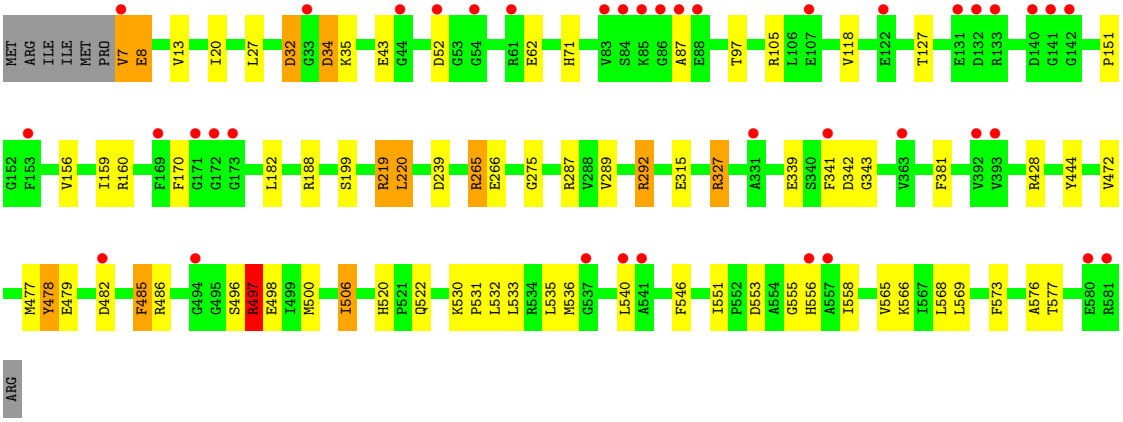
Chain C:





• Molecule 1: Acylamino-acid-releasing enzyme





4 Data and refinement statistics (i)

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 24.63 – 1.82	Depositor EDS
% Data completeness (in resolution range)	95.3 (24.62-1.82) 95.3 (24.63-1.82)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	10388 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 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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: 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	1.03	17/4457 (0.4%)	1.06	30/6050 (0.5%)
1	B	1.05	17/4354 (0.4%)	1.12	24/5917 (0.4%)
1	C	1.00	16/4410 (0.4%)	1.04	22/5994 (0.4%)
1	D	1.05	23/4382 (0.5%)	1.13	22/5953 (0.4%)
All	All	1.03	73/17603 (0.4%)	1.09	98/23914 (0.4%)

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 (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	TYR	CE2-CZ	-15.53	1.18	1.38
1	B	444	TYR	CE2-CZ	-15.21	1.18	1.38
1	A	444	TYR	CE1-CZ	-14.69	1.19	1.38
1	B	444	TYR	CE1-CZ	-14.48	1.19	1.38
1	C	444	TYR	CE2-CZ	-14.27	1.20	1.38
1	C	444	TYR	CE1-CZ	-14.24	1.20	1.38
1	A	287	ARG	CZ-NH1	-14.09	1.14	1.33
1	D	265	ARG	CZ-NH1	-14.08	1.14	1.33
1	B	485	PHE	CE1-CZ	-14.02	1.10	1.37
1	D	498	GLU	CD-OE1	13.99	1.41	1.25
1	B	265	ARG	CZ-NH1	-13.57	1.15	1.33
1	B	105	ARG	CZ-NH1	-13.48	1.15	1.33
1	A	444	TYR	CG-CD1	-13.40	1.21	1.39
1	D	444	TYR	CE1-CZ	-13.26	1.21	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	287	ARG	CZ-NH1	-12.85	1.16	1.33
1	B	444	TYR	CG-CD1	-12.77	1.22	1.39
1	B	160	ARG	CZ-NH1	-12.76	1.16	1.33
1	D	444	TYR	CG-CD1	-12.70	1.22	1.39
1	D	105	ARG	CZ-NH1	-12.66	1.16	1.33
1	D	485	PHE	CE1-CZ	-12.64	1.13	1.37
1	A	9	PHE	CE2-CZ	-12.57	1.13	1.37
1	D	444	TYR	CE2-CZ	-12.52	1.22	1.38
1	D	485	PHE	CE2-CZ	-12.52	1.13	1.37
1	A	444	TYR	CG-CD2	-12.20	1.23	1.39
1	B	485	PHE	CE2-CZ	-12.19	1.14	1.37
1	B	444	TYR	CG-CD2	-12.18	1.23	1.39
1	C	9	PHE	CE1-CZ	-12.11	1.14	1.37
1	D	444	TYR	CG-CD2	-12.05	1.23	1.39
1	C	444	TYR	CG-CD2	-11.81	1.23	1.39
1	A	17	GLU	CB-CG	-11.70	1.29	1.52
1	C	444	TYR	CG-CD1	-11.66	1.24	1.39
1	C	9	PHE	CE2-CZ	-11.61	1.15	1.37
1	C	17	GLU	CB-CG	-11.31	1.30	1.52
1	A	9	PHE	CE1-CZ	-11.31	1.15	1.37
1	D	485	PHE	CG-CD2	-10.92	1.22	1.38
1	D	160	ARG	CZ-NH1	-10.89	1.18	1.33
1	C	9	PHE	CG-CD2	-10.80	1.22	1.38
1	D	485	PHE	CG-CD1	-10.79	1.22	1.38
1	C	9	PHE	CG-CD1	-10.71	1.22	1.38
1	A	292	ARG	CZ-NH1	-10.68	1.19	1.33
1	A	268	ARG	CZ-NH2	-10.59	1.19	1.33
1	D	292	ARG	CZ-NH1	-10.33	1.19	1.33
1	B	485	PHE	CG-CD2	-10.21	1.23	1.38
1	C	292	ARG	CZ-NH1	-10.19	1.19	1.33
1	A	292	ARG	CZ-NH2	-10.18	1.19	1.33
1	A	268	ARG	CZ-NH1	-10.16	1.19	1.33
1	A	9	PHE	CG-CD1	-10.13	1.23	1.38
1	C	268	ARG	CZ-NH2	-10.11	1.20	1.33
1	A	9	PHE	CG-CD2	-9.53	1.24	1.38
1	C	268	ARG	CZ-NH1	-9.47	1.20	1.33
1	B	292	ARG	CZ-NH2	-9.44	1.20	1.33
1	C	292	ARG	CZ-NH2	-9.26	1.21	1.33
1	D	292	ARG	CZ-NH2	-9.02	1.21	1.33
