Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:32 PM GMT

PDB ID	:	1KSI
Title	:	CRYSTAL STRUCTURE OF A EUKARYOTIC (PEA SEEDLING) COPPER-CONTAINING AMINE OXIDASE AT 2.2A RESOLUTION
Authors	:	Wilce, M.C.J.; Kumar, V.; Freeman, H.C.; Guss, J.M.
Deposited on	:	1996-07-20
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

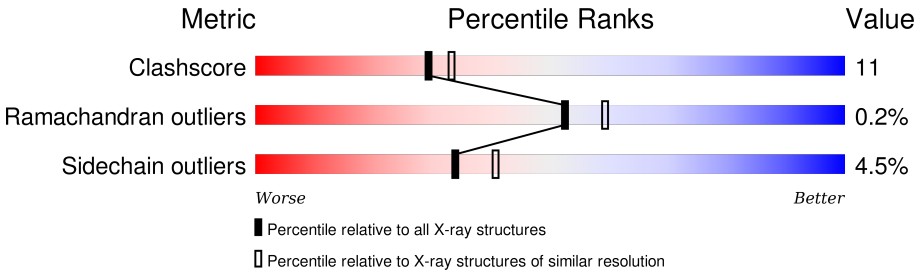
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	642	66% 31% .
1	B	642	73% 22% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	655	X	-	X	-
2	NAG	A	656	X	-	X	-
2	NAG	A	657	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	655	X	-	-	-
2	NAG	B	656	X	-	-	-
2	NAG	B	657	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10995 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.

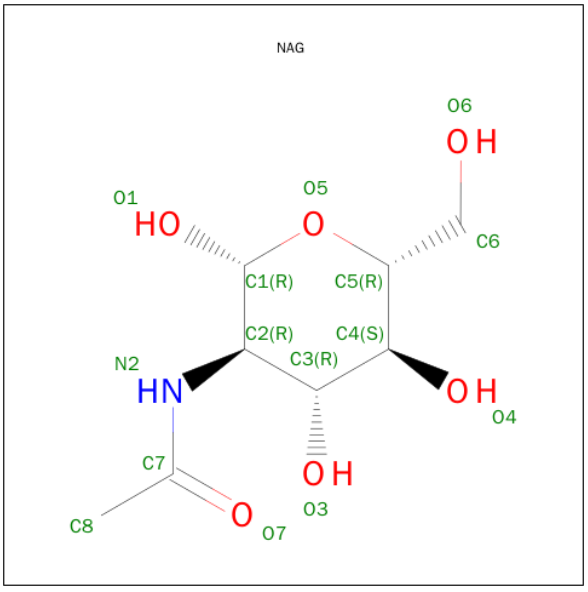
- Molecule 1 is a protein called COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	10	1	0
			5168	3319	877	961	11			
1	B	642	Total	C	N	O	S	12	1	0
			5168	3319	877	961	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	TPQ	TYR	MODIFIED RESIDUE	UNP Q43077
B	387	TPQ	TYR	MODIFIED RESIDUE	UNP Q43077

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cu 1 1	0	0
3	A	1	Total Cu 1 1	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mn 1 1	0	0
4	A	1	Total Mn 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	280	Total O 280 280	0	0
5	B	291	Total O 291 291	0	0

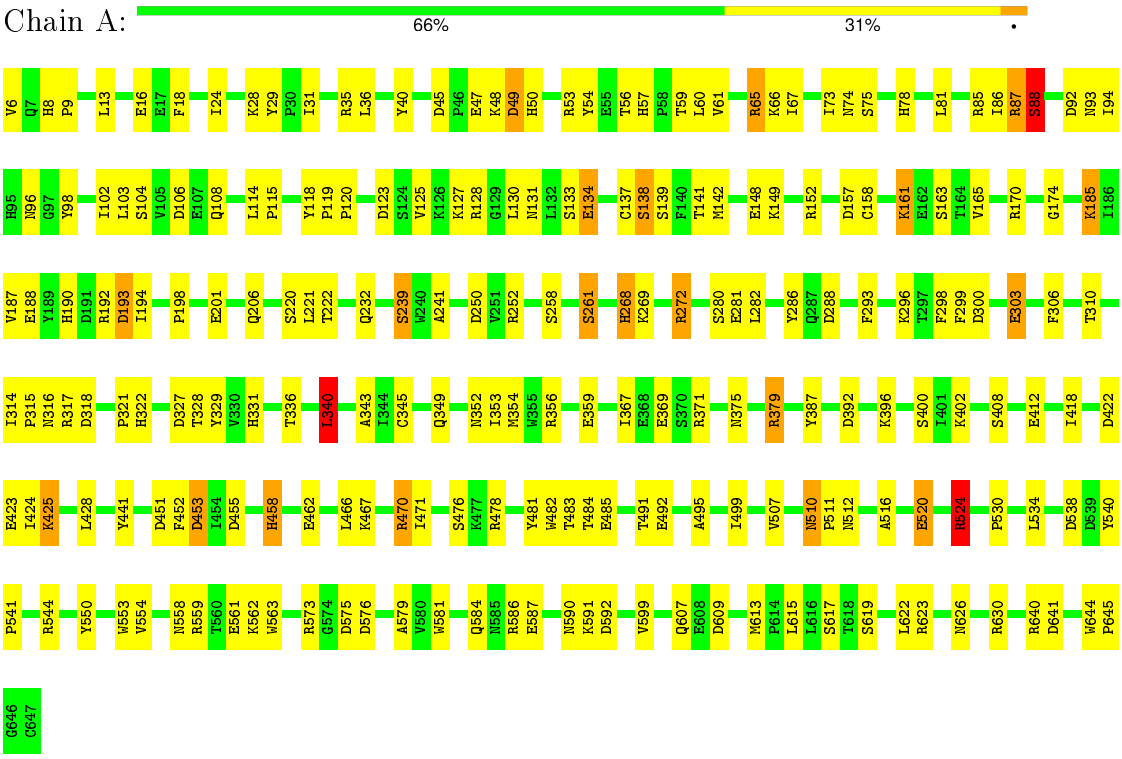
3 Residue-property plots (i)

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

Note EDS was not executed.

