Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:04 PM GMT

PDB ID	:	1NDV
Title	:	Crystal Structure of Adenosine Deaminase complexed with FR117016
Authors	:	Kinoshita, T.
Deposited on	:	2002-12-09
Resolution	:	2.30 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:

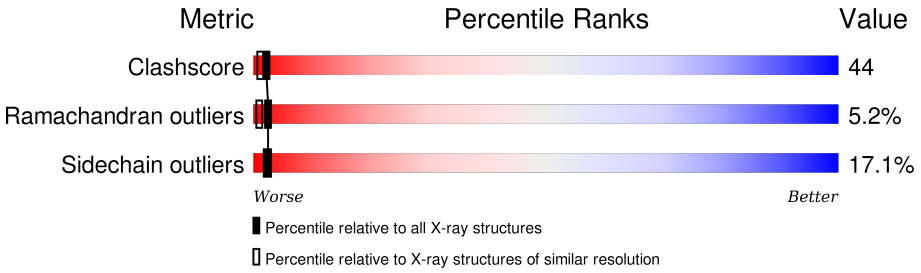
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	356	23% 38% 29% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3272 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 Adenosine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2788	1772	471	533	12			

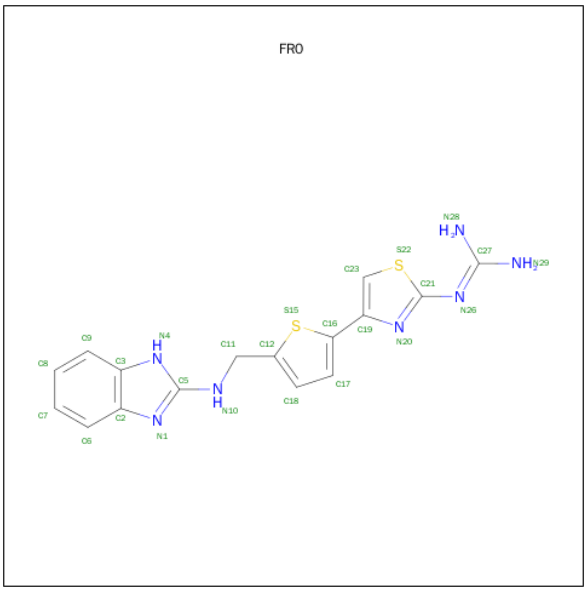
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	ASN	SEE REMARK 999	UNP P56658
A	32	LYS	ARG	SEE REMARK 999	UNP P56658
A	33	ARG	LYS	SEE REMARK 999	UNP P56658
A	57	THR	SER	SEE REMARK 999	UNP P56658
A	60	ASP	GLU	SEE REMARK 999	UNP P56658
A	77	ASP	GLU	SEE REMARK 999	UNP P56658
A	79	ILE	VAL	SEE REMARK 999	UNP P56658
A	199	GLN	LYS	SEE REMARK 999	UNP P56658
A	246	THR	ALA	SEE REMARK 999	UNP P56658
A	261	ILE	VAL	SEE REMARK 999	UNP P56658
A	279	ALA	PRO	SEE REMARK 999	UNP P56658
A	281	ILE	VAL	SEE REMARK 999	UNP P56658
A	313	LYS	ASN	SEE REMARK 999	UNP P56658
A	314	ASP	GLU	SEE REMARK 999	UNP P56658
A	352	ARG	GLY	SEE REMARK 999	UNP P56658

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N''-(4-(5-((1H-BENZIMIDAZOL-2-YLAMINO)METHYL)-2-THIENYL)-1,3-THIAZOL-2-YL)GUANIDINE (three-letter code: FR0) (formula: $C_{16}H_{15}N_7S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			25	16	7	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	458	Total	O	0	0
			458	458		

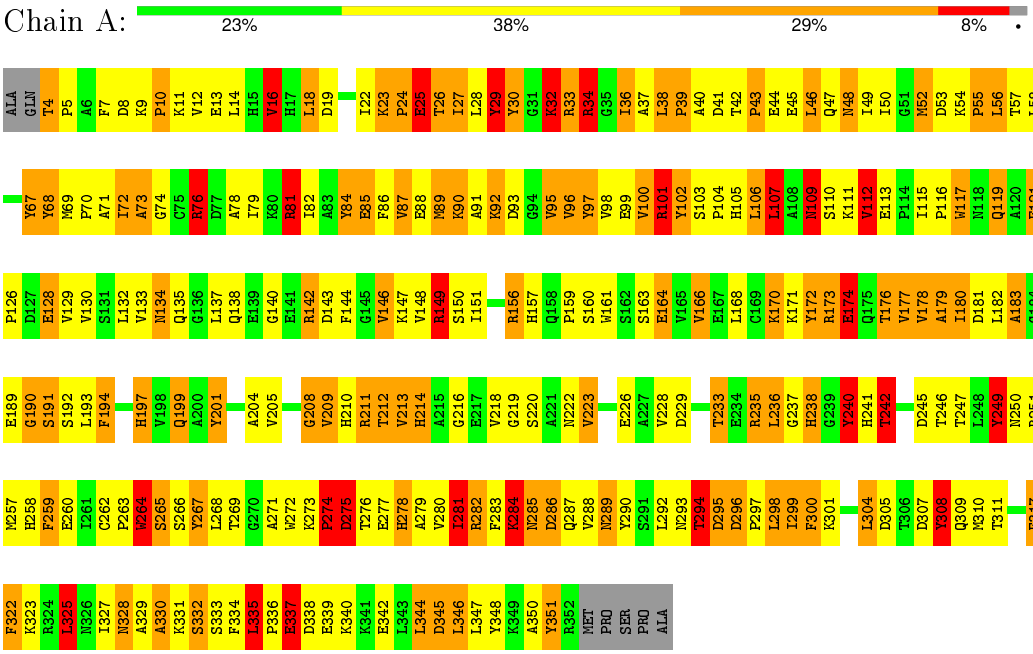
3 Residue-property plots (i)