1	B	485	PHE	CG-CD1	-8.89	1.25	1.38
1	B	292	ARG	CZ-NH1	-8.54	1.22	1.33
1	D	498	GLU	CD-OE2	8.07	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	339	GLU	C-O	7.86	1.38	1.23
1	B	160	ARG	CZ-NH2	-7.79	1.23	1.33
1	A	140	ASP	CB-CG	-7.25	1.36	1.51
1	D	339	GLU	CD-OE1	-7.18	1.17	1.25
1	C	55	GLU	CD-OE1	-6.84	1.18	1.25
1	D	160	ARG	CZ-NH2	-6.74	1.24	1.33
1	C	55	GLU	CD-OE2	-6.55	1.18	1.25
1	D	496	SER	CB-OG	6.28	1.50	1.42
1	A	455	LEU	CG-CD1	-6.22	1.28	1.51
1	D	339	GLU	CD-OE2	-6.19	1.18	1.25
1	D	32	ASP	C-O	-5.58	1.12	1.23
1	D	43	GLU	CD-OE1	-5.55	1.19	1.25
1	B	43	GLU	CD-OE2	-5.53	1.19	1.25
1	B	339	GLU	CD-OE2	-5.48	1.19	1.25
1	D	8	GLU	CD-OE1	-5.45	1.19	1.25
1	D	87	ALA	C-O	-5.36	1.13	1.23
1	A	102	GLU	CD-OE2	-5.15	1.20	1.25

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	265	ARG	NE-CZ-NH1	-28.30	106.15	120.30
1	B	265	ARG	NE-CZ-NH2	28.02	134.31	120.30
1	D	265	ARG	NE-CZ-NH2	27.67	134.14	120.30
1	D	265	ARG	NE-CZ-NH1	-25.82	107.39	120.30
1	C	287	ARG	NE-CZ-NH2	24.99	132.79	120.30
1	D	105	ARG	NE-CZ-NH2	22.91	131.75	120.30
1	A	287	ARG	NE-CZ-NH2	22.04	131.32	120.30
1	B	105	ARG	NE-CZ-NH2	21.87	131.23	120.30
1	C	268	ARG	NE-CZ-NH2	17.39	128.99	120.30
1	A	292	ARG	NE-CZ-NH2	16.73	128.66	120.30
1	B	292	ARG	NE-CZ-NH1	16.55	128.58	120.30
1	C	292	ARG	NE-CZ-NH2	16.53	128.56	120.30
1	A	268	ARG	NE-CZ-NH1	15.55	128.07	120.30
1	C	292	ARG	NE-CZ-NH1	15.49	128.04	120.30
1	A	292	ARG	NE-CZ-NH1	15.43	128.01	120.30
1	A	292	ARG	NH1-CZ-NH2	-14.84	103.08	119.40
1	C	292	ARG	NH1-CZ-NH2	-14.80	103.12	119.40
1	D	160	ARG	NE-CZ-NH2	14.61	127.61	120.30
1	D	292	ARG	NE-CZ-NH2	14.24	127.42	120.30
1	C	268	ARG	NH1-CZ-NH2	-13.94	104.07	119.40
1	C	268	ARG	NE-CZ-NH1	13.26	126.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	268	ARG	NH1-CZ-NH2	-12.81	105.30	119.40
1	B	160	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	A	140	ASP	CB-CG-OD2	-12.27	107.26	118.30
1	A	268	ARG	NE-CZ-NH2	12.22	126.41	120.30
1	C	287	ARG	NE-CZ-NH1	-11.96	114.32	120.30
1	D	292	ARG	NH1-CZ-NH2	-11.38	106.88	119.40
1	D	292	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	B	292	ARG	NH1-CZ-NH2	-10.64	107.70	119.40
1	A	61	ARG	NE-CZ-NH1	10.29	125.45	120.30
1	C	140	ASP	CB-CG-OD2	-9.70	109.57	118.30
1	D	160	ARG	NH1-CZ-NH2	-9.66	108.78	119.40
1	B	160	ARG	NH1-CZ-NH2	-9.49	108.96	119.40
1	B	553	ASP	CB-CG-OD1	9.41	126.77	118.30
1	A	287	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	A	140	ASP	N-CA-CB	-8.83	94.70	110.60
1	B	569	LEU	CB-CG-CD1	8.67	125.73	111.00
1	D	220	LEU	CB-CG-CD2	8.52	125.48	111.00
1	C	324	GLU	OE1-CD-OE2	-7.88	113.84	123.30
1	B	105	ARG	NH1-CZ-NH2	-7.81	110.81	119.40
1	C	122	GLU	CG-CD-OE2	-7.76	102.78	118.30
1	B	455	LEU	CB-CG-CD2	7.73	124.14	111.00
1	B	428	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	D	62	GLU	OE1-CD-OE2	-7.53	114.26	123.30
1	B	62	GLU	OE1-CD-OE2	-7.41	114.41	123.30