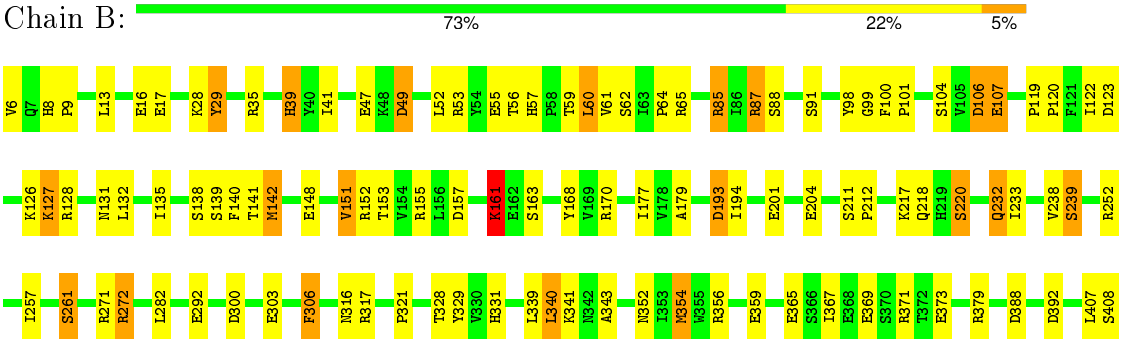
- Molecule 1: COPPER AMINE OXIDASE

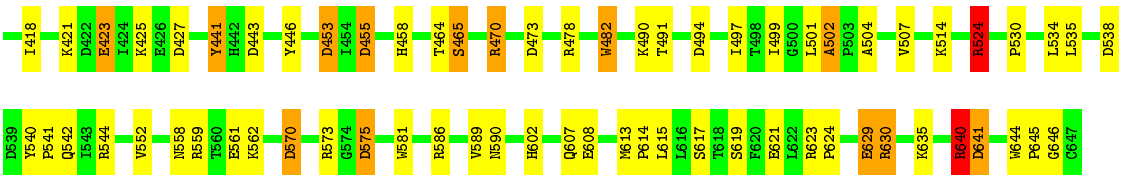
Chain A:



- Molecule 1: COPPER AMINE OXIDASE

Chain B:




I418
K421
D422
E423
I424
K425
E426
D427
Y441
H442
D443
Y446
D453
I454
D455
H458
T464
S465
R470
D473
R478
W482
K490
T491
D494
I497
T498
I499
G500
L501
A502
P503
A504
V507
K514
R524
P530
L534
L535
D538
D539
Y540
P541
Q542
I543
R544
V552
N558
R559
T560
E561
K562
D570
R573
G574
D575
W581
R586
V589
N590
H602
Q607
E608
M613
P614
L615
L616
S617
T618
S619
F620
E621
L622
R623
P624
E629
R630
K635
R640
D641
W644
P645
G646
C647

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.37Å 114.64Å 199.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	86.5 (7.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10995	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, TPQ, CU, NAG

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	0.80	1/5297 (0.0%)	1.75	102/7211 (1.4%)
1	B	0.82	4/5297 (0.1%)	1.68	91/7211 (1.3%)
All	All	0.81	5/10594 (0.0%)	1.72	193/14422 (1.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	640	ARG	NE-CZ	10.87	1.47	1.33
1	B	148	GLU	CA-CB	7.35	1.70	1.53
1	B	640	ARG	CD-NE	6.34	1.57	1.46
1	B	148	GLU	CD-OE2	5.17	1.31	1.25
1	A	258	SER	CA-CB	5.14	1.60	1.52

