Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:01 PM GMT

PDB ID	:	1IEI
Title	:	CRYSTAL STRUCTURE OF HUMAN ALDOSE REDUCTASE COMPLEXED WITH THE INHIBITOR ZENARESTAT.
Authors	:	Kinoshita, T.; Miyake, H.; Fujii, T.; Takakura, S.; Goto, T.
Deposited on	:	2001-04-09
Resolution	:	2.50 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:

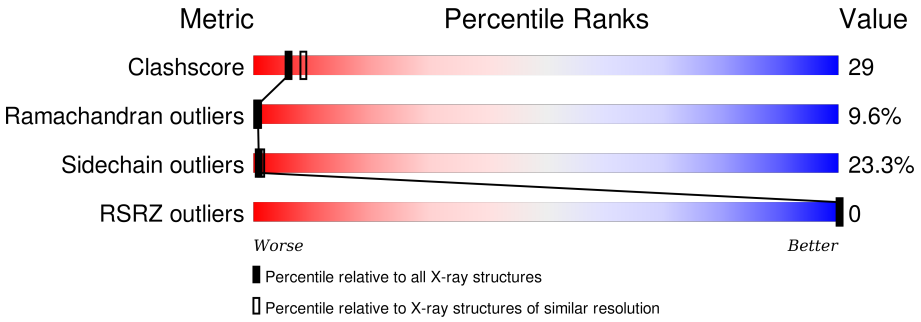
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	316	32% 35% 24% 9%

2 Entry composition

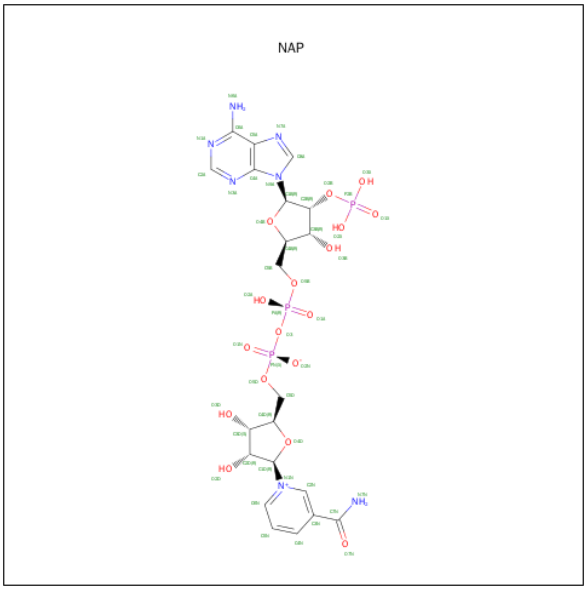
There are 4 unique types of molecules in this entry. The entry contains 2773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALDOSE REDUCTASE.

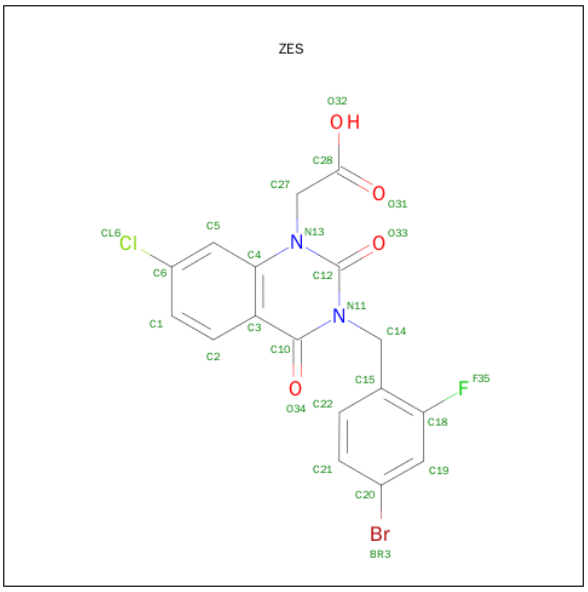
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2513	1615	424	462	12			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is [3-(4-BROMO-2-FLUORO-BENZYL)-7-CHLORO-2,4-DIOXO-3,4-DIHYDRO-2H-QUINAZOLIN-1-YL]-ACETIC ACID (three-letter code: ZES) (formula: $C_{17}H_{11}BrClFN_2O_4$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Br	C	Cl	F	N	O	0	0
			26	1	17	1	1	2	4		

- Molecule 4 is water.

