Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:08 PM GMT

PDB ID	:	1E8H
Title	:	STRUCTURE OF THE H61T MUTANT OF THE FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN THE APO FORM COMPLEXED BY ADP
Authors	:	Mattevi, A.; Fraaije, M.W.
Deposited on	:	2000-09-20
Resolution	:	2.60 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 (1)) were used in the production of this report:

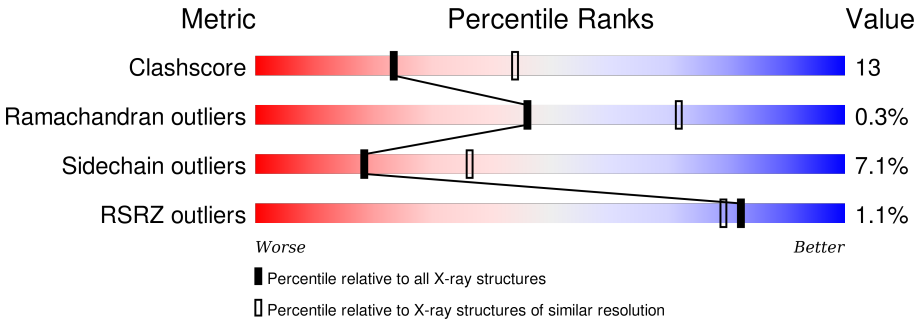
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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.

Mol	Chain	Length	Quality of chain
1	A	560	% 63% 29%
1	B	560	% 65% 27%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8765 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.

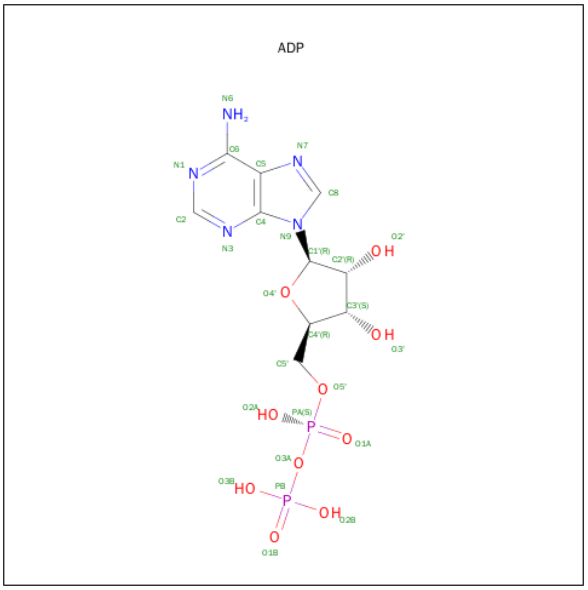
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	125	0	0
			4311	2768	737	782	24			
1	B	545	Total	C	N	O	S	125	0	0
			4311	2768	737	782	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	THR	HIS	ENGINEERED	UNP P56216
B	61	THR	HIS	ENGINEERED	UNP P56216

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

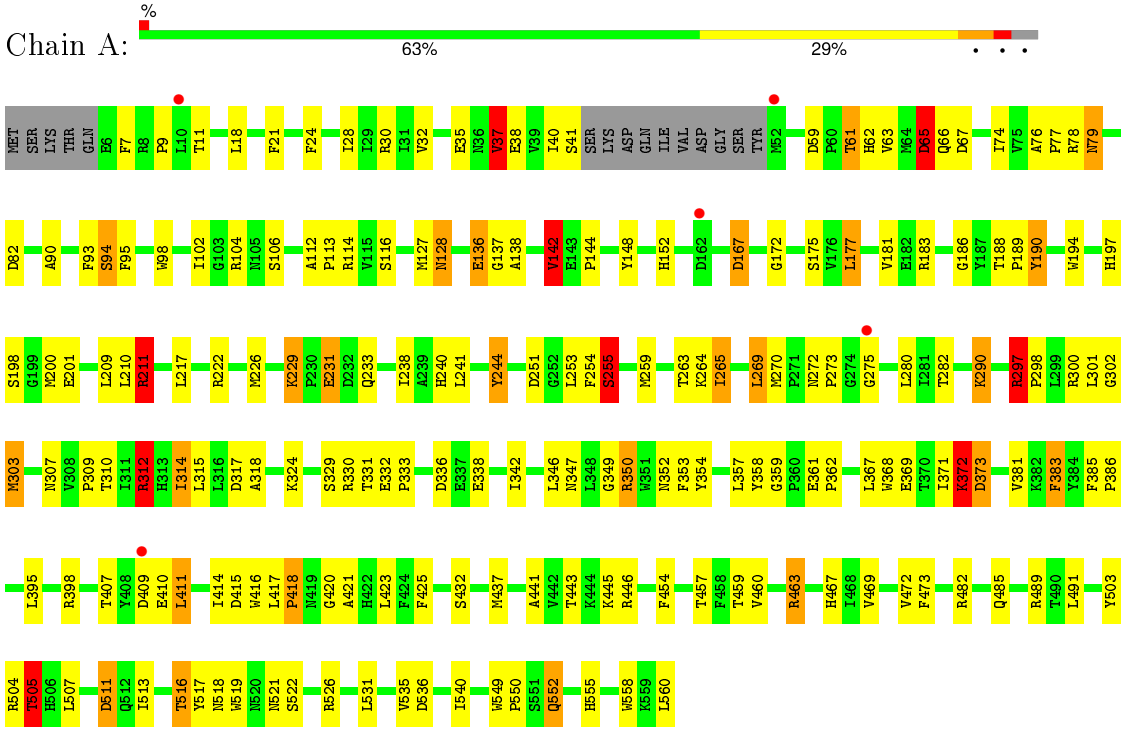
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	43	Total	O	0	0
			43	43		

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.