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: Adenosine deaminase

Chain A:



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 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	78.03Å 78.03Å 136.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.225 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3272	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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: ZN, FR0

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	1.72	34/2852 (1.2%)	2.58	190/3866 (4.9%)

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	A	0	23

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	GLU	CG-CD	9.71	1.66	1.51
1	A	253	ARG	NE-CZ	9.60	1.45	1.33
1	A	85	GLU	CG-CD	6.60	1.61	1.51
1	A	213	VAL	CA-CB	6.58	1.68	1.54
1	A	103	SER	CA-CB	6.46	1.62	1.52
1	A	103	SER	CB-OG	6.26	1.50	1.42
1	A	253	ARG	CD-NE	6.19	1.56	1.46
1	A	339	GLU	CG-CD	-6.15	1.42	1.51
1	A	238	HIS	C-N	6.13	1.44	1.33
1	A	260	GLU	CD-OE1	-6.06	1.19	1.25
1	A	253	ARG	CG-CD	6.04	1.67	1.51
1	A	339	GLU	CD-OE1	-5.82	1.19	1.25
1	A	190	GLY	CA-C	5.81	1.61	1.51
1	A	102	TYR	CB-CG	5.75	1.60	1.51
1	A	247	THR	CA-CB	5.74	1.68	1.53
1	A	282	ARG	NE-CZ	5.71	1.40	1.33
1	A	188	ILE	CA-CB	-5.54	1.42	1.54
1	A	99	GLU	CG-CD	5.47	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	GLY	CA-C	5.45	1.60	1.51
1	A	128	GLU	CG-CD	5.41	1.60	1.51
1	A	265	SER	CA-CB	-5.38	1.44	1.52
1	A	88	GLU	CD-OE1	-5.32	1.19	1.25
1	A	191	SER	CB-OG	5.29	1.49	1.42
1	A	199	GLN	CG-CD	5.28	1.63	1.51
1	A	157	HIS	CG-CD2	5.26	1.44	1.35
1	A	201	TYR	CE2-CZ	5.24	1.45	1.38
1	A	174	GLU	CB-CG	5.23	1.62	1.52
1	A	97	TYR	C-N	-5.21	1.22	1.34
1	A	240	TYR	CE2-CZ	5.21	1.45	1.38
1	A	181	ASP	CB-CG	5.15	1.62	1.51
1	A	201	TYR	CG-CD2	5.14	1.45	1.39
1	A	102	TYR	CE1-CZ	5.07	1.45	1.38
1	A	134	ASN	CB-CG	5.05	1.62	1.51
1	A	211	ARG	CZ-NH1	-5.05	1.26	1.33