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	152	ARG	CD-NE-CZ	20.12	151.76	123.60
1	A	317	ARG	NE-CZ-NH1	19.41	130.01	120.30
1	A	478	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	A	575	ASP	CB-CG-OD1	16.53	133.17	118.30
1	A	478	ARG	NE-CZ-NH2	-16.32	112.14	120.30
1	B	317	ARG	NE-CZ-NH2	-15.36	112.62	120.30
1	A	252	ARG	NE-CZ-NH1	-14.59	113.00	120.30
1	A	252	ARG	NE-CZ-NH2	14.33	127.46	120.30
1	A	371	ARG	NE-CZ-NH1	13.71	127.15	120.30
1	A	85	ARG	CD-NE-CZ	13.65	142.71	123.60
1	B	640	ARG	NE-CZ-NH1	13.12	126.86	120.30
1	B	379	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	B	559	ARG	NE-CZ-NH1	12.49	126.54	120.30
1	A	623	ARG	CD-NE-CZ	12.22	140.71	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	640	ARG	NE-CZ-NH1	-11.96	114.32	120.30
1	B	317	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	A	85	ARG	NE-CZ-NH1	11.51	126.06	120.30
1	A	106	ASP	CB-CG-OD2	-11.31	108.12	118.30
1	A	524	ARG	NE-CZ-NH2	-11.19	114.70	120.30
1	B	388	ASP	CB-CG-OD2	-10.41	108.93	118.30
1	B	570	ASP	CB-CG-OD2	-10.23	109.09	118.30
1	A	92	ASP	CB-CG-OD1	10.17	127.45	118.30
1	A	35	ARG	NE-CZ-NH2	10.11	125.35	120.30
1	A	152	ARG	NE-CZ-NH1	10.03	125.32	120.30
1	B	272	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	B	170	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	B	524	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	B	470	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	A	128	ARG	NE-CZ-NH2	9.70	125.15	120.30
1	A	157	ASP	CB-CG-OD1	9.66	126.99	118.30
1	A	193	ASP	CB-CG-OD1	-9.47	109.78	118.30
1	A	87	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	379	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	A	106	ASP	CB-CG-OD1	9.12	126.51	118.30
1	B	640	ARG	NH1-CZ-NH2	-9.12	109.37	119.40
1	A	87	ARG	CD-NE-CZ	9.08	136.31	123.60
1	B	85	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	B	148	GLU	N-CA-CB	9.00	126.80	110.60
1	A	524	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	A	640	ARG	NE-CZ-NH2	8.80	124.70	120.30
1	B	106	ASP	CB-CG-OD1	8.72	126.15	118.30
1	A	128	ARG	NE-CZ-NH1	-8.70	115.95	120.30
1	B	630	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	A	371	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	B	478	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	B	87	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	B	575	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	379	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	85	ARG	CD-NE-CZ	8.29	135.20	123.60
1	B	392	ASP	CB-CG-OD1	8.13	125.62	118.30
1	A	641	ASP	CB-CG-OD1	-8.04	111.06	118.30
1	B	544	ARG	NE-CZ-NH2	8.01	124.31	120.30
1	B	640	ARG	CA-CB-CG	7.90	130.78	113.40
1	B	453	ASP	CB-CG-OD1	7.80	125.32	118.30
1	A	317	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	B	271	ARG	NE-CZ-NH2	-7.77	116.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	392	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	35	ARG	NE-CZ-NH1	-7.39	116.61	120.30
1	A	272	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	A	617	SER	N-CA-CB	-7.33	99.50	110.50
1	B	586	ARG	NE-CZ-NH1	-7.15	116.72	120.30
1	A	575	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	250	ASP	CB-CG-OD1	-6.94	112.05	118.30
1	B	87	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	470	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	640	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	B	300	ASP	CB-CG-OD1	6.87	124.48	118.30
1	B	478	ARG	CD-NE-CZ	6.85	133.19	123.60
1	B	640	ARG	CD-NE-CZ	6.84	133.18	123.60
1	B	106	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	B	470	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	142	MET	CA-CB-CG	6.78	124.83	113.30
1	A	619	SER	N-CA-CB	-6.78	100.33	110.50
1	A	451	ASP	CB-CG-OD2	6.72	124.35	118.30
1	B	128	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	586	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	B	204	GLU	OE1-CD-OE2	6.62	131.24	123.30
1	A	157	ASP	OD1-CG-OD2	-6.61	110.74	123.30
1	B	29	TYR	CB-CG-CD2	-6.59	117.04	121.00
1	B	35	ARG	CD-NE-CZ	6.56	132.78	123.60
1	A	98	TYR	CB-CG-CD1	-6.50	117.10	121.00
1	B	453	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	49	ASP	CB-CA-C	-6.47	97.45	110.40
1	B	157	ASP	CB-CG-OD1	6.44	124.10	118.30
1	B	39	HIS	CA-CB-CG	-6.43	102.66	113.60
1	B	559	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	354	MET	CG-SD-CE	6.32	110.32	100.20
1	A	161	LYS	C-N-CA	-6.32	105.91	121.70
1	A	329	TYR	CA-CB-CG	-6.32	101.40	113.40
1	A	327	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	B	619	SER	N-CA-CB	-6.26	101.12	110.50
1	A	138	SER	N-CA-CB	-6.25	101.12	110.50
1	B	49	ASP	CB-CA-C	-6.24	97.91	110.40
1	B	640	ARG	CB-CA-C	6.23	122.86	110.40
1	A	85	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	239	SER	CA-CB-OG	-6.20	94.45	111.20