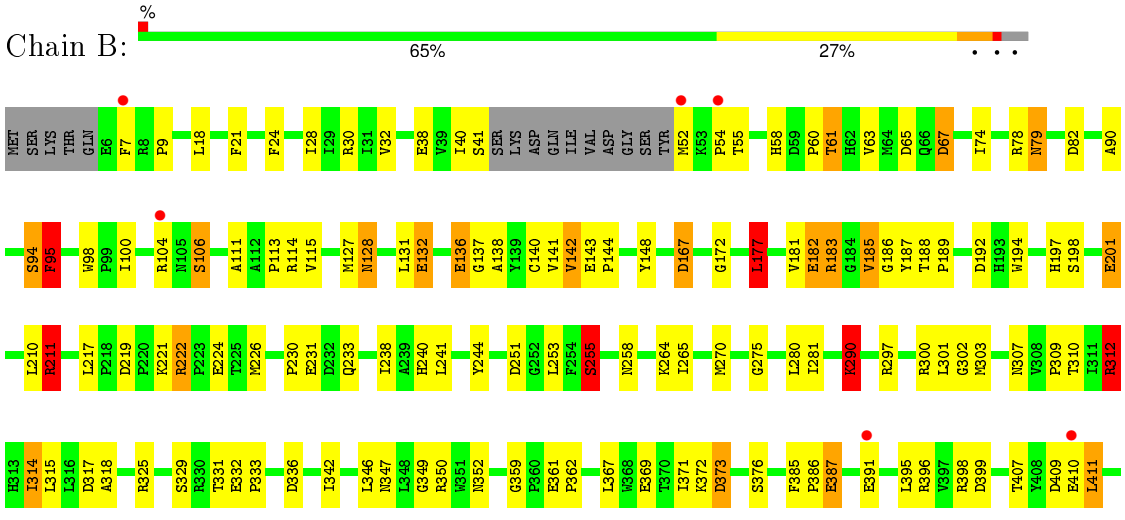
- Molecule 1: VANILLYL-ALCOHOL OXIDASE

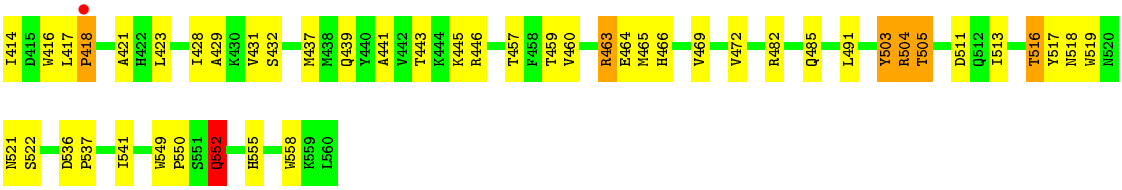
Chain A:



- Molecule 1: VANILLYL-ALCOHOL OXIDASE

Chain B:




I414
D415
W416
L417
P418
A421
H422
L423
I428
A429
K430
V431
S432
M437
M438
Q439
Y440
A441
V442
T443
K444
K445
R446
T457
F458
T459
V460
R463
E464
M465
H466
V469
V472
R482
Q485
L491
Y503
R504
T505
D511
Q512
I513
T516
Y517
N518
W519
N520
N521
S522
D536
P537
I541
W549
P550
S551
Q552
H555
W558
K559
L560

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	130.34Å 130.34Å 134.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.60) 99.5 (19.70-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.303 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.9	EDS
Estimated twinning fraction	0.000 for l,-k,h 0.000 for -l,-k,-h 0.012 for -h,-l,-k 0.000 for -h,l,k 0.025 for -h,k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 34149 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8765	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 3.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ADP

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	0.62	3/4428 (0.1%)	1.66	67/6018 (1.1%)
1	B	0.64	5/4428 (0.1%)	1.56	48/6018 (0.8%)
All	All	0.63	8/8856 (0.1%)	1.61	115/12036 (1.0%)