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	ARG	NE-CZ-NH1	-20.31	110.15	120.30
1	A	308	TYR	CB-CG-CD2	-20.21	108.87	121.00
1	A	251	ARG	NE-CZ-NH1	-16.83	111.88	120.30
1	A	211	ARG	NE-CZ-NH2	16.64	128.62	120.30
1	A	76	ARG	NE-CZ-NH1	14.58	127.59	120.30
1	A	34	ARG	NE-CZ-NH2	-14.01	113.29	120.30
1	A	282	ARG	NE-CZ-NH1	13.44	127.02	120.30
1	A	223	VAL	CA-CB-CG2	13.27	130.80	110.90
1	A	282	ARG	NE-CZ-NH2	11.95	126.27	120.30
1	A	164	GLU	CA-CB-CG	11.67	139.08	113.40
1	A	68	TYR	CB-CG-CD2	-11.57	114.06	121.00
1	A	282	ARG	NH1-CZ-NH2	-11.55	106.70	119.40
1	A	81	ARG	NE-CZ-NH2	10.96	125.78	120.30
1	A	251	ARG	NE-CZ-NH2	10.84	125.72	120.30
1	A	294	THR	CA-CB-CG2	10.64	127.30	112.40
1	A	325	LEU	CB-CG-CD2	10.51	128.86	111.00
1	A	100	VAL	CG1-CB-CG2	-10.46	94.17	110.90
1	A	279	ALA	N-CA-CB	-10.26	95.74	110.10
1	A	242	THR	CA-CB-CG2	9.73	126.02	112.40
1	A	30	TYR	CB-CG-CD1	-9.49	115.31	121.00
1	A	149	ARG	CD-NE-CZ	-9.42	110.41	123.60
1	A	201	TYR	CB-CG-CD2	-9.30	115.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	ARG	CB-CA-C	9.28	128.95	110.40
1	A	235	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	156	ARG	CD-NE-CZ	8.99	136.19	123.60
1	A	76	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	A	32	LYS	CB-CA-C	8.63	127.66	110.40
1	A	334	PHE	CB-CG-CD2	-8.49	114.86	120.80
1	A	179	ALA	N-CA-CB	8.30	121.72	110.10
1	A	340	LYS	CA-CB-CG	8.19	131.41	113.40
1	A	156	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	A	299	ILE	CB-CA-C	8.15	127.90	111.60
1	A	279	ALA	CB-CA-C	7.93	122.00	110.10
1	A	34	ARG	CD-NE-CZ	-7.88	112.56	123.60
1	A	174	GLU	CA-CB-CG	7.80	130.55	113.40
1	A	253	ARG	CA-CB-CG	7.78	130.51	113.40
1	A	308	TYR	CB-CG-CD1	7.72	125.63	121.00
1	A	32	LYS	N-CA-CB	-7.69	96.77	110.60
1	A	290	TYR	CB-CG-CD2	-7.64	116.41	121.00
1	A	186	GLU	CB-CA-C	-7.63	95.13	110.40
1	A	346	LEU	CB-CA-C	-7.63	95.70	110.20
1	A	32	LYS	CA-CB-CG	7.60	130.12	113.40
1	A	101	ARG	CD-NE-CZ	-7.42	113.21	123.60
1	A	166	VAL	CG1-CB-CG2	7.39	122.73	110.90
1	A	183	ALA	CB-CA-C	-7.39	99.02	110.10
1	A	33	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	96	VAL	CG1-CB-CG2	-7.37	99.10	110.90
1	A	179	ALA	CB-CA-C	-7.37	99.05	110.10
1	A	33	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	12	VAL	CG1-CB-CG2	-7.21	99.37	110.90
1	A	16	VAL	CG1-CB-CG2	7.13	122.31	110.90
1	A	26	THR	CA-CB-CG2	-7.12	102.43	112.40
1	A	278	HIS	N-CA-CB	7.12	123.41	110.60
1	A	295	ASP	N-CA-C	7.08	130.12	111.00
1	A	95	VAL	CA-CB-CG2	6.98	121.37	110.90
1	A	60	ASP	CB-CG-OD1	6.95	124.55	118.30
1	A	36	ILE	N-CA-C	6.88	129.59	111.00
1	A	29	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	107	LEU	C-N-CA	-6.84	104.60	121.70
1	A	101	ARG	NE-CZ-NH1	-6.83	116.88	120.30
1	A	34	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	308	TYR	CD1-CG-CD2	6.71	125.28	117.90
1	A	177	VAL	O-C-N	6.71	133.44	122.70
1	A	249	TYR	CB-CG-CD1	-6.67	117.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	350	ALA	CB-CA-C	-6.67	100.09	110.10
1	A	10	PRO	O-C-N	6.62	133.29	122.70
1	A	143	ASP	CB-CG-OD1	-6.61	112.36	118.30
1	A	299	ILE	CA-CB-CG2	6.58	124.06	110.90
1	A	106	LEU	CA-CB-CG	-6.55	100.23	115.30
1	A	330	ALA	CB-CA-C	-6.53	100.31	110.10
1	A	329	ALA	N-CA-C	6.48	128.49	111.00
1	A	339	GLU	CA-CB-CG	-6.47	99.15	113.40
1	A	193	LEU	CA-CB-CG	6.46	130.16	115.30
1	A	166	VAL	CB-CA-C	-6.45	99.15	111.40
1	A	38	LEU	CB-CG-CD2	-6.45	100.04	111.00
1	A	7	PHE	CB-CG-CD2	-6.31	116.38	120.80
1	A	119	GLN	CB-CA-C	-6.29	97.82	110.40
1	A	23	LYS	CA-CB-CG	-6.29	99.56	113.40
1	A	337	GLU	N-CA-CB	6.25	121.85	110.60
1	A	124	LEU	CB-CG-CD2	6.23	121.60	111.00
1	A	259	PHE	O-C-N	-6.21	112.77	122.70
1	A	310	MET	CG-SD-CE	-6.20	90.28	100.20
1	A	93	ASP	C-N-CA	-6.17	109.36	122.30
1	A	89	MET	CB-CA-C	-6.14	98.11	110.40
1	A	335	LEU	CD1-CG-CD2	6.13	128.91	110.50
1	A	185	ASP	N-CA-CB	-6.10	99.62	110.60
1	A	36	ILE	C-N-CA	6.10	136.95	121.70
1	A	218	VAL	CA-CB-CG2	6.09	120.04	110.90
1	A	300	PHE	CB-CG-CD2	-6.09	116.53	120.80
1	A	18	LEU	CB-CG-CD1	6.09	121.36	111.00
1	A	166	VAL	CA-CB-CG1	6.08	120.03	110.90
1	A	333	SER	C-N-CA	-6.08	106.50	121.70
1	A	142	ARG	CB-CG-CD	6.08	127.39	111.60
1	A	253	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	A	73	ALA	CB-CA-C	-6.03	101.06	110.10
1	A	10	PRO	CA-C-N	-6.01	103.97	117.20
1	A	197	HIS	CA-CB-CG	-6.01	103.38	113.60
1	A	142	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	177	VAL	CG1-CB-CG2	5.96	120.44	110.90
1	A	157	HIS	CB-CA-C	5.95	122.29	110.40
1	A	194	PHE	CB-CA-C	-5.93	98.53	110.40