1	D	105	ARG	NH1-CZ-NH2	-7.38	111.28	119.40
1	D	485	PHE	CB-CG-CD1	7.34	125.94	120.80
1	D	553	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	140	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	287	ARG	CG-CD-NE	7.01	126.52	111.80
1	A	52	ASP	CB-CG-OD1	6.90	124.51	118.30
1	D	105	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	C	455	LEU	CB-CG-CD2	6.70	122.39	111.00
1	A	102	GLU	OE1-CD-OE2	-6.68	115.28	123.30
1	B	292	ARG	NE-CZ-NH2	6.65	123.63	120.30
1	B	315	GLU	OE1-CD-OE2	-6.64	115.33	123.30
1	C	444	TYR	CB-CG-CD2	6.54	124.93	121.00
1	C	55	GLU	OE1-CD-OE2	-6.52	115.48	123.30
1	D	497	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	C	287	ARG	NH1-CZ-NH2	-6.46	112.29	119.40
1	B	497	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	34	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	D	315	GLU	OE1-CD-OE2	-6.43	115.59	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	538	GLU	CA-CB-CG	6.42	127.53	113.40
1	A	287	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
1	A	492	LEU	CB-CG-CD2	6.35	121.79	111.00
1	D	8	GLU	OE1-CD-OE2	-6.32	115.72	123.30
1	C	287	ARG	CG-CD-NE	6.29	125.02	111.80
1	C	122	GLU	OE1-CD-OE2	6.04	130.54	123.30
1	A	444	TYR	CB-CG-CD1	6.03	124.62	121.00
1	D	87	ALA	N-CA-C	5.98	127.13	111.00
1	A	61	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	444	TYR	CZ-CE2-CD2	5.91	125.12	119.80
1	C	17	GLU	CB-CA-C	-5.90	98.61	110.40
1	B	160	ARG	CD-NE-CZ	5.79	131.70	123.60
1	D	444	TYR	CB-CG-CD2	5.73	124.44	121.00
1	A	52	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	489	ILE	CG1-CB-CG2	-5.62	99.05	111.40
1	B	444	TYR	CB-CG-CD1	5.58	124.35	121.00
1	A	324	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	A	9	PHE	CB-CG-CD2	5.49	124.64	120.80
1	A	191	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	102	GLU	OE1-CD-OE2	-5.49	116.72	123.30
1	B	160	ARG	CG-CD-NE	-5.44	100.38	111.80
1	D	482	ASP	CB-CG-OD2	5.39	123.16	118.30
1	A	444	TYR	CD1-CG-CD2	-5.38	111.98	117.90
1	B	160	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	C	538	GLU	CA-CB-CG	5.30	125.07	113.40
1	D	569	LEU	CB-CG-CD1	5.25	119.92	111.00
1	D	444	TYR	CD1-CE1-CZ	5.21	124.48	119.80
1	B	8	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	B	219	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	C	444	TYR	CD1-CE1-CZ	5.11	124.39	119.80
1	B	444	TYR	CD1-CG-CD2	-5.10	112.29	117.90
1	A	406	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	C	444	TYR	CD1-CG-CD2	-5.04	112.35	117.90
1	B	264	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	A	122	GLU	OE1-CD-OE2	-5.01	117.29	123.30

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4350	0	4298	45	0
1	B	4255	0	4151	63	0
1	C	4309	0	4209	78	0