1	A	185	LYS	N-CA-CB	-6.16	99.51	110.60
1	B	365	GLU	OE1-CD-OE2	6.16	130.69	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	ARG	CD-NE-CZ	6.13	132.18	123.60
1	B	88	SER	N-CA-CB	-6.10	101.35	110.50
1	A	422	ASP	CB-CA-C	-6.09	98.22	110.40
1	B	441	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	B	107	GLU	OE1-CD-OE2	-6.06	116.03	123.30
1	A	123	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	B	369	GLU	OE1-CD-OE2	-6.03	116.07	123.30
1	A	340	LEU	CB-CA-C	6.02	121.63	110.20
1	B	371	ARG	CD-NE-CZ	6.00	132.00	123.60
1	A	40	TYR	CB-CG-CD2	5.96	124.57	121.00
1	A	478	ARG	CD-NE-CZ	5.95	131.93	123.60
1	A	149	LYS	CB-CA-C	5.92	122.24	110.40
1	A	239	SER	CA-CB-OG	-5.89	95.30	111.20
1	A	232	GLN	CB-CG-CD	5.88	126.90	111.60
1	A	310	THR	CA-CB-CG2	5.88	120.64	112.40
1	B	123	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	B	152	ARG	CD-NE-CZ	5.87	131.82	123.60
1	A	65	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	B	142	MET	CA-CB-CG	5.85	123.25	113.30
1	A	481	TYR	CB-CG-CD2	-5.84	117.49	121.00
1	B	53	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	193	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	B	482	TRP	CA-CB-CG	5.80	124.72	113.70
1	A	16	GLU	CA-CB-CG	5.76	126.08	113.40
1	B	201	GLU	N-CA-CB	-5.76	100.23	110.60
1	B	201	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	B	608	GLU	OE1-CD-OE2	-5.73	116.42	123.30
1	B	379	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	455	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	B	220	SER	N-CA-CB	5.66	118.99	110.50
1	A	241	ALA	N-CA-CB	5.66	118.02	110.10
1	B	292	GLU	CG-CD-OE2	5.65	129.59	118.30
1	A	261	SER	CB-CA-C	-5.63	99.40	110.10
1	B	220	SER	CA-C-N	-5.61	104.87	117.20
1	B	98	TYR	CA-CB-CG	-5.60	102.76	113.40
1	A	49	ASP	O-C-N	5.59	131.65	122.70
1	A	520	GLU	OE1-CD-OE2	-5.59	116.59	123.30
1	B	272	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	617	SER	N-CA-CB	-5.56	102.16	110.50
1	B	624	PRO	O-C-N	-5.54	113.83	122.70
1	A	576	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	A	453	ASP	CB-CG-OD1	5.52	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	220	SER	CB-CA-C	-5.51	99.64	110.10
1	B	232	GLN	CB-CG-CD	5.50	125.91	111.60
1	B	423	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	B	443	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	524	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	354	MET	CG-SD-CE	5.45	108.92	100.20
1	B	220	SER	CA-C-O	5.45	131.54	120.10
1	A	641	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	300	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	379	ARG	CD-NE-CZ	5.38	131.14	123.60
1	A	609	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	49	ASP	N-CA-CB	5.34	120.22	110.60
1	A	550	TYR	CA-CB-CG	-5.34	103.25	113.40
1	B	573	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	232	GLN	CA-CB-CG	5.33	125.13	113.40
1	B	641	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	A	544	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	134	GLU	OE1-CD-OE2	-5.32	116.92	123.30
1	A	317	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
1	A	300	ASP	CA-C-O	-5.28	109.02	120.10
1	A	609	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	B	261	SER	CB-CA-C	-5.27	100.09	110.10
1	A	516	ALA	CB-CA-C	5.26	117.99	110.10
1	B	140	PHE	CB-CG-CD1	5.25	124.47	120.80
1	A	579	ALA	O-C-N	-5.24	114.31	122.70
1	A	170	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	427	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	161	LYS	CA-C-N	5.20	128.65	117.20
1	B	161	LYS	CA-C-N	5.20	128.65	117.20
1	A	303	GLU	OE1-CD-OE2	5.19	129.53	123.30
1	B	562	LYS	CB-CA-C	-5.18	100.04	110.40
1	A	317	ARG	CD-NE-CZ	-5.16	116.38	123.60
1	B	570	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	268	HIS	CA-CB-CG	-5.14	104.85	113.60
1	B	329	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	A	573	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	179	ALA	N-CA-CB	5.13	117.29	110.10
1	B	161	LYS	C-N-CA	-5.13	108.88	121.70
1	A	88	SER	N-CA-CB	-5.12	102.83	110.50
1	A	318	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	54	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	A	96	ASN	CA-C-N	5.10	126.40	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	599	VAL	CA-C-N	5.09	126.39	116.20
1	A	369	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	B	257	ILE	C-N-CA	-5.07	109.02	121.70
1	A	299	PHE	N-CA-CB	5.07	119.72	110.60
1	A	553	TRP	CA-CB-CG	5.06	123.31	113.70
1	B	514	LYS	CA-CB-CG	-5.06	102.27	113.40
1	B	356	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	53	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	458	HIS	CA-CB-CG	-5.03	105.06	113.60
1	A	53	ARG	CG-CD-NE	5.01	122.32	111.80
1	A	98	TYR	CA-CB-CG	-5.01	103.88	113.40