1	A	146	VAL	C-N-CA	-5.93	106.87	121.70
1	A	259	PHE	CB-CG-CD2	-5.92	116.66	120.80
1	A	109	ASN	CB-CA-C	5.89	122.18	110.40
1	A	296	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	205	VAL	CA-CB-CG1	-5.87	102.09	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	TYR	CZ-CE2-CD2	-5.87	114.52	119.80
1	A	132	LEU	CB-CG-CD1	-5.87	101.03	111.00
1	A	180	ILE	CB-CG1-CD1	-5.85	97.52	113.90
1	A	90	LYS	CD-CE-NZ	-5.83	98.28	111.70
1	A	264	TRP	CH2-CZ2-CE2	5.80	123.20	117.40
1	A	143	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	157	HIS	CA-CB-CG	-5.77	103.80	113.60
1	A	185	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	188	ILE	CG1-CB-CG2	5.69	123.91	111.40
1	A	73	ALA	C-N-CA	-5.69	110.36	122.30
1	A	281	ILE	CA-CB-CG1	5.69	121.80	111.00
1	A	61	PHE	CB-CG-CD2	-5.68	116.82	120.80
1	A	68	TYR	CB-CA-C	-5.65	99.09	110.40
1	A	185	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	205	VAL	CA-CB-CG2	5.63	119.35	110.90
1	A	87	VAL	CA-C-N	-5.63	104.81	117.20
1	A	87	VAL	CA-CB-CG2	5.62	119.32	110.90
1	A	209	VAL	CA-CB-CG2	5.60	119.30	110.90
1	A	30	TYR	CD1-CG-CD2	5.57	124.02	117.90
1	A	212	THR	N-CA-CB	5.55	120.84	110.30
1	A	299	ILE	N-CA-CB	-5.55	98.04	110.80
1	A	209	VAL	N-CA-C	5.54	125.96	111.00
1	A	247	THR	CA-CB-OG1	5.53	120.60	109.00
1	A	284	LYS	C-N-CA	-5.51	107.92	121.70
1	A	298	LEU	CA-C-N	-5.50	105.09	117.20
1	A	223	VAL	CA-CB-CG1	5.50	119.14	110.90
1	A	30	TYR	CG-CD2-CE2	-5.49	116.91	121.30
1	A	197	HIS	N-CA-CB	5.49	120.49	110.60
1	A	220	SER	CB-CA-C	-5.46	99.73	110.10
1	A	246	THR	CA-CB-CG2	5.46	120.04	112.40
1	A	237	GLY	N-CA-C	5.45	126.71	113.10
1	A	186	GLU	CA-CB-CG	5.44	125.37	113.40
1	A	236	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	A	296	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	176	THR	CB-CA-C	-5.42	96.98	111.60
1	A	310	MET	N-CA-CB	-5.41	100.86	110.60
1	A	111	LYS	N-CA-C	5.41	125.60	111.00
1	A	68	TYR	CB-CG-CD1	5.40	124.24	121.00
1	A	44	GLU	CB-CA-C	-5.37	99.66	110.40
1	A	344	LEU	CB-CG-CD1	-5.37	101.88	111.00
1	A	92	LYS	CB-CA-C	-5.36	99.69	110.40
1	A	251	ARG	CB-CG-CD	-5.33	97.74	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	THR	CA-CB-CG2	5.33	119.86	112.40
1	A	332	SER	CA-CB-OG	-5.33	96.82	111.20
1	A	170	LYS	CB-CG-CD	-5.33	97.75	111.60
1	A	274	PRO	N-CA-CB	-5.32	96.75	102.60
1	A	345	ASP	O-C-N	5.30	131.19	122.70
1	A	119	GLN	C-N-CA	-5.28	108.49	121.70
1	A	192	SER	CA-C-N	-5.27	105.61	117.20
1	A	91	ALA	C-N-CA	-5.26	108.55	121.70
1	A	288	VAL	CA-CB-CG2	-5.24	103.04	110.90
1	A	204	ALA	N-CA-CB	5.24	117.44	110.10
1	A	275	ASP	C-N-CA	-5.23	108.63	121.70
1	A	181	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	283	PHE	CB-CG-CD1	5.21	124.45	120.80
1	A	68	TYR	CG-CD1-CE1	-5.20	117.14	121.30
1	A	194	PHE	N-CA-CB	5.20	119.96	110.60
1	A	253	ARG	CD-NE-CZ	5.20	130.88	123.60
1	A	122	GLY	CA-C-O	5.19	129.94	120.60
1	A	25	GLU	O-C-N	-5.18	114.42	122.70
1	A	87	VAL	CA-C-O	5.17	130.95	120.10
1	A	84	TYR	CG-CD1-CE1	-5.16	117.17	121.30
1	A	308	TYR	CG-CD1-CE1	-5.16	117.17	121.30
1	A	298	LEU	CB-CG-CD2	5.15	119.75	111.00
1	A	189	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	A	81	ARG	CB-CG-CD	5.13	124.94	111.60
1	A	201	TYR	CZ-CE2-CD2	-5.12	115.19	119.80
1	A	229	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	334	PHE	CG-CD1-CE1	-5.09	115.20	120.80
1	A	26	THR	CA-C-N	-5.09	106.00	117.20
1	A	27	ILE	C-N-CA	-5.09	108.98	121.70
1	A	253	ARG	CG-CD-NE	5.08	122.47	111.80
1	A	338	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	304	LEU	CB-CG-CD1	5.08	119.63	111.00
1	A	245	ASP	N-CA-CB	-5.07	101.47	110.60
1	A	267	TYR	C-N-CA	-5.07	109.02	121.70
1	A	11	LYS	CA-CB-CG	5.07	124.55	113.40
1	A	293	ASN	N-CA-CB	5.07	119.72	110.60
1	A	223	VAL	CB-CA-C	5.07	121.02	111.40
1	A	299	ILE	CG1-CB-CG2	-5.06	100.26	111.40
1	A	124	LEU	N-CA-CB	5.05	120.51	110.40
1	A	262	CYS	N-CA-C	5.05	124.63	111.00
1	A	25	GLU	C-N-CA	-5.02	109.14	121.70
1	A	262	CYS	CA-CB-SG	-5.02	104.96	114.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	142	ARG	Sidechain
1	A	149	ARG	Sidechain
1	A	172	TYR	Sidechain
1	A	19	ASP	Peptide
1	A	201	TYR	Sidechain
1	A	208	GLY	Peptide
1	A	211	ARG	Sidechain
1	A	214	HIS	Sidechain
1	A	240	TYR	Sidechain
1	A	249	TYR	Sidechain
1	A	259	PHE	Sidechain
1	A	264	TRP	Peptide
1	A	275	ASP	Peptide
1	A	29	TYR	Sidechain
1	A	317	PHE	Sidechain
1	A	328	ASN	Mainchain
1	A	34	ARG	Sidechain
1	A	348	TYR	Sidechain
1	A	351	TYR	Sidechain
1	A	45	GLU	Peptide
1	A	55	PRO	Peptide
1	A	67	TYR	Sidechain