1	D	4287	0	4191	64	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	7	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	243	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 (243) 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: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:HE1	1:C:565:VAL:CG2	1.68	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:A:32[A]:ASP:CG	1:A:33:GLY:H	1.49	1.09
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:MET:CE	1:B:528:PRO:HD2	1.97	0.95
1:C:561[B]:MET:HE2	1:C:565:VAL:CG2	1.95	0.95
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:B:477:MET:HE3	1:B:528:PRO:HD2	1.52	0.89
1:C:561[B]:MET:HE1	1:C:565:VAL:HG21	0.90	0.88
1:D:497:ARG:HG2	1:D:497:ARG:HH11	1.38	0.88
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:A:32[A]:ASP:CG	1:A:33:GLY:N	2.27	0.83
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:561[B]:MET:HE2	1:C:565:VAL:HG23	1.62	0.79
1:C:561[B]:MET:CE	1:C:565:VAL:HG23	2.12	0.78
1:C:521[A]:PRO:CB	1:C:524:ALA:CB	2.61	0.77
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:32:ASP:O	1:D:32:ASP:CG	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:MET:N	1:C:6:PRO:HD2	2.07	0.70
1:B:477:MET:HE1	1:B:528:PRO:HD2	1.75	0.68
1:B:477:MET:CE	1:B:528:PRO:CD	2.70	0.67
1:D:7:VAL:HG23	1:D:8:GLU:N	2.10	0.67
1:B:477:MET:HE3	1:B:528:PRO:CD	2.24	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:521[A]:PRO:CG	1:C:524:ALA:HB2	2.27	0.63
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: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:B:477:MET:HE1	1:B:528:PRO:CD	2.32	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
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:A:558:ILE:HD11	1:A:567:ILE:CD1	2.33	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:D:7:VAL:HG21	1:D:576:ALA:HB1	1.88	0.56
1:D:478:TYR:CD1	1:D:478:TYR:C	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:TYR:CD1	1:B:478:TYR:C	2.80	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:B:477:MET:HE1	1:B:528:PRO:CG	2.38	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: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: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: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:B:478:TYR:HD1	1:B:478:TYR:C	2.13	0.51
1:C:457:MET:HE3	4:C:672:HOH:O	2.10	0.51
1:A:562:GLU:HG3	4:A:707:HOH:O	2.11	0.51
1:D:32:ASP:HB2	1:D:97:THR:OG1	2.10	0.51
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: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: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:D:533:LEU:HD23	1:D:536:MET:HE1	1.90	0.49
1:B:341:PHE:CG	1:B:342:ASP:N	2.80	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:457:MET:HE1	1:A:508:HIS:CG	2.48	0.48
1:A:272:PHE:HA	1:A:276:GLU:O	2.13	0.48
1:D:52:ASP:CG	1:D:292:ARG:HH12	2.17	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:C:457:MET:HE1	1:C:508:HIS:CG	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: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:B:162:ASP:OD2	1:B:183:SER:OG	2.33	0.47