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	5168	0	5085	119	1
1	B	5168	0	5085	102	1
2	A	42	0	39	32	0
2	B	42	0	38	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	280	0	0	7	0
5	B	291	0	0	6	0
All	All	10995	0	10247	226	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (226) 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:A:558:ASN:HD21	2:A:657:NAG:C1	1.07	1.58
1:B:558:ASN:HD21	2:B:657:NAG:C1	1.27	1.45
1:A:558:ASN:HD21	2:A:657:NAG:C2	1.34	1.41
1:A:558:ASN:ND2	2:A:657:NAG:H2	1.40	1.36
1:B:558:ASN:HD21	2:B:657:NAG:C2	1.47	1.25
2:A:655:NAG:C3	2:A:656:NAG:H82	1.69	1.21
2:A:655:NAG:C4	2:A:656:NAG:H82	1.73	1.17
2:A:655:NAG:C2	2:A:656:NAG:H82	1.79	1.12
2:A:655:NAG:H4	2:A:656:NAG:H82	1.37	1.04
2:A:655:NAG:H4	2:A:656:NAG:C8	1.87	1.04
1:B:558:ASN:ND2	2:B:657:NAG:C2	2.18	1.03
2:A:655:NAG:H4	2:A:656:NAG:C7	1.89	1.03
1:B:558:ASN:ND2	2:B:657:NAG:H2	1.77	1.00
2:A:655:NAG:H2	2:A:656:NAG:H82	1.49	0.93
2:A:655:NAG:H2	2:A:656:NAG:C8	1.99	0.92
1:B:558:ASN:HB3	1:B:561:GLU:HG3	1.51	0.90
1:A:558:ASN:ND2	2:A:657:NAG:H4	1.92	0.84
2:A:655:NAG:C4	2:A:656:NAG:C8	2.50	0.83
1:B:558:ASN:ND2	2:B:657:NAG:H4	1.96	0.79
1:B:151:VAL:HG23	1:B:153:THR:HG23	1.65	0.79
1:A:499:ILE:HG22	1:A:530:PRO:HG3	1.65	0.78
1:A:28:LYS:HG2	1:A:29:TYR:CE2	2.20	0.77
2:A:655:NAG:HO4	2:A:656:NAG:C1	1.93	0.77
1:B:132:LEU:HA	1:B:135:ILE:HD12	1.66	0.76
1:A:558:ASN:ND2	2:A:657:NAG:C4	2.50	0.75
1:A:424:ILE:HG12	1:A:428:LEU:HD11	1.70	0.74
1:B:28:LYS:HG2	1:B:29:TYR:CE1	2.24	0.73
1:A:558:ASN:ND2	2:A:657:NAG:C3	2.52	0.73
2:A:655:NAG:C3	2:A:656:NAG:C8	2.60	0.72
1:B:161:LYS:O	1:B:161:LYS:HG2	1.91	0.71
1:A:558:ASN:HD22	2:A:657:NAG:H2	1.49	0.71
2:A:655:NAG:C4	2:A:656:NAG:C7	2.66	0.71
1:B:131:ASN:ND2	2:B:655:NAG:C2	2.55	0.69
1:B:272:ARG:NH2	1:B:453:ASP:OD2	2.26	0.69
1:B:644:TRP:CH2	1:B:646:GLY:HA2	2.29	0.67
1:B:630:ARG:HD2	5:B:856:HOH:O	1.94	0.67
2:A:655:NAG:O4	2:A:656:NAG:C2	2.43	0.67
2:A:655:NAG:C2	2:A:656:NAG:C8	2.60	0.67
1:B:122:ILE:O	1:B:126:LYS:HG3	1.95	0.66
1:B:644:TRP:CZ3	1:B:646:GLY:HA2	2.30	0.66
1:A:59:THR:C	1:A:60:LEU:HG	2.16	0.65
1:A:458:HIS:HB3	1:A:590:ASN:OD1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:ASN:CB	1:B:561:GLU:HG3	2.27	0.65
1:A:510:ASN:HD21	1:A:512:ASN:HD22	1.45	0.65
1:A:558:ASN:HD22	2:A:657:NAG:H4	1.64	0.63
1:A:161:LYS:HG2	1:A:161:LYS:O	1.98	0.63
1:B:233:ILE:HG12	1:B:238:VAL:HG22	1.81	0.63
1:A:6:VAL:HG11	1:A:65:ARG:NH2	2.12	0.63
2:A:655:NAG:O4	2:A:656:NAG:O5	2.17	0.62
1:A:119:PRO:N	1:A:120:PRO:CD	2.62	0.62
1:B:359:GLU:HB3	1:B:367:ILE:HB	1.81	0.62
1:A:558:ASN:HD22	2:A:657:NAG:C2	2.01	0.61
1:A:86:ILE:HG13	1:A:88:SER:HB3	1.81	0.61
1:A:534:LEU:HB2	1:B:482:TRP:CD1	2.35	0.61
1:B:127:LYS:HD2	1:B:194:ILE:HD11	1.83	0.61
1:A:470:ARG:HH22	1:B:538:ASP:CG	2.04	0.61
1:A:272:ARG:NH2	1:A:453:ASP:OD2	2.32	0.60
1:B:100:PHE:HB3	1:B:101:PRO:HD2	1.83	0.60
1:B:575:ASP:OD1	5:B:887:HOH:O	2.16	0.60
2:A:655:NAG:C4	2:A:656:NAG:N2	2.64	0.60
1:A:45:ASP:O	1:A:559:ARG:NH1	2.34	0.59
1:B:558:ASN:ND2	2:B:657:NAG:C4	2.65	0.59
1:B:119:PRO:HB2	1:B:120:PRO:HD3	1.85	0.59
1:A:467:LYS:HD3	1:A:485:GLU:OE1	2.03	0.58
1:B:408:SER:HB2	1:B:615:LEU:HD12	1.84	0.58
1:B:352:ASN:HB2	5:B:709:HOH:O	2.04	0.58
1:B:490:LYS:HA	1:B:589:VAL:CG2	2.34	0.58
1:A:316:ASN:ND2	1:A:321:PRO:HA	2.19	0.57
1:B:558:ASN:CG	2:B:657:NAG:C1	2.73	0.57
1:A:630:ARG:HA	1:B:607:GLN:O	2.04	0.57
1:A:316:ASN:HD22	1:A:321:PRO:HA	1.70	0.57