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	2788	0	2743	244	0
2	A	1	0	0	0	0
3	A	25	0	15	6	0
4	A	458	0	0	86	0
All	All	3272	0	2758	245	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 44.

All (245) 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:36:ILE:HD12	1:A:37:ALA:HA	1.38	1.02
1:A:278:HIS:HD2	1:A:280:VAL:H	1.15	0.94
1:A:337:GLU:HA	4:A:1395:HOH:O	1.67	0.94
1:A:294:THR:HG23	1:A:297:PRO:HD3	1.59	0.85
1:A:330:ALA:HB3	4:A:1072:HOH:O	1.77	0.84
1:A:105:HIS:HA	4:A:1301:HOH:O	1.76	0.83
1:A:68:TYR:OH	1:A:299:ILE:HD11	1.78	0.82
1:A:151:ILE:HG12	1:A:179:ALA:HB3	1.63	0.81
1:A:182:LEU:HD23	4:A:1421:HOH:O	1.79	0.81
1:A:164:GLU:HB3	4:A:1432:HOH:O	1.82	0.79
1:A:269:THR:HG22	3:A:1001:FR0:C9	2.13	0.78
1:A:76:ARG:HB2	1:A:76:ARG:HH11	1.47	0.78
1:A:331:LYS:HG3	1:A:344:LEU:HD21	1.66	0.78
1:A:258:HIS:HA	1:A:289:ASN:O	1.84	0.77
1:A:298:LEU:HD22	4:A:1414:HOH:O	1.83	0.77
1:A:236:LEU:HD23	4:A:1367:HOH:O	1.86	0.76
1:A:125:THR:HG23	1:A:128:GLU:HB2	1.68	0.75
1:A:110:SER:O	1:A:112:VAL:HG12	1.87	0.74
1:A:174:GLU:O	1:A:176:THR:HA	1.87	0.74
1:A:27:ILE:HG21	4:A:1062:HOH:O	1.87	0.73
1:A:106:LEU:HB3	1:A:117:TRP:HZ2	1.52	0.73
1:A:301:LYS:HE3	4:A:1194:HOH:O	1.88	0.73
1:A:102:TYR:CZ	1:A:133:VAL:HG21	2.23	0.72
1:A:347:LEU:HD13	4:A:1307:HOH:O	1.90	0.72
1:A:116:PRO:HD2	4:A:1359:HOH:O	1.90	0.71
1:A:342:GLU:O	1:A:345:ASP:HB3	1.90	0.71
1:A:278:HIS:CD2	1:A:280:VAL:H	2.04	0.71
1:A:266:SER:OG	1:A:278:HIS:HE1	1.75	0.70
1:A:14:LEU:HD12	4:A:1416:HOH:O	1.91	0.69
1:A:174:GLU:HA	4:A:1327:HOH:O	1.92	0.69
1:A:87:VAL:HG21	1:A:140:GLY:HA3	1.73	0.69
1:A:89:MET:SD	4:A:1289:HOH:O	2.50	0.69
1:A:97:TYR:CE1	4:A:1408:HOH:O	2.47	0.68
1:A:100:VAL:HG23	4:A:1211:HOH:O	1.94	0.67
1:A:308:TYR:CD2	1:A:322:PHE:CD2	2.82	0.67
1:A:183:ALA:HB3	4:A:1335:HOH:O	1.93	0.66
1:A:171:LYS:HD3	1:A:172:TYR:CZ	2.29	0.66
1:A:188:ILE:HB	4:A:1396:HOH:O	1.95	0.66
1:A:30:TYR:O	1:A:34:ARG:HB2	1.96	0.66
1:A:16:VAL:HG13	4:A:1211:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HG	4:A:1036:HOH:O	1.96	0.65
1:A:22:ILE:HB	4:A:1414:HOH:O	1.97	0.65
1:A:212:THR:HA	1:A:233:THR:HG22	1.79	0.64
1:A:277:GLU:HA	4:A:1118:HOH:O	1.97	0.64
1:A:129:VAL:O	1:A:133:VAL:HG23	1.97	0.64
1:A:125:THR:O	1:A:129:VAL:HG23	1.97	0.64
1:A:133:VAL:HG22	4:A:1013:HOH:O	1.98	0.64
1:A:275:ASP:OD1	1:A:276:THR:HB	1.97	0.64
1:A:323:LYS:HB3	1:A:351:TYR:CD1	2.33	0.63
1:A:178:VAL:HG21	4:A:1244:HOH:O	1.97	0.63
1:A:67:TYR:HB2	4:A:1278:HOH:O	1.97	0.63
1:A:308:TYR:CD2	1:A:322:PHE:CE2	2.86	0.63
1:A:34:ARG:HB3	1:A:36:ILE:HG23	1.79	0.63
1:A:298:LEU:HB3	1:A:299:ILE:HG13	1.80	0.62
1:A:346:LEU:HB2	4:A:1179:HOH:O	1.99	0.62
1:A:238:HIS:HB3	1:A:240:TYR:CZ	2.33	0.62
1:A:50:ILE:HD12	1:A:298:LEU:HD21	1.83	0.61
1:A:134:ASN:O	1:A:138:GLN:HG3	2.02	0.59
1:A:327:ILE:HD13	1:A:347:LEU:HD23	1.85	0.59
1:A:161:TRP:HH2	4:A:1089:HOH:O	1.84	0.59
1:A:147:LYS:HE3	4:A:1333:HOH:O	2.03	0.59
1:A:228:VAL:HG22	4:A:1231:HOH:O	2.03	0.59
1:A:210:HIS:HB2	4:A:1441:HOH:O	2.01	0.58
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.40	0.57
1:A:115:ILE:HA	4:A:1359:HOH:O	2.05	0.57
1:A:79:ILE:HD13	1:A:124:LEU:HD11	1.87	0.56
1:A:235:ARG:HD3	1:A:332:SER:O	2.05	0.56
1:A:61:PHE:CE1	3:A:1001:FR0:H9	2.40	0.56
1:A:87:VAL:HB	4:A:1249:HOH:O	2.04	0.56
1:A:188:ILE:HD12	4:A:1396:HOH:O	2.06	0.56
1:A:86:PHE:CE2	1:A:90:LYS:HE3	2.40	0.56
1:A:76:ARG:NH1	1:A:76:ARG:HB2	2.17	0.56
1:A:109:ASN:HB2	4:A:1106:HOH:O	2.04	0.56
1:A:106:LEU:HB3	1:A:117:TRP:CZ2	2.37	0.56
1:A:156:ARG:HD3	1:A:191:SER:OG	2.05	0.56
1:A:137:LEU:HG	1:A:148:VAL:HG11	1.88	0.56
1:A:254:GLN:HB3	4:A:1066:HOH:O	2.06	0.55
1:A:271:ALA:HA	4:A:1027:HOH:O	2.06	0.55