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	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	372	LYS	CG-CD	-7.15	1.28	1.52
1	A	35	GLU	CB-CG	6.69	1.64	1.52
1	B	221	LYS	CG-CD	-6.50	1.30	1.52
1	B	95	PHE	CB-CG	-6.38	1.40	1.51
1	A	67	ASP	CA-CB	-6.09	1.40	1.53
1	B	67	ASP	CA-CB	-5.99	1.40	1.53
1	B	325	ARG	CB-CG	-5.42	1.38	1.52
1	A	229	LYS	CG-CD	-5.26	1.34	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	211	ARG	CD-NE-CZ	28.35	163.29	123.60
1	A	211	ARG	CD-NE-CZ	25.97	159.96	123.60
1	A	312	ARG	NE-CZ-NH2	-20.73	109.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	312	ARG	NE-CZ-NH1	16.83	128.71	120.30
1	B	312	ARG	NE-CZ-NH2	-14.88	112.86	120.30
1	A	211	ARG	NE-CZ-NH1	14.48	127.54	120.30
1	B	312	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	B	104	ARG	CD-NE-CZ	12.74	141.44	123.60
1	A	463	ARG	NE-CZ-NH2	-12.09	114.25	120.30
1	B	211	ARG	CA-CB-CG	11.85	139.47	113.40
1	A	211	ARG	NE-CZ-NH2	-11.83	114.39	120.30
1	B	183	ARG	CD-NE-CZ	11.54	139.76	123.60
1	A	190	TYR	CB-CG-CD1	11.52	127.91	121.00
1	A	211	ARG	CA-CB-CG	11.44	138.56	113.40
1	A	504	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	A	190	TYR	CB-CG-CD2	-10.91	114.45	121.00
1	A	244	TYR	CB-CG-CD1	10.65	127.39	121.00
1	A	104	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	A	350	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	B	221	LYS	CB-CG-CD	9.70	136.83	111.60
1	B	463	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	104	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	B	7	PHE	N-CA-C	9.22	135.90	111.00
1	B	300	ARG	CD-NE-CZ	9.21	136.49	123.60
1	A	222	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	A	104	ARG	CD-NE-CZ	8.64	135.69	123.60
1	B	504	ARG	CD-NE-CZ	8.45	135.43	123.60
1	A	7	PHE	N-CA-C	8.34	133.52	111.00
1	A	425	PHE	CB-CG-CD2	-8.23	115.04	120.80
1	A	467	HIS	O-C-N	-8.23	109.53	122.70
1	B	463	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	A	297	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	A	255	SER	N-CA-CB	8.06	122.59	110.50
1	A	37	VAL	CA-C-N	8.02	134.85	117.20
1	B	446	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	127	MET	C-N-CA	7.91	141.49	121.70
1	B	78	ARG	NE-CZ-NH1	-7.89	116.35	120.30
1	B	372	LYS	CG-CD-CE	7.78	135.25	111.90
1	B	244	TYR	CB-CG-CD1	7.74	125.64	121.00
1	A	373	ASP	CB-CG-OD1	-7.67	111.40	118.30
1	A	177	LEU	CA-CB-CG	7.60	132.78	115.30
1	B	127	MET	C-N-CA	7.57	140.63	121.70
1	B	226	MET	CA-CB-CG	7.55	126.14	113.30
1	A	297	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	526	ARG	NE-CZ-NH2	7.48	124.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	255	SER	N-CA-CB	7.36	121.54	110.50
1	A	446	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	B	128	ASN	CB-CA-C	-7.11	96.18	110.40
1	A	300	ARG	CD-NE-CZ	7.08	133.52	123.60
1	B	482	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	B	167	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	128	ASN	CB-CA-C	-6.81	96.78	110.40