1:B:497:ILE:HB	1:B:552:VAL:HB	1.87	0.56
1:B:104:SER:OG	1:B:107:GLU:HG2	2.06	0.56
1:A:499:ILE:CG2	1:A:530:PRO:HG3	2.36	0.56
1:A:452:PHE:HZ	1:A:622:LEU:HD22	1.71	0.56
1:B:64:PRO:HB3	1:B:85:ARG:HD3	1.89	0.55
1:A:510:ASN:ND2	1:A:512:ASN:H	2.04	0.54
1:A:296:LYS:HE2	5:A:716:HOH:O	2.06	0.54
1:A:104:SER:O	1:A:108:GLN:HG3	2.08	0.54
1:A:201:GLU:OE1	1:A:201:GLU:HA	2.08	0.54
1:A:510:ASN:HD22	1:A:512:ASN:H	1.56	0.53
1:B:491:THR:O	1:B:494:ASP:HB2	2.08	0.53
1:B:131:ASN:ND2	2:B:655:NAG:O5	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:O	1:B:55:GLU:HB2	2.09	0.52
1:A:322:HIS:HB3	5:A:875:HOH:O	2.10	0.52
1:B:217:LYS:HG3	1:B:218:GLN:N	2.25	0.52
1:B:340:LEU:HG	1:B:343:ALA:HB2	1.92	0.52
1:A:558:ASN:HD22	2:A:657:NAG:C3	2.20	0.52
1:B:59:THR:O	1:B:60:LEU:HD13	2.10	0.52
1:A:328:THR:HG22	5:A:741:HOH:O	2.10	0.52
1:A:558:ASN:HD22	2:A:657:NAG:C4	2.20	0.52
1:A:148:GLU:OE1	1:A:148:GLU:HA	2.10	0.51
1:B:499:ILE:HG22	1:B:530:PRO:HG3	1.92	0.51
1:B:151:VAL:CG2	1:B:153:THR:HG23	2.39	0.51
1:A:206:GLN:NE2	1:B:367:ILE:HG23	2.26	0.51
1:A:188:GLU:OE2	1:A:190:HIS:HE1	1.93	0.51
1:A:48:LYS:HE2	1:A:453:ASP:OD2	2.11	0.51
1:A:507:VAL:HG22	1:A:524:ARG:HB2	1.92	0.51
1:A:118:TYR:CD2	1:A:120:PRO:HD2	2.46	0.50
1:A:296:LYS:HE3	1:A:298:PHE:CZ	2.46	0.50
2:A:655:NAG:O3	2:A:656:NAG:C8	2.59	0.50
1:A:322:HIS:HD2	5:A:784:HOH:O	1.94	0.50
1:B:57:HIS:O	1:B:61:VAL:HG23	2.11	0.50
1:A:408:SER:HB2	1:A:615:LEU:HD12	1.94	0.50
1:A:28:LYS:HG2	1:A:29:TYR:CD2	2.46	0.50
1:A:495:ALA:HB1	1:A:554:VAL:HB	1.94	0.50
1:B:407:LEU:HD21	1:B:446:TYR:OH	2.12	0.49
1:A:558:ASN:CG	2:A:657:NAG:C1	2.73	0.49
1:B:39:HIS:HB3	1:B:101:PRO:HB2	1.93	0.49
1:B:316:ASN:HD22	1:B:321:PRO:HA	1.78	0.49
1:A:540:TYR:HB2	1:A:541:PRO:HD3	1.94	0.48
1:B:621:GLU:OE2	1:B:623:ARG:HD2	2.12	0.48
1:B:57:HIS:HB3	1:B:60:LEU:HD23	1.96	0.48
1:A:141:THR:HG21	1:A:303:GLU:HB3	1.94	0.48
1:B:418:ILE:HA	1:B:423:GLU:OE1	2.14	0.48
1:B:561:GLU:HB3	1:B:581:TRP:CZ3	2.48	0.48
1:A:288:ASP:HB3	1:A:293:PHE:HB2	1.95	0.48
1:A:78:HIS:CE1	1:A:94:ILE:HD11	2.49	0.48
1:B:490:LYS:HA	1:B:589:VAL:HG23	1.95	0.48
1:B:490:LYS:HD3	1:B:589:VAL:HG21	1.96	0.48
1:A:471:ILE:HD13	1:A:476:SER:HB3	1.95	0.48
1:A:127:LYS:HE3	1:A:194:ILE:HD11	1.95	0.48
1:B:458:HIS:HB3	1:B:590:ASN:OD1	2.13	0.48
1:A:538:ASP:OD2	1:B:470:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HG13	1:A:87:ARG:HH21	1.79	0.47
1:B:28:LYS:HG2	1:B:29:TYR:CD1	2.49	0.47
1:A:119:PRO:N	1:A:120:PRO:HD3	2.30	0.47
1:B:644:TRP:HA	1:B:645:PRO:HD2	1.73	0.47
1:B:6:VAL:HG11	1:B:65:ARG:NH2	2.30	0.47
1:B:119:PRO:N	1:B:120:PRO:CD	2.77	0.47
1:B:8:HIS:CG	1:B:9:PRO:HD2	2.50	0.47
1:A:36:LEU:CD1	1:A:73:ILE:HG12	2.45	0.47
1:A:31:ILE:HG12	5:A:805:HOH:O	2.15	0.47
1:B:354:MET:HB2	1:B:373:GLU:HB3	1.97	0.46
2:A:655:NAG:C1	2:A:656:NAG:H82	2.45	0.46
1:B:142:MET:HG2	1:B:155:ARG:HG2	1.96	0.46
1:B:316:ASN:ND2	1:B:321:PRO:HA	2.30	0.46
1:A:359:GLU:OE1	1:B:168:TYR:HE2	1.97	0.46
1:A:340:LEU:HG	1:A:343:ALA:HB2	1.96	0.46
1:A:221:LEU:HG	1:A:222:THR:N	2.31	0.46
1:A:281:GLU:HG3	1:A:282:LEU:O	2.16	0.46
1:A:352:ASN:HB2	5:A:771:HOH:O	2.16	0.46
1:A:626:ASN:OD1	1:B:607:GLN:HG3	2.15	0.46
1:A:538:ASP:OD1	1:B:470:ARG:NH2	2.49	0.46
1:A:458:HIS:HD2	1:A:590:ASN:O	1.99	0.45
1:A:8:HIS:CG	1:A:9:PRO:HD2	2.52	0.45
1:B:558:ASN:HD22	2:B:657:NAG:H4	1.78	0.45
2:A:655:NAG:O3	2:A:656:NAG:H82	2.08	0.45
1:B:540:TYR:HB2	1:B:541:PRO:HD3	1.98	0.45