1:A:39:PRO:HA	4:A:1439:HOH:O	2.07	0.55
1:A:124:LEU:HA	4:A:1222:HOH:O	2.06	0.55
1:A:292:LEU:HD22	4:A:1266:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:TYR:CD1	1:A:78:ALA:HB2	2.42	0.55
1:A:171:LYS:HD3	1:A:172:TYR:CE2	2.42	0.54
1:A:289:ASN:OD1	1:A:328:ASN:HB3	2.08	0.54
1:A:308:TYR:HD2	1:A:322:PHE:CE2	2.25	0.54
1:A:36:ILE:HG12	1:A:71:ALA:HB2	1.90	0.54
1:A:210:HIS:HE1	4:A:1343:HOH:O	1.90	0.54
1:A:46:LEU:HA	4:A:1283:HOH:O	2.08	0.54
1:A:79:ILE:HG13	1:A:107:LEU:HG	1.90	0.53
1:A:117:TRP:HD1	1:A:119:GLN:NE2	2.06	0.53
1:A:272:TRP:CD1	1:A:277:GLU:O	2.61	0.53
1:A:86:PHE:HD1	4:A:1025:HOH:O	1.92	0.53
1:A:174:GLU:C	1:A:176:THR:HA	2.29	0.53
1:A:48:ASN:OD1	1:A:48:ASN:N	2.41	0.53
1:A:23:LYS:O	1:A:27:ILE:HG13	2.10	0.52
1:A:98:VAL:CG1	1:A:148:VAL:HG22	2.39	0.52
1:A:49:ILE:HB	4:A:1283:HOH:O	2.08	0.52
1:A:26:THR:HG21	1:A:81:ARG:NH2	2.25	0.52
1:A:272:TRP:CD1	1:A:278:HIS:HA	2.45	0.52
1:A:79:ILE:HG23	4:A:1013:HOH:O	2.10	0.52
1:A:328:ASN:O	1:A:331:LYS:HB2	2.10	0.52
1:A:28:LEU:O	1:A:29:TYR:C	2.45	0.52
1:A:281:ILE:HD13	4:A:1041:HOH:O	2.09	0.52
1:A:222:ASN:O	1:A:226:GLU:HG3	2.10	0.52
1:A:266:SER:OG	1:A:278:HIS:CE1	2.60	0.52
1:A:105:HIS:CE1	4:A:1432:HOH:O	2.63	0.52
1:A:179:ALA:HB2	4:A:1441:HOH:O	2.09	0.51
1:A:33:ARG:HB3	4:A:1086:HOH:O	2.09	0.51
1:A:107:LEU:HB2	1:A:129:VAL:HG11	1.91	0.51
1:A:284:LYS:HD2	1:A:317:PHE:HZ	1.75	0.51
1:A:156:ARG:HB3	4:A:1396:HOH:O	2.10	0.51
1:A:50:ILE:HG21	4:A:1278:HOH:O	2.10	0.50
1:A:69:MET:N	1:A:70:PRO:HD2	2.26	0.50
1:A:170:LYS:O	1:A:173:ARG:HG2	2.12	0.50
1:A:173:ARG:HD3	4:A:1068:HOH:O	2.12	0.50
1:A:14:LEU:HB2	4:A:1416:HOH:O	2.12	0.50
1:A:47:GLN:NE2	1:A:301:LYS:HG2	2.26	0.49
1:A:23:LYS:HB2	1:A:85:GLU:OE2	2.13	0.49
1:A:305:ASP:O	1:A:309:GLN:HB2	2.12	0.49
1:A:117:TRP:HD1	1:A:119:GLN:HE21	1.61	0.49
1:A:346:LEU:HD22	4:A:1153:HOH:O	2.12	0.49
1:A:311:THR:O	1:A:317:PHE:HD1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:THR:HB	1:A:5:PRO:CD	2.43	0.49
1:A:249:TYR:HE2	4:A:1295:HOH:O	1.94	0.49
1:A:250:ASN:O	1:A:254:GLN:HG3	2.13	0.48
1:A:22:ILE:HG23	1:A:82:ILE:CG2	2.43	0.48
1:A:213:VAL:HG23	1:A:233:THR:HG23	1.94	0.48
1:A:13:GLU:OE1	1:A:294:THR:HB	2.13	0.48
1:A:61:PHE:CZ	3:A:1001:FR0:H9	2.49	0.48
1:A:84:TYR:CZ	1:A:144:PHE:CE1	3.01	0.48
1:A:292:LEU:HD13	4:A:1418:HOH:O	2.13	0.48
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.29	0.48
1:A:117:TRP:CE3	4:A:1363:HOH:O	2.56	0.48
1:A:29:TYR:C	1:A:29:TYR:CD1	2.87	0.48
1:A:287:GLN:HA	4:A:1186:HOH:O	2.14	0.48
1:A:72:ILE:HD13	1:A:72:ILE:H	1.77	0.48
1:A:149:ARG:HD3	1:A:178:VAL:CG1	2.43	0.48
1:A:149:ARG:HD3	1:A:178:VAL:HG11	1.96	0.48
1:A:147:LYS:HB3	4:A:1254:HOH:O	2.13	0.48
1:A:68:TYR:HD2	4:A:1278:HOH:O	1.96	0.47
1:A:84:TYR:CZ	1:A:144:PHE:CZ	3.02	0.47
1:A:250:ASN:HA	1:A:253:ARG:HD3	1.96	0.47
1:A:34:ARG:NH2	1:A:73:ALA:O	2.48	0.47
1:A:18:LEU:HD22	4:A:1082:HOH:O	2.14	0.47
1:A:186:GLU:OE1	1:A:216:GLY:N	2.41	0.47
1:A:101:ARG:HA	4:A:1310:HOH:O	2.15	0.47
1:A:72:ILE:HG23	1:A:72:ILE:HD12	1.62	0.47
1:A:273:LYS:HE3	4:A:1334:HOH:O	2.15	0.46
1:A:156:ARG:HA	1:A:197:HIS:CE1	2.50	0.46
1:A:267:TYR:CE1	1:A:268:LEU:HD23	2.51	0.46
1:A:10:PRO:HB3	1:A:96:VAL:HG13	1.98	0.46
1:A:47:GLN:O	1:A:301:LYS:HD3	2.15	0.46
1:A:36:ILE:HD11	1:A:38:LEU:HD11	1.97	0.46
1:A:130:VAL:HG11	1:A:172:TYR:CD2	2.51	0.46
1:A:319:GLU:O	1:A:323:LYS:HG3	2.16	0.46
1:A:257:MET:HE2	4:A:1380:HOH:O	2.15	0.46
1:A:97:TYR:HB2	4:A:1254:HOH:O	2.16	0.45
1:A:40:ALA:HB3	1:A:46:LEU:HD13	1.98	0.45
1:A:56:LEU:HD22	1:A:60:ASP:OD1	2.16	0.45
1:A:235:ARG:HD2	1:A:258:HIS:CD2	2.52	0.45
1:A:52:MET:CE	1:A:268:LEU:HB3	2.47	0.45
1:A:263:PRO:HD2	1:A:307:ASP:OD2	2.16	0.45