1	A	350	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	211	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	A	383	PHE	N-CA-CB	-6.62	98.68	110.60
1	A	167	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	222	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	59	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	504	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	200	MET	CA-CB-CG	6.37	124.13	113.30
1	A	372	LYS	CG-CD-CE	6.21	130.54	111.90
1	A	489	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	536	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	511	ASP	CB-CG-OD1	-6.16	112.75	118.30
1	A	142	VAL	N-CA-CB	-6.16	97.95	111.50
1	B	244	TYR	CA-C-N	6.12	128.43	116.20
1	A	37	VAL	O-C-N	-6.10	112.93	122.70
1	B	552	GLN	CA-CB-CG	6.09	126.79	113.40
1	B	373	ASP	CB-CG-OD1	-6.03	112.87	118.30
1	A	128	ASN	N-CA-CB	-5.95	99.90	110.60
1	B	485	GLN	OE1-CD-NE2	-5.90	108.34	121.90
1	A	211	ARG	N-CA-CB	5.88	121.19	110.60
1	B	536	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	222	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	259	MET	CA-C-N	5.74	127.69	116.20
1	B	187	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	B	185	VAL	CB-CA-C	-5.71	100.56	111.40
1	B	132	GLU	OE1-CD-OE2	-5.68	116.48	123.30
1	A	485	GLN	OE1-CD-NE2	-5.64	108.92	121.90
1	B	312	ARG	CD-NE-CZ	5.59	131.43	123.60
1	A	244	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	B	177	LEU	CA-CB-CG	5.57	128.11	115.30
1	B	201	GLU	OE1-CD-OE2	5.56	129.97	123.30
1	B	224	GLU	OE1-CD-OE2	-5.56	116.63	123.30
1	A	354	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	A	383	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	A	560	LEU	CA-C-O	-5.53	108.50	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	LEU	CB-CG-CD1	5.49	120.33	111.00
1	A	226	MET	CA-CB-CG	5.47	122.60	113.30
1	A	24	PHE	CA-CB-CG	5.46	127.00	113.90
1	B	128	ASN	N-CA-CB	-5.45	100.79	110.60
1	B	290	LYS	CB-CG-CD	5.42	125.70	111.60
1	B	372	LYS	CD-CE-NZ	5.40	124.12	111.70
1	A	358	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	A	136	GLU	CA-CB-CG	5.35	125.18	113.40
1	B	142	VAL	N-CA-CB	-5.34	99.75	111.50
1	B	24	PHE	CA-CB-CG	5.34	126.71	113.90
1	A	244	TYR	CA-C-N	5.33	126.86	116.20
1	B	244	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	244	TYR	CG-CD2-CE2	5.26	125.51	121.30
1	B	183	ARG	O-C-N	-5.26	114.26	123.20
1	A	526	ARG	NH1-CZ-NH2	-5.26	113.61	119.40
1	B	463	ARG	CD-NE-CZ	5.25	130.95	123.60
1	A	229	LYS	CB-CG-CD	5.23	125.20	111.60
1	A	425	PHE	CB-CG-CD1	5.21	124.44	120.80
1	A	505	THR	CB-CA-C	-5.19	97.58	111.60
1	A	354	TYR	CB-CG-CD1	5.18	124.11	121.00
1	A	254	PHE	CB-CG-CD1	-5.15	117.19	120.80
1	A	482	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	182	GLU	CA-C-O	5.13	130.87	120.10
1	A	290	LYS	CB-CG-CD	5.06	124.75	111.60
1	B	536	ASP	CA-CB-CG	5.04	124.50	113.40
1	B	537	PRO	CA-C-N	5.02	128.24	117.20
1	A	65	ASP	N-CA-CB	-5.01	101.58	110.60
1	B	192	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	LEU	Mainchain
1	A	37	VAL	Mainchain