1:D:478:TYR:CE1	1:D:486:ARG:CG	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:533:LEU:HD23	1:B:536:MET:HE1	1.96	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:B:416:CYS:HG	1:B:453:CYS:HG	1.65	0.45
1:B:13:VAL:HG22	1:B:569:LEU:HD21	1.99	0.45
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:410:LYS:NZ	4:A:734:HOH:O	2.49	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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:475:GLU:HA	1:A:500:MET:HE1	2.02	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
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:D:555:GLY:C	1:D:556:HIS:CD2	2.95	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:478:TYR:CD2	1:D:500:MET:HE2	2.56	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%)	41 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	574/582 (99%)	554 (96%)	19 (3%)	1 (0%)	47 33
1	C	580/582 (100%)	569 (98%)	11 (2%)	0	100 100
1	D	574/582 (99%)	553 (96%)	19 (3%)	2 (0%)	41 27
All	All	2307/2328 (99%)	2242 (97%)	60 (3%)	5 (0%)	47 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 (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	450/468 (96%)	433 (96%)	17 (4%)	33 18
1	B	425/468 (91%)	412 (97%)	13 (3%)	40 25
1	C	434/468 (93%)	416 (96%)	18 (4%)	30 15
1	D	434/468 (93%)	421 (97%)	13 (3%)	41 26
All	All	1743/1872 (93%)	1682 (96%)	61 (4%)	36 20

All (61) 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

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Mol	Chain	Res	Type
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	520	HIS
1	A	538	GLU
1	A	558	ILE
1	B	20	ILE
1	B	34	ASP
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	477	MET
1	B	478	TYR
1	B	497	ARG
1	B	506	ILE
1	B	525	SER
1	C	34	ASP
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	419	GLU
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	558	ILE

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Mol	Chain	Res	Type
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	477	MET
1	D	478	TYR
1	D	485	PHE
1	D	497	ARG
1	D	506	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	89	GLN
1	A	508	HIS
1	A	556	HIS
1	B	556	HIS
1	C	28	GLN
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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	A	583[A]	-	5,5,5	0.58	0	5,5,5	0.55	0
2	GOL	B	584	-	5,5,5	0.44	0	5,5,5	0.68	0
2	GOL	A	583[B]	-	5,5,5	0.63	0	5,5,5	0.57	0
2	GOL	D	585	-	5,5,5	0.48	0	5,5,5	0.36	0
2	GOL	A	584	-	5,5,5	0.32	0	5,5,5	1.28	0
2	GOL	D	584	-	5,5,5	0.61	0	5,5,5	0.90	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	GOL	A	583[A]	-	-	4/4/4/4	-
2	GOL	B	584	-	-	4/4/4/4	-
2	GOL	A	583[B]	-	-	4/4/4/4	-
2	GOL	D	585	-	-	4/4/4/4	-
2	GOL	A	584	-	-	1/4/4/4	-
2	GOL	D	584	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) 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	A	584	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