1:A:159:PRO:HG3	1:A:194:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLN:HB3	4:A:1122:HOH:O	2.17	0.45
1:A:163:SER:HB3	4:A:1209:HOH:O	2.16	0.45
1:A:280:VAL:HG22	4:A:1370:HOH:O	2.17	0.45
1:A:68:TYR:OH	1:A:299:ILE:CD1	2.59	0.45
1:A:9:LYS:HG2	1:A:9:LYS:H	1.44	0.45
1:A:30:TYR:CE1	1:A:78:ALA:HB2	2.52	0.44
1:A:156:ARG:CB	4:A:1396:HOH:O	2.65	0.44
1:A:39:PRO:O	1:A:40:ALA:HB2	2.17	0.44
1:A:282:ARG:HD2	1:A:286:ASP:OD1	2.17	0.44
1:A:68:TYR:CE1	1:A:69:MET:SD	3.10	0.44
1:A:116:PRO:HB2	1:A:117:TRP:CE2	2.53	0.44
1:A:308:TYR:HD2	1:A:322:PHE:CD2	2.30	0.44
1:A:27:ILE:HA	4:A:1133:HOH:O	2.17	0.44
1:A:183:ALA:HB2	1:A:214:HIS:CE1	2.52	0.44
1:A:281:ILE:O	1:A:281:ILE:HD12	2.18	0.44
1:A:32:LYS:HE3	4:A:1356:HOH:O	2.18	0.44
1:A:188:ILE:HA	4:A:1393:HOH:O	2.17	0.43
1:A:28:LEU:HD22	1:A:46:LEU:HD21	1.99	0.43
1:A:272:TRP:NE1	1:A:277:GLU:O	2.51	0.43
1:A:84:TYR:OH	1:A:144:PHE:CZ	2.68	0.43
1:A:61:PHE:CD1	3:A:1001:FR0:C9	3.01	0.43
1:A:137:LEU:HG	1:A:148:VAL:CG1	2.47	0.43
1:A:320:GLU:H	1:A:320:GLU:HG3	1.48	0.43
1:A:4:THR:HB	1:A:5:PRO:HD3	2.00	0.43
1:A:62:LEU:HB3	4:A:1375:HOH:O	2.19	0.43
1:A:317:PHE:N	1:A:317:PHE:CD1	2.86	0.43
1:A:150:SER:HB2	4:A:1310:HOH:O	2.18	0.43
1:A:273:LYS:HA	1:A:274:PRO:HD2	1.76	0.43
1:A:121:GLU:HB3	1:A:122:GLY:H	1.61	0.43
1:A:187:THR:O	1:A:188:ILE:C	2.57	0.43
1:A:112:VAL:HG13	4:A:1359:HOH:O	2.18	0.43
1:A:264:TRP:HA	4:A:1145:HOH:O	2.18	0.43
1:A:24:PRO:O	1:A:25:GLU:C	2.57	0.43
1:A:27:ILE:HG12	4:A:1133:HOH:O	2.19	0.43
1:A:16:VAL:CG1	4:A:1211:HOH:O	2.60	0.43
1:A:272:TRP:NE1	1:A:278:HIS:HA	2.33	0.43
1:A:69:MET:HB3	4:A:1455:HOH:O	2.18	0.43
1:A:219:GLY:O	1:A:241:HIS:ND1	2.51	0.43
1:A:241:HIS:O	1:A:242:THR:C	2.56	0.43
1:A:104:PRO:O	1:A:105:HIS:C	2.54	0.43
1:A:212:THR:HA	1:A:233:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:HD2	1:A:317:PHE:CZ	2.54	0.43
1:A:296:ASP:HB2	1:A:300:PHE:CE2	2.54	0.43
1:A:285:ASN:HB2	4:A:1059:HOH:O	2.19	0.43
1:A:106:LEU:HD21	4:A:1089:HOH:O	2.18	0.42
1:A:210:HIS:CE1	4:A:1343:HOH:O	2.68	0.42
1:A:74:GLY:HA2	1:A:109:ASN:HB3	2.01	0.42
1:A:61:PHE:CG	3:A:1001:FR0:C9	3.03	0.42
1:A:97:TYR:HE1	4:A:1408:HOH:O	1.96	0.42
1:A:32:LYS:HE2	1:A:32:LYS:O	2.19	0.42
1:A:125:THR:HA	1:A:126:PRO:HD3	1.86	0.42
1:A:115:ILE:HA	1:A:116:PRO:HD2	1.87	0.42
1:A:325:LEU:HB2	4:A:1329:HOH:O	2.19	0.42
1:A:42:THR:HA	1:A:43:PRO:HD2	1.75	0.42
1:A:185:ASP:OD2	1:A:187:THR:OG1	2.28	0.41
1:A:116:PRO:HB2	1:A:117:TRP:CD1	2.56	0.41
1:A:23:LYS:HB3	1:A:25:GLU:HG2	2.01	0.41
1:A:134:ASN:O	1:A:137:LEU:HB2	2.21	0.41
1:A:92:LYS:HZ3	1:A:92:LYS:HG3	1.72	0.41
1:A:185:ASP:CG	1:A:187:THR:HG1	2.20	0.41
1:A:188:ILE:H	1:A:188:ILE:HG13	1.58	0.41
1:A:95:VAL:O	1:A:146:VAL:HG13	2.20	0.41
1:A:23:LYS:HD3	1:A:85:GLU:OE2	2.20	0.41
1:A:134:ASN:C	1:A:138:GLN:HG3	2.40	0.41
1:A:298:LEU:CB	1:A:299:ILE:HG13	2.49	0.41
3:A:1001:FR0:S22	4:A:1386:HOH:O	2.62	0.41
1:A:36:ILE:H	1:A:36:ILE:HG13	1.39	0.41
1:A:116:PRO:HB2	1:A:117:TRP:CD2	2.56	0.41
1:A:335:LEU:HA	1:A:336:PRO:HD2	1.83	0.41
1:A:72:ILE:HB	1:A:78:ALA:HB1	2.03	0.41
1:A:123:ASP:O	1:A:125:THR:HG22	2.20	0.41
1:A:148:VAL:CA	4:A:1408:HOH:O	2.68	0.41
1:A:264:TRP:HE1	1:A:300:PHE:HB3	1.86	0.41
1:A:52:MET:HE2	1:A:268:LEU:HB3	2.02	0.41
1:A:327:ILE:HA	4:A:1072:HOH:O	2.21	0.40
1:A:36:ILE:HD11	1:A:38:LEU:CD1	2.51	0.40
1:A:74:GLY:C	1:A:124:LEU:HD12	2.41	0.40
1:A:323:LYS:HB3	1:A:351:TYR:CE1	2.56	0.40
1:A:36:ILE:HG12	1:A:71:ALA:CB	2.52	0.40
1:A:130:VAL:CG1	1:A:172:TYR:CD2	3.05	0.40
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.77	0.40
1:A:32:LYS:O	1:A:33:ARG:C	2.59	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	347/356 (98%)	289 (83%)	40 (12%)	18 (5%)	2 1