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	4311	0	4259	120	3
1	B	4311	0	4260	117	2
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	46	0	0	5	0
3	B	43	0	0	2	0
All	All	8765	0	8543	220	4

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 13.

All (220) 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:B:63:VAL:HG11	1:B:423:LEU:HD11	1.35	1.09
1:A:63:VAL:HG11	1:A:423:LEU:HD11	1.43	1.01
1:B:40:ILE:HD11	1:B:74:ILE:HD11	1.54	0.89
1:A:550:PRO:HB2	1:A:552:GLN:NE2	1.94	0.82
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.62	0.81
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.64	0.79
1:B:181:VAL:O	1:B:255:SER:HB3	1.85	0.77
1:A:552:GLN:H	1:A:552:GLN:NE2	1.83	0.76
1:B:550:PRO:HB2	1:B:552:GLN:NE2	2.00	0.76
1:B:349:GLY:H	1:B:352:ASN:HD21	1.34	0.76
1:B:552:GLN:NE2	1:B:552:GLN:H	1.86	0.73
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.70	0.72
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.72	0.71
1:A:189:PRO:HG2	1:A:270:MET:HE1	1.71	0.71
1:B:79:ASN:ND2	1:B:82:ASP:H	1.90	0.70
1:A:40:ILE:HD11	1:A:74:ILE:HD11	1.72	0.70
1:A:79:ASN:HD22	1:A:82:ASP:H	1.42	0.68
1:B:189:PRO:HG2	1:B:270:MET:HE1	1.76	0.68
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.58	0.67
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.74	0.67
1:A:181:VAL:O	1:A:255:SER:HB3	1.95	0.66
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.78	0.65
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.26	0.65
1:A:79:ASN:ND2	1:A:82:ASP:H	1.94	0.65
1:B:275:GLY:HA3	1:B:359:GLY:O	1.97	0.65
1:A:315:LEU:HA	1:A:318:ALA:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.78	0.65
1:B:167:ASP:OD1	1:B:186:GLY:HA3	1.95	0.65
1:B:79:ASN:HD22	1:B:82:ASP:H	1.45	0.64
1:A:411:LEU:O	1:A:414:ILE:HG12	1.98	0.63
1:B:407:THR:HB	1:B:409:ASP:OD1	1.98	0.63
1:B:183:ARG:HH11	1:B:255:SER:HB2	1.64	0.63
1:B:552:GLN:HE21	1:B:552:GLN:H	1.47	0.62
1:A:349:GLY:H	1:A:352:ASN:HD21	1.44	0.62
1:A:369:GLU:O	1:A:373:ASP:HB2	1.99	0.62
1:A:552:GLN:H	1:A:552:GLN:HE21	1.48	0.62
1:B:280:LEU:HB3	1:B:395:LEU:HD22	1.82	0.62
1:A:275:GLY:HA3	1:A:359:GLY:O	1.99	0.61
1:B:315:LEU:HA	1:B:318:ALA:HB3	1.83	0.61
1:B:513:ILE:O	1:B:516:THR:HB	2.01	0.61
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.31	0.60
1:A:183:ARG:NH1	1:A:255:SER:HB2	2.15	0.60
1:B:369:GLU:O	1:B:373:ASP:HB2	2.02	0.60
1:B:346:LEU:O	1:B:347:ASN:HB2	2.02	0.60
1:B:310:THR:HG22	1:B:459:THR:HG22	1.84	0.60
1:A:346:LEU:O	1:A:347:ASN:HB2	2.02	0.60
1:B:201:GLU:OE2	1:B:264:LYS:NZ	2.34	0.59
1:A:136:GLU:HG2	3:A:2005:HOH:O	2.02	0.59
1:B:194:TRP:O	1:B:197:HIS:HD2	1.84	0.59
1:A:65:ASP:OD1	1:A:66:GLN:N	2.36	0.59
1:A:189:PRO:HG2	1:A:270:MET:CE	2.32	0.59
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.02	0.59
1:A:381:VAL:HG12	3:A:2026:HOH:O	2.02	0.59
1:B:411:LEU:O	1:B:414:ILE:HG12	2.03	0.58
1:A:513:ILE:O	1:A:516:THR:HB	2.03	0.58
1:B:189:PRO:HG2	1:B:270:MET:CE	2.32	0.58
1:A:194:TRP:O	1:A:197:HIS:HD2	1.86	0.58
1:B:521:ASN:O	1:B:522:SER:HB2	2.03	0.57
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.87	0.57
1:A:519:TRP:CE3	1:B:211:ARG:HG2	2.40	0.57
1:B:416:TRP:HB3	1:B:472:VAL:HG21	1.86	0.57
1:A:521:ASN:O	1:A:522:SER:HB2	2.04	0.57
1:B:148:TYR:HB2	1:B:172:GLY:O	2.05	0.57
1:A:290:LYS:HB2	1:A:437:MET:HG3	1.88	0.56
1:A:188:THR:HB	1:A:189:PRO:CD	2.36	0.56
1:A:211:ARG:HG2	1:B:519:TRP:CE3	2.41	0.56