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	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

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, 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	576/582 (98%)	-0.26	5 (0%) 84 82	29, 39, 51, 63	0
1	B	574/582 (98%)	0.11	41 (7%) 16 12	31, 44, 66, 91	0
1	C	577/582 (99%)	0.07	26 (4%) 33 27	27, 45, 68, 87	0
1	D	575/582 (98%)	0.13	39 (6%) 17 13	29, 46, 71, 84	0
All	All	2302/2328 (98%)	0.01	111 (4%) 30 25	27, 43, 66, 91	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	141	GLY	10.2
1	C	142	GLY	7.0
1	D	141	GLY	6.6
1	B	556	HIS	6.4
1	D	86	GLY	5.7
1	D	87	ALA	5.2
1	D	84	SER	5.0
1	C	5	MET	4.9
1	C	558	ILE	4.9
1	D	33	GLY	4.8
1	C	556	HIS	4.7
1	B	555	GLY	4.5
1	D	556	HIS	4.5
1	A	142	GLY	4.4
1	B	478	TYR	4.4
1	B	557	ALA	4.3
1	B	132	ASP	4.3
1	B	7	VAL	4.2
1	C	494	GLY	4.1
1	D	341	PHE	3.9
1	B	54	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	87	ALA	3.8
1	D	153	PHE	3.7
1	B	481	SER	3.7
1	B	484	ALA	3.6
1	D	540	LEU	3.6
1	D	61	ARG	3.5
1	D	85	LYS	3.5
1	B	479	GLU	3.5
1	C	122	GLU	3.4
1	C	480	LEU	3.4
1	D	54	GLY	3.3
1	C	140	ASP	3.3
1	D	132	ASP	3.2
1	D	142	GLY	3.2
1	D	83	VAL	3.2
1	B	172	GLY	3.1
1	B	341	PHE	3.1
1	C	524	ALA	3.1
1	D	541	ALA	3.1
1	D	173	GLY	3.1
1	B	482	ASP	3.1
1	C	6	PRO	3.0
1	A	141	GLY	3.0
1	B	33	GLY	3.0
1	D	44	GLY	3.0
1	C	557	ALA	3.0
1	B	365	LEU	2.9
1	B	525	SER	2.9
1	B	495	GLY	2.9
1	D	140	ASP	2.9
1	C	526	ARG	2.9
1	B	429	TRP	2.8
1	C	483	ALA	2.8
1	C	488	PHE	2.8
1	B	86	GLY	2.7
1	B	393	VAL	2.7
1	D	580	GLU	2.7
1	C	151	PRO	2.6
1	C	183	SER	2.6
1	B	483	ALA	2.6
1	B	524	ALA	2.6
1	C	497	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	357	PRO	2.6
1	D	581	ARG	2.5
1	B	580	GLU	2.5
1	D	131	GLU	2.5
1	C	153	PHE	2.5
1	B	494	GLY	2.5
1	B	85	LYS	2.5
1	B	194	GLU	2.5
1	D	122	GLU	2.5
1	D	88	GLU	2.4
1	C	495	GLY	2.4
1	D	107	GLU	2.4
1	B	359	PRO	2.4
1	B	385	LEU	2.4
1	C	478	TYR	2.4
1	B	342	ASP	2.4
1	A	6	PRO	2.4
1	D	169	PHE	2.4
1	D	331	ALA	2.4
1	C	98	SER	2.3
1	D	393	VAL	2.3
1	C	33	GLY	2.3
1	D	494	GLY	2.3
1	D	537	GLY	2.3
1	A	341	PHE	2.2
1	D	172	GLY	2.2
1	C	529[A]	LEU	2.2
1	D	133	ARG	2.2
1	C	132	ASP	2.2
1	B	343	GLY	2.2
1	D	171	GLY	2.2
1	B	452	LEU	2.2
1	B	433	SER	2.2
1	B	44	GLY	2.2
1	D	392	VAL	2.2
1	D	557	ALA	2.2
1	B	131	GLU	2.2
1	D	7	VAL	2.2
1	B	437	SER	2.1
1	C	525	SER	2.1
1	B	392	VAL	2.1
1	D	52	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	434	GLY	2.1
1	B	447	GLY	2.1
1	B	554	ALA	2.1
1	B	356	ALA	2.0
1	D	363	VAL	2.0
1	D	482	ASP	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	GOL	B	584	6/6	0.72	0.17	48,55,57,60	0
2	GOL	D	584	6/6	0.82	0.13	36,46,48,53	0
2	GOL	A	584	6/6	0.86	0.13	45,57,58,62	0
2	GOL	D	585	6/6	0.89	0.14	34,52,57,59	0
2	GOL	A	583[A]	6/6	0.90	0.16	29,31,34,34	6
2	GOL	A	583[B]	6/6	0.90	0.16	29,32,34,34	6
3	NA	D	583	1/1	0.96	0.06	39,39,39,39	0
3	NA	B	583	1/1	0.97	0.04	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.