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	56	LEU
1	A	121	GLU
1	A	135	GLN
1	A	289	ASN
1	A	322	PHE
1	A	24	PRO
1	A	242	THR
1	A	274	PRO
1	A	43	PRO
1	A	55	PRO
1	A	190	GLY
1	A	295	ASP
1	A	39	PRO
1	A	318	THR
1	A	321	GLU
1	A	112	VAL
1	A	188	ILE

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	304/309 (98%)	252 (83%)	52 (17%)	2 2

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

Mol	Chain	Res	Type
1	A	4	THR
1	A	8	ASP
1	A	16	VAL
1	A	25	GLU
1	A	32	LYS
1	A	41	ASP
1	A	46	LEU
1	A	48	ASN
1	A	52	MET
1	A	53	ASP
1	A	54	LYS
1	A	57	THR
1	A	72	ILE
1	A	76	ARG
1	A	81	ARG
1	A	107	LEU
1	A	109	ASN
1	A	112	VAL
1	A	113	GLU
1	A	117	TRP
1	A	123	ASP
1	A	124	LEU
1	A	125	THR
1	A	149	ARG
1	A	160	SER
1	A	166	VAL
1	A	168	LEU
1	A	173	ARG
1	A	174	GLU
1	A	177	VAL
1	A	178	VAL
1	A	180	ILE
1	A	199	GLN
1	A	209	VAL
1	A	223	VAL

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Mol	Chain	Res	Type
1	A	233	THR
1	A	253	ARG
1	A	265	SER
1	A	274	PRO
1	A	281	ILE
1	A	284	LYS
1	A	285	ASN
1	A	286	ASP
1	A	294	THR
1	A	304	LEU
1	A	308	TYR
1	A	318	THR
1	A	320	GLU
1	A	321	GLU
1	A	325	LEU
1	A	335	LEU
1	A	337	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	119	GLN
1	A	157	HIS
1	A	197	HIS
1	A	278	HIS
1	A	309	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	FR0	A	1001	-	20,28,28	2.77	5 (25%)	13,39,39	3.07	4 (30%)

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
3	FR0	A	1001	-	-	0/1/13/13	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR0	C19-C16	-5.65	1.36	1.49
3	A	1001	FR0	C11-C12	-2.69	1.47	1.51
3	A	1001	FR0	C7-C6	2.46	1.42	1.36
3	A	1001	FR0	C19-N20	3.99	1.50	1.37
3	A	1001	FR0	C5-N10	8.77	1.48	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	FR0	C11-C12-C18	-4.00	120.27	128.63
3	A	1001	FR0	C12-C11-N10	-2.66	106.97	112.66
3	A	1001	FR0	C19-C23-S22	6.50	119.78	111.79
3	A	1001	FR0	C23-C19-C16	6.91	154.03	128.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	FR0	6	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.