1:A:373:ASP:HB3	3:A:2024:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:CD2	1:B:253:LEU:HD21	2.35	0.55
1:B:307:ASN:O	1:B:309:PRO:HD3	2.07	0.55
1:B:115:VAL:HG13	3:B:2040:HOH:O	2.05	0.55
1:A:37:VAL:HG12	1:A:37:VAL:O	2.06	0.55
1:A:518:ASN:O	1:A:519:TRP:C	2.44	0.55
1:A:269:LEU:O	1:B:463:ARG:NH2	2.39	0.55
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.88	0.54
1:A:443:THR:HG21	1:A:469:VAL:CG2	2.37	0.54
1:A:420:GLY:HA2	1:A:473:PHE:O	2.08	0.54
1:A:253:LEU:HD21	1:B:253:LEU:CD2	2.36	0.54
1:A:183:ARG:HH11	1:A:255:SER:HB2	1.72	0.54
1:A:241:LEU:HB3	1:B:463:ARG:O	2.08	0.54
1:A:253:LEU:HD21	1:B:253:LEU:HD11	1.89	0.53
1:B:183:ARG:NH1	1:B:255:SER:HB2	2.21	0.53
1:A:312:ARG:NH2	1:A:410:GLU:OE1	2.41	0.53
1:B:201:GLU:HB3	1:B:264:LYS:HB2	1.89	0.53
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.89	0.53
1:A:148:TYR:HB2	1:A:172:GLY:O	2.09	0.53
1:A:416:TRP:HB3	1:A:472:VAL:HG21	1.90	0.53
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.44	0.53
1:A:152:HIS:HD2	3:A:2029:HOH:O	1.91	0.52
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.91	0.52
1:B:290:LYS:HB2	1:B:437:MET:HG3	1.90	0.52
1:A:463:ARG:O	1:B:241:LEU:HB3	2.09	0.52
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.45	0.51
1:A:443:THR:HA	1:A:491:LEU:HD21	1.93	0.51
1:A:61:THR:OG1	1:A:421:ALA:HB1	2.10	0.51
1:A:516:THR:HG23	1:B:217:LEU:CD2	2.41	0.51
1:B:309:PRO:HG2	1:B:460:VAL:HB	1.92	0.51
1:B:185:VAL:HG12	1:B:186:GLY:N	2.24	0.51
1:A:531:LEU:O	1:A:535:VAL:HG22	2.11	0.51
1:A:188:THR:CB	1:A:189:PRO:CD	2.90	0.50
1:B:516:THR:HG21	3:B:2032:HOH:O	2.11	0.50
1:A:505:THR:HG23	3:A:2031:HOH:O	2.11	0.50
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.41	0.50
1:B:290:LYS:HB2	1:B:437:MET:CG	2.41	0.50
1:B:518:ASN:O	1:B:519:TRP:C	2.48	0.50
1:B:312:ARG:HD3	1:B:317:ASP:OD1	2.12	0.49
1:A:11:THR:HG21	1:A:116:SER:HB3	1.95	0.49
1:A:38:GLU:HB3	1:A:74:ILE:HD13	1.95	0.49
1:A:290:LYS:HB2	1:A:437:MET:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:NH2	1:A:511:ASP:OD2	2.46	0.49
1:B:219:ASP:OD2	1:B:222:ARG:NH1	2.46	0.48
1:B:443:THR:HA	1:B:491:LEU:HD21	1.95	0.48
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.95	0.48
1:A:361:GLU:N	1:A:362:PRO:HD2	2.28	0.48
1:A:407:THR:HB	1:A:409:ASP:OD1	2.14	0.48
1:B:280:LEU:CB	1:B:395:LEU:HD22	2.43	0.48
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.76	0.48
1:B:137:GLY:O	1:B:138:ALA:HB3	2.12	0.47
1:B:443:THR:HG21	1:B:469:VAL:CG2	2.42	0.47
1:A:367:LEU:O	1:A:371:ILE:HG13	2.14	0.47
1:B:441:ALA:O	1:B:445:LYS:HG3	2.15	0.47
1:A:142:VAL:HG12	1:A:265:ILE:HG22	1.97	0.47
1:B:302:GLY:O	1:B:303:MET:HB2	2.15	0.46
1:B:90:ALA:HB1	1:B:95:PHE:O	2.16	0.46
1:B:52:MET:O	1:B:54:PRO:HD3	2.15	0.46
1:B:63:VAL:CG1	1:B:423:LEU:HD11	2.25	0.46
1:B:312:ARG:NH2	1:B:410:GLU:OE1	2.49	0.46
1:A:415:ASP:O	1:A:416:TRP:C	2.52	0.46
1:B:28:ILE:O	1:B:32:VAL:HG22	2.14	0.46
1:A:197:HIS:HE1	1:A:251:ASP:OD2	1.99	0.46
1:B:188:THR:HB	1:B:189:PRO:CD	2.45	0.46
1:A:229:LYS:O	1:A:233:GLN:HG3	2.15	0.45
1:B:177:LEU:HB2	1:B:265:ILE:CG2	2.45	0.45
1:B:61:THR:HA	1:B:421:ALA:HB1	1.98	0.45
1:B:38:GLU:HB3	1:B:74:ILE:HD13	1.98	0.45
1:B:38:GLU:O	1:B:74:ILE:HD12	2.16	0.45
1:B:361:GLU:N	1:B:362:PRO:HD2	2.31	0.45
1:A:297:ARG:HH21	1:B:136:GLU:HA	1.80	0.45
1:A:201:GLU:HB3	1:A:264:LYS:HB2	1.99	0.45
1:A:244:TYR:CD2	1:B:183:ARG:HD2	2.52	0.45
1:B:332:GLU:CB	1:B:333:PRO:HD2	2.43	0.45
1:A:137:GLY:O	1:A:138:ALA:HB3	2.16	0.45
1:B:61:THR:OG1	1:B:421:ALA:HB1	2.16	0.45