1:A:510:ASN:HD22	1:A:510:ASN:C	2.19	0.45
1:A:510:ASN:HD22	1:A:511:PRO:HD2	1.82	0.44
1:B:491:THR:O	1:B:494:ASP:N	2.44	0.44
1:A:375:ASN:OD1	1:A:396:LYS:HG2	2.17	0.44
1:B:252:ARG:O	1:B:306:PHE:HB2	2.17	0.44
1:A:562:LYS:HE2	1:A:563:TRP:CZ2	2.52	0.44
1:B:282:LEU:HD11	1:B:306:PHE:CZ	2.52	0.44
1:B:613:MET:HE3	5:B:930:HOH:O	2.17	0.44
1:A:286:TYR:OH	1:A:387:TPQ:O5	2.36	0.44
1:B:465:SER:HA	1:B:504:ALA:HA	2.00	0.44
1:A:467:LYS:N	1:A:483:THR:O	2.48	0.44
1:A:296:LYS:HE3	1:A:298:PHE:CE1	2.52	0.44
1:B:41:ILE:H	1:B:331:HIS:CE1	2.35	0.44
1:A:482:TRP:CH2	1:B:441:TYR:HB3	2.52	0.44
1:A:114:LEU:HB2	1:A:115:PRO:HD3	2.00	0.44
1:B:13:LEU:HA	1:B:17:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:HD21	1:B:341:LYS:HD3	1.99	0.43
1:B:211:SER:HB2	1:B:212:PRO:HD2	2.00	0.43
1:B:328:THR:HG22	5:B:788:HOH:O	2.18	0.43
1:A:174:GLY:O	1:A:192:ARG:HB2	2.17	0.43
1:A:185:LYS:O	1:A:187:VAL:HG13	2.18	0.43
1:A:607:GLN:HB3	1:B:629:GLU:O	2.18	0.43
1:A:102:ILE:HD13	1:A:102:ILE:HG21	1.79	0.43
1:A:125:VAL:HG13	1:A:130:LEU:HB2	2.00	0.43
1:B:418:ILE:HG23	1:B:423:GLU:HB2	2.00	0.43
1:A:587:GLU:O	1:A:591:LYS:HD3	2.17	0.43
1:A:441:TYR:HB3	1:B:482:TRP:CH2	2.54	0.43
1:B:16:GLU:CD	1:B:16:GLU:H	2.23	0.43
1:A:331:HIS:HA	1:A:336:THR:O	2.19	0.43
1:B:141:THR:HG21	1:B:303:GLU:HB3	2.01	0.43
1:A:13:LEU:HD12	1:A:18:PHE:CE1	2.54	0.43
1:A:561:GLU:HB3	1:A:581:TRP:CZ3	2.54	0.42
1:A:131:ASN:OD1	1:A:133:SER:HB2	2.18	0.42
1:A:510:ASN:HD22	1:A:511:PRO:CD	2.32	0.42
1:A:402:LYS:HE3	5:A:849:HOH:O	2.19	0.42
1:A:644:TRP:HA	1:A:645:PRO:HD2	1.81	0.42
1:A:66:LYS:C	1:A:67:ILE:HD13	2.39	0.42
1:A:67:ILE:O	1:A:81:LEU:HD12	2.19	0.42
1:A:418:ILE:HA	1:A:423:GLU:OE1	2.19	0.42
1:B:119:PRO:CB	1:B:120:PRO:HD3	2.47	0.42
1:A:201:GLU:CA	1:A:201:GLU:OE1	2.68	0.42
1:A:491:THR:O	1:A:492:GLU:C	2.58	0.42
1:A:359:GLU:HB3	1:A:367:ILE:HB	2.02	0.41
1:A:220:SER:HB2	1:B:640:ARG:O	2.20	0.41
1:B:507:VAL:HG22	1:B:524:ARG:HB2	2.02	0.41
1:A:165:VAL:HG21	1:B:367:ILE:HG21	2.02	0.41
1:A:102:ILE:HG22	1:A:103:LEU:O	2.21	0.41
1:A:314:ILE:HA	1:A:315:PRO:HD3	1.92	0.41
1:A:137:CYS:HA	1:A:158:CYS:HA	2.02	0.41
1:B:421:LYS:NZ	5:B:850:HOH:O	2.52	0.41
1:A:57:HIS:O	1:A:61:VAL:HG23	2.20	0.41
1:B:535:LEU:HD12	1:B:542:GLN:HE21	1.85	0.41
1:A:495:ALA:CB	1:A:554:VAL:HB	2.50	0.41
1:B:558:ASN:HD21	2:B:657:NAG:C4	2.30	0.41
1:B:464:THR:O	1:B:504:ALA:HA	2.20	0.41
1:B:507:VAL:HG22	1:B:524:ARG:CB	2.50	0.41
1:A:134:GLU:HA	1:A:134:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:LYS:HE2	1:B:635:LYS:HB3	1.90	0.41
1:B:161:LYS:HE3	1:B:161:LYS:HB3	1.59	0.41
1:A:74:ASN:O	1:A:75:SER:HB2	2.19	0.41
1:A:462:GLU:OE2	1:A:520:GLU:OE1	2.39	0.41
1:A:293:PHE:HE1	1:A:412:GLU:OE2	2.03	0.41
1:A:584:GLN:NE2	2:A:657:NAG:O4	2.48	0.41
1:A:48:LYS:NZ	1:A:592:ASP:OD2	2.51	0.41
1:A:353:ILE:O	1:B:615:LEU:HD22	2.20	0.41
1:A:466:LEU:HD22	1:A:484:THR:HG22	2.02	0.41
1:B:177:ILE:HG21	1:B:177:ILE:HD13	1.90	0.41
1:B:534:LEU:HD12	1:B:602:HIS:CE1	2.56	0.41
1:B:99:GLY:HA2	1:B:570:ASP:O	2.21	0.41
1:A:78:HIS:HA	1:A:93:ASN:O	2.20	0.40
1:B:613:MET:HA	1:B:614:PRO:HD3	1.84	0.40
1:B:501:LEU:O	1:B:502:ALA:HB2	2.21	0.40
1:A:345:CYS:SG	1:A:379:ARG:HB3	2.61	0.40
1:A:558:ASN:OD1	1:A:558:ASN:C	2.60	0.40
1:B:558:ASN:OD1	2:B:657:NAG:C1	2.69	0.40
1:A:510:ASN:HA	1:A:511:PRO:HD3	1.96	0.40
1:A:425:LYS:HD3	1:A:425:LYS:HA	1.60	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:HIS:NE2	1:B:640:ARG:NH1[4_455]	1.95	0.25