1:A:357:LEU:CD1	1:A:368:TRP:HB2	2.47	0.45
1:B:198:SER:O	1:B:240:HIS:HD2	1.99	0.44
1:B:60:PRO:HG2	1:B:106:SER:HB2	1.99	0.44
1:B:280:LEU:HD12	1:B:281:ILE:N	2.32	0.44
1:B:114:ARG:NH2	1:B:511:ASP:OD2	2.46	0.44
1:A:280:LEU:HB3	1:A:395:LEU:HD22	1.98	0.44
1:B:79:ASN:HD22	1:B:79:ASN:C	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:CB	1:B:189:PRO:CD	2.95	0.44
1:A:385:PHE:HB3	1:A:386:PRO:CD	2.43	0.44
1:B:395:LEU:O	1:B:399:ASP:N	2.50	0.44
1:B:387:GLU:HA	1:B:396:ARG:NH2	2.32	0.44
1:B:367:LEU:O	1:B:371:ILE:HG13	2.18	0.44
1:A:114:ARG:HB2	1:A:507:LEU:HD22	1.99	0.44
1:B:9:PRO:HG3	1:B:21:PHE:CE2	2.53	0.44
1:B:230:PRO:HA	1:B:233:GLN:NE2	2.33	0.44
1:A:398:ARG:NH1	1:A:410:GLU:OE2	2.51	0.44
1:B:516:THR:HG22	1:B:517:TYR:CD1	2.53	0.43
1:B:314:ILE:HD12	1:B:342:ILE:HG22	2.01	0.43
1:B:505:THR:HG21	1:B:513:ILE:CD1	2.48	0.43
1:A:238:ILE:HG21	1:B:428:ILE:HG21	2.01	0.43
1:A:357:LEU:HD11	1:A:368:TRP:HB2	2.00	0.43
1:A:63:VAL:CG1	1:A:423:LEU:HD11	2.32	0.43
1:A:372:LYS:HG2	1:A:383:PHE:CZ	2.52	0.43
1:A:309:PRO:HB2	1:A:353:PHE:CE1	2.53	0.43
1:A:540:ILE:H	1:A:540:ILE:HG13	1.67	0.43
1:A:310:THR:O	1:A:353:PHE:HA	2.19	0.43
1:B:55:THR:HG21	1:B:58:HIS:CE1	2.53	0.43
1:A:307:ASN:O	1:A:309:PRO:HD3	2.19	0.43
1:B:74:ILE:HD12	1:B:74:ILE:N	2.33	0.43
1:A:210:LEU:C	1:A:210:LEU:HD23	2.39	0.43
1:A:198:SER:O	1:A:240:HIS:HD2	2.01	0.43
1:A:63:VAL:HG11	1:A:423:LEU:CD1	2.32	0.43
1:B:258:ASN:HB2	1:B:541:ILE:O	2.19	0.43
1:B:398:ARG:NH1	1:B:410:GLU:OE2	2.50	0.42
1:B:177:LEU:HB2	1:B:265:ILE:HG21	2.01	0.42
1:A:454:PHE:C	1:A:454:PHE:CD1	2.93	0.42
1:A:324:LYS:HD2	1:A:416:TRP:NE1	2.34	0.42
1:A:314:ILE:HD12	1:A:342:ILE:HG22	2.01	0.42
1:B:100:ILE:HD13	1:B:111:ALA:HB1	2.01	0.42
1:B:417:LEU:HB3	1:B:418:PRO:CD	2.46	0.42
1:B:63:VAL:HG11	1:B:423:LEU:CD1	2.26	0.42
1:A:61:THR:HA	1:A:421:ALA:HB1	2.02	0.42
1:A:28:ILE:O	1:A:32:VAL:HG22	2.19	0.42
1:B:210:LEU:HD23	1:B:211:ARG:N	2.35	0.42
1:A:144:PRO:HD3	1:A:263:THR:O	2.20	0.42
1:A:93:PHE:O	1:A:94:SER:HB2	2.19	0.42
1:A:441:ALA:O	1:A:445:LYS:HG3	2.20	0.42
1:A:282:THR:HA	1:A:352:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ALA:O	1:A:507:LEU:HD11	2.19	0.41
1:A:190:TYR:CD1	1:A:270:MET:HB2	2.56	0.41
1:B:431:VAL:HG22	1:B:465:MET:HG3	2.02	0.41
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.55	0.41
1:A:309:PRO:HG2	1:A:460:VAL:HB	2.02	0.41
1:A:90:ALA:HB1	1:A:95:PHE:O	2.20	0.41
1:A:272:ASN:HA	1:A:273:PRO:HD3	1.92	0.41
1:A:76:ALA:HA	1:A:77:PRO:HD2	1.92	0.41
1:A:302:GLY:O	1:A:303:MET:HB2	2.20	0.41
1:B:177:LEU:HD12	1:B:177:LEU:C	2.41	0.41
1:A:209:LEU:HD23	1:A:209:LEU:HA	1.92	0.41
1:B:429:ALA:HB2	1:B:439:GLN:NE2	2.36	0.41
1:A:78:ARG:HB2	1:A:82:ASP:OD2	2.21	0.41
1:A:516:THR:HG22	1:A:517:TYR:CD1	2.56	0.41
1:A:312:ARG:HD3	1:A:317:ASP:OD1	2.21	0.41
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.56	0.41
1:B:90:ALA:O	1:B:94:SER:N	2.54	0.41
1:B:503:TYR:O	1:B:504:ARG:HB2	2.20	0.41
1:B:464:GLU:OE1	1:B:466:HIS:ND1	2.47	0.41
1:B:131:LEU:HD12	1:B:141:VAL:HG12	2.03	0.41
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.56	0.41
1:B:238:ILE:HG22	1:B:238:ILE:O	2.22	0.40
1:B:197:HIS:HE1	1:B:251:ASP:OD2	2.05	0.40
1:A:138:ALA:O	1:B:463:ARG:NH2	2.50	0.40
1:A:231:GLU:H	1:A:231:GLU:HG3	1.30	0.40
1:A:9:PRO:HG3	1:A:21:PHE:CE2	2.56	0.40
1:A:210:LEU:HD23	1:A:211:ARG:N	2.36	0.40
1:A:211:ARG:HG2	1:B:519:TRP:CZ3	2.57	0.40
1:A:310:THR:HG22	1:A:459:THR:HG22	2.03	0.40
1:B:132:GLU:O	1:B:140:CYS:HA	2.22	0.40

All (4) 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:18:LEU:CD2	1:A:30:ARG:NH1[3_655]	1.68	0.52
1:A:330:ARG:NH2	1:A:338:GLU:OE2[2_765]	1.71	0.49
1:A:37:VAL:O	1:B:391:GLU:OE2[6_655]	2.04	0.16
1:B:18:LEU:CD2	1:B:30:ARG:NH1[4_565]	2.10	0.10

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	541/560 (97%)	504 (93%)	36 (7%)	1 (0%)	52 77
1	B	541/560 (97%)	506 (94%)	33 (6%)	2 (0%)	39 65
All	All	1082/1120 (97%)	1010 (93%)	69 (6%)	3 (0%)	46 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	PRO
1	B	67	ASP
1	B	418	PRO

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	466/481 (97%)	434 (93%)	32 (7%)	19 38
1	B	466/481 (97%)	432 (93%)	34 (7%)	17 35
All	All	932/962 (97%)	866 (93%)	66 (7%)	18 36

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	61	THR
1	A	62	HIS

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Mol	Chain	Res	Type
1	A	65	ASP
1	A	79	ASN
1	A	94	SER
1	A	106	SER
1	A	128	ASN
1	A	142	VAL
1	A	177	LEU
1	A	211	ARG
1	A	231	GLU
1	A	255	SER
1	A	265	ILE
1	A	297	ARG
1	A	301	LEU
1	A	303	MET
1	A	312	ARG
1	A	314	ILE
1	A	329	SER
1	A	331	THR
1	A	336	ASP
1	A	350	ARG
1	A	372	LYS
1	A	411	LEU
1	A	432	SER
1	A	457	THR
1	A	503	TYR
1	A	505	THR
1	A	516	THR
1	A	552	GLN
1	A	555	HIS
1	B	41	SER
1	B	61	THR
1	B	65	ASP
1	B	79	ASN
1	B	94	SER
1	B	95	PHE
1	B	106	SER
1	B	128	ASN
1	B	136	GLU
1	B	142	VAL
1	B	177	LEU
1	B	182	GLU
1	B	211	ARG

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Mol	Chain	Res	Type
1	B	231	GLU
1	B	255	SER
1	B	290	LYS
1	B	297	ARG
1	B	301	LEU
1	B	312	ARG
1	B	314	ILE
1	B	329	SER
1	B	331	THR
1	B	336	ASP
1	B	350	ARG
1	B	376	SER
1	B	387	GLU
1	B	411	LEU
1	B	432	SER
1	B	457	THR
1	B	503	TYR
1	B	505	THR
1	B	516	THR
1	B	552	GLN
1	B	555	HIS

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	62	HIS
1	A	79	ASN
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	520	ASN
1	A	552	GLN
1	B	62	HIS
1	B	79	ASN
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	439	GLN
1	B	467	HIS
1	B	520	ASN
1	B	552	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	600	-	22,29,29	1.66	5 (22%)	27,45,45	1.59	5 (18%)
2	ADP	B	600	-	22,29,29	1.69	6 (27%)	27,45,45	1.77	6 (22%)

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	ADP	A	600	-	-	0/12/32/32	0/3/3/3
2	ADP	B	600	-	-	0/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ADP	C8-N7	-4.18	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	ADP	O4'-C1'	-3.56	1.36	1.41
2	A	600	ADP	C8-N7	-3.26	1.28	1.34
2	A	600	ADP	C5-N7	-2.48	1.31	1.39
2	B	600	ADP	C5-N7	-2.46	1.31	1.39
2	B	600	ADP	O4'-C1'	-2.25	1.38	1.41
2	B	600	ADP	PB-O2B	-2.07	1.47	1.54
2	A	600	ADP	C2-N1	2.15	1.38	1.33
2	B	600	ADP	C2-N1	2.47	1.38	1.33
2	A	600	ADP	PB-O1B	2.84	1.60	1.51
2	B	600	ADP	PB-O1B	3.75	1.63	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	ADP	N3-C2-N1	-3.49	126.22	128.89
2	A	600	ADP	C2'-C3'-C4'	-2.64	97.19	102.61
2	A	600	ADP	O2'-C2'-C3'	-2.44	103.89	111.83
2	B	600	ADP	O5'-PA-O1A	-2.08	101.56	109.62
2	B	600	ADP	O3B-PB-O1B	2.04	117.16	110.58
2	B	600	ADP	O3A-PA-O5'	2.09	108.49	102.94
2	A	600	ADP	O3B-PB-O1B	2.38	118.25	110.58
2	B	600	ADP	O4'-C1'-N9	2.85	114.07	108.10
2	B	600	ADP	C1'-N9-C4	3.44	132.13	126.94
2	A	600	ADP	C4-C5-N7	3.69	112.87	109.48
2	B	600	ADP	C4-C5-N7	4.89	113.97	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	545/560 (97%)	-0.35	5 (0%)	85	83	24, 43, 67, 78	27 (4%)
1	B	545/560 (97%)	-0.31	7 (1%)	79	75	24, 43, 67, 78	27 (4%)
All	All	1090/1120 (97%)	-0.33	12 (1%)	82	79	24, 43, 68, 78	54 (4%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	PHE	3.4
1	B	391	GLU	3.2
1	B	104	ARG	3.0
1	B	410	GLU	2.8
1	B	418	PRO	2.7
1	B	52	MET	2.7
1	A	10	LEU	2.5
1	A	52	MET	2.5
1	A	162	ASP	2.4
1	A	409	ASP	2.3
1	B	54	PRO	2.0
1	A	275	GLY	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	ADP	A	600	27/27	0.95	0.14	-0.04	47,50,61,63	0
2	ADP	B	600	27/27	0.92	0.14	-0.16	47,50,61,63	0

6.5 Other polymers

There are no such residues in this entry.