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	640/642 (100%)	612 (96%)	28 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	640/642 (100%)	605 (94%)	33 (5%)	2 (0%)	46 50
All	All	1280/1284 (100%)	1217 (95%)	61 (5%)	2 (0%)	52 59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	473	ASP
1	B	502	ALA

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	576/575 (100%)	552 (96%)	24 (4%)	36 44
1	B	576/575 (100%)	548 (95%)	28 (5%)	31 36
All	All	1152/1150 (100%)	1100 (96%)	52 (4%)	34 41

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	49	ASP
1	A	50	HIS
1	A	56	THR
1	A	88	SER
1	A	138	SER
1	A	139	SER
1	A	163	SER
1	A	193	ASP
1	A	198	PRO
1	A	239	SER
1	A	261	SER
1	A	269	LYS
1	A	280	SER

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Mol	Chain	Res	Type
1	A	306	PHE
1	A	340	LEU
1	A	349	GLN
1	A	356	ARG
1	A	400	SER
1	A	425	LYS
1	A	455	ASP
1	A	510	ASN
1	A	524	ARG
1	A	613	MET
1	B	47	GLU
1	B	49	ASP
1	B	56	THR
1	B	60	LEU
1	B	62	SER
1	B	87	ARG
1	B	91	SER
1	B	106	ASP
1	B	127	LYS
1	B	138	SER
1	B	139	SER
1	B	151	VAL
1	B	161	LYS
1	B	163	SER
1	B	193	ASP
1	B	220	SER
1	B	232	GLN
1	B	239	SER
1	B	261	SER
1	B	306	PHE
1	B	340	LEU
1	B	425	LYS
1	B	455	ASP
1	B	465	SER
1	B	524	ARG
1	B	629	GLU
1	B	640	ARG
1	B	641	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	190	HIS
1	A	206	GLN
1	A	316	ASN
1	A	458	HIS
1	A	510	ASN
1	A	542	GLN
1	A	549	ASN
1	A	558	ASN
1	B	190	HIS
1	B	316	ASN
1	B	331	HIS
1	B	360	ASN
1	B	542	GLN
1	B	549	ASN
1	B	558	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPQ	A	387	1	13,14,15	2.47	5 (38%)	15,19,21	2.78	8 (53%)
1	TPQ	B	387	1	13,14,15	2.57	5 (38%)	15,19,21	2.55	5 (33%)

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
1	TPQ	A	387	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	387	1	-	0/4/22/24	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	387	TPQ	C1-C2	-6.09	1.41	1.49
1	A	387	TPQ	C1-C2	-5.36	1.42	1.49
1	B	387	TPQ	C6-C1	2.35	1.40	1.34
1	A	387	TPQ	C6-C1	2.35	1.40	1.34
1	B	387	TPQ	C3-C4	2.61	1.39	1.35
1	A	387	TPQ	C3-C4	2.73	1.40	1.35
1	A	387	TPQ	O2-C2	3.55	1.34	1.24
1	A	387	TPQ	O5-C5	3.56	1.34	1.24
1	B	387	TPQ	O2-C2	3.60	1.34	1.24
1	B	387	TPQ	O5-C5	3.68	1.34	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	387	TPQ	C1-C6-C5	-7.20	118.58	122.97
1	A	387	TPQ	C1-C6-C5	-6.36	119.09	122.97
1	A	387	TPQ	O-C-CA	-4.08	114.87	125.49
1	B	387	TPQ	O-C-CA	-3.67	115.92	125.49
1	A	387	TPQ	C4-C3-C2	-2.44	117.66	120.77
1	A	387	TPQ	O5-C5-C4	-2.25	115.57	119.16
1	A	387	TPQ	O2-C2-C3	-2.18	116.97	121.89
1	B	387	TPQ	C6-C1-C2	2.16	119.96	118.44
1	A	387	TPQ	C6-C5-C4	2.16	121.05	117.34
1	A	387	TPQ	CA-CB-C1	2.23	118.10	113.63
1	B	387	TPQ	C6-C5-C4	2.25	121.19	117.34
1	B	387	TPQ	C3-C2-C1	3.55	120.96	118.30
1	A	387	TPQ	C3-C2-C1	5.61	122.50	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	387	TPQ	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 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	NAG	A	655	1,2	14,14,15	1.30	1 (7%)	15,19,21	2.15	4 (26%)
2	NAG	A	656	2	14,14,15	1.30	1 (7%)	15,19,21	2.16	4 (26%)
2	NAG	A	657	1	14,14,15	1.30	1 (7%)	15,19,21	2.15	4 (26%)
2	NAG	B	655	1,2	14,14,15	1.53	3 (21%)	15,19,21	1.45	2 (13%)
2	NAG	B	656	2	14,14,15	1.17	2 (14%)	15,19,21	1.04	1 (6%)
2	NAG	B	657	1	14,14,15	1.29	1 (7%)	15,19,21	2.15	4 (26%)

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	NAG	A	655	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	656	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	657	1	-	0/6/23/26	0/1/1/1
2	NAG	B	655	1,2	2/2/5/7	0/6/23/26	0/1/1/1
2	NAG	B	656	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	657	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	656	NAG	O7-C7	-3.17	1.15	1.23
2	A	657	NAG	O7-C7	-3.17	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	655	NAG	O7-C7	-3.17	1.15	1.23
2	B	657	NAG	O7-C7	-3.17	1.15	1.23
2	B	656	NAG	O5-C1	-2.04	1.40	1.43
2	B	655	NAG	O5-C1	2.82	1.48	1.43
2	B	655	NAG	C1-C2	3.28	1.57	1.52
2	B	656	NAG	C8-C7	3.47	1.57	1.50
2	B	655	NAG	C8-C7	3.64	1.57	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	656	NAG	C4-C3-C2	-3.99	105.02	111.23
2	B	657	NAG	C4-C3-C2	-3.98	105.04	111.23
2	A	655	NAG	C4-C3-C2	-3.98	105.05	111.23
2	A	657	NAG	C4-C3-C2	-3.97	105.06	111.23
2	A	657	NAG	C3-C4-C5	-3.71	103.74	110.20
2	A	656	NAG	C3-C4-C5	-3.70	103.74	110.20
2	A	655	NAG	C3-C4-C5	-3.69	103.77	110.20
2	B	657	NAG	C3-C4-C5	-3.69	103.77	110.20
2	B	655	NAG	C3-C2-N2	-3.00	103.37	110.56
2	B	656	NAG	C1-O5-C5	2.43	115.33	112.25
2	A	657	NAG	O3-C3-C2	3.11	115.27	109.11
2	B	657	NAG	O3-C3-C2	3.12	115.28	109.11
2	A	655	NAG	O3-C3-C2	3.13	115.32	109.11
2	A	656	NAG	O3-C3-C2	3.15	115.35	109.11
2	B	655	NAG	C1-O5-C5	3.57	116.78	112.25
2	A	657	NAG	C1-O5-C5	4.51	117.97	112.25
2	B	657	NAG	C1-O5-C5	4.52	117.98	112.25
2	A	655	NAG	C1-O5-C5	4.52	117.98	112.25
2	A	656	NAG	C1-O5-C5	4.53	118.00	112.25

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	655	NAG	C1
2	B	655	NAG	C2
2	B	656	NAG	C1
2	A	656	NAG	C1
2	A	655	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	655	NAG	19	0
2	A	656	NAG	19	0
2	A	657	NAG	13	0
2	B	655	NAG	2	0
2	B	657	NAG	10	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.