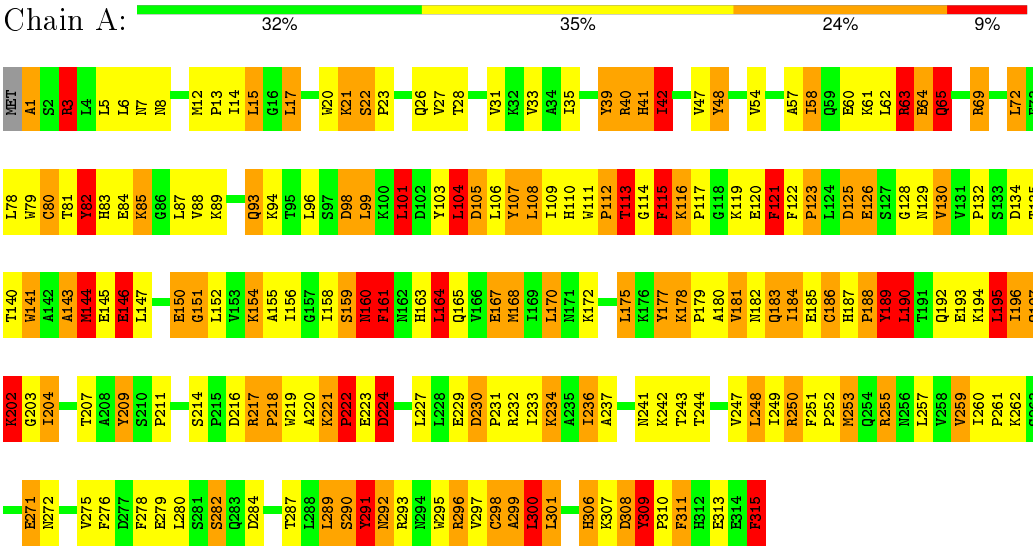
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total	O	0	0
			186	186		

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: ALDOSE REDUCTASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	40.40Å 47.97Å 47.66Å 76.20° 76.70° 67.50°	Depositor
Resolution (Å)	10.00 – 2.50 32.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 44.9 (32.34-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.82 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.178 , 0.199 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	1.1	Xtriage
Anisotropy	1.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 127.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 9831 reflections	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	2773	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.25% 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: ZES, NAP

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	1.76	21/2575 (0.8%)	2.23	101/3496 (2.9%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	LEU	CG-CD2	-22.19	0.69	1.51
1	A	306	HIS	CA-CB	-10.90	1.29	1.53
1	A	151	GLY	CA-C	7.98	1.64	1.51
1	A	39	TYR	CE2-CZ	6.88	1.47	1.38
1	A	58	ILE	CB-CG2	-6.37	1.33	1.52
1	A	222	PRO	N-CD	6.26	1.56	1.47
1	A	311	PHE	CG-CD1	5.93	1.47	1.38
1	A	122	PHE	CG-CD1	5.91	1.47	1.38
1	A	211	PRO	CA-CB	-5.79	1.42	1.53
1	A	282	SER	CB-OG	-5.58	1.34	1.42
1	A	63	ARG	NE-CZ	5.54	1.40	1.33
1	A	291	TYR	CE2-CZ	5.49	1.45	1.38
1	A	311	PHE	CA-CB	5.48	1.66	1.53
1	A	144	MET	CA-CB	-5.42	1.42	1.53
1	A	293	ARG	CZ-NH2	5.37	1.40	1.33
1	A	217	ARG	NE-CZ	5.30	1.40	1.33
1	A	222	PRO	CA-CB	5.22	1.64	1.53
1	A	267	GLU	CG-CD	5.16	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	TYR	CG-CD1	5.10	1.45	1.39
1	A	146	GLU	CG-CD	5.10	1.59	1.51
1	A	289	LEU	C-N	5.02	1.45	1.34

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	LEU	CB-CG-CD2	-20.85	75.55	111.00
1	A	217	ARG	NE-CZ-NH1	18.41	129.50	120.30
1	A	217	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	A	309	TYR	CB-CG-CD1	-11.44	114.14	121.00
1	A	296	ARG	NE-CZ-NH2	11.42	126.01	120.30
1	A	232	ARG	NE-CZ-NH1	-11.34	114.63	120.30
1	A	12	MET	CG-SD-CE	-9.48	85.03	100.20
1	A	69	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	A	3	ARG	CD-NE-CZ	-9.17	110.77	123.60
1	A	224	ASP	CB-CA-C	8.92	128.23	110.40
1	A	201	SER	N-CA-CB	8.79	123.69	110.50
1	A	115	PHE	CB-CG-CD1	-8.25	115.03	120.80
1	A	297	VAL	CA-CB-CG1	8.03	122.94	110.90
1	A	105	ASP	CB-CG-OD2	7.95	125.46	118.30
1	A	82	TYR	CB-CG-CD2	-7.85	116.29	121.00
1	A	64	GLU	CA-CB-CG	7.76	130.48	113.40
1	A	267	GLU	CA-CB-CG	7.74	130.42	113.40
1	A	40	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	217	ARG	CD-NE-CZ	7.42	133.99	123.60
1	A	198	TYR	CG-CD1-CE1	-7.34	115.43	121.30
1	A	216	ASP	CA-CB-CG	7.20	129.23	113.40
1	A	160	ASN	C-N-CA	6.99	139.18	121.70
1	A	315	PHE	CB-CG-CD2	-6.98	115.92	120.80
1	A	299	ALA	N-CA-C	6.85	129.51	111.00
1	A	232	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	A	141	TRP	N-CA-CB	-6.75	98.44	110.60
1	A	42	ILE	CA-CB-CG2	-6.72	97.45	110.90
1	A	128	GLY	N-CA-C	6.67	129.77	113.10
1	A	220	ALA	C-N-CA	-6.61	105.17	121.70
1	A	198	TYR	CB-CG-CD2	-6.61	117.04	121.00
1	A	188	PRO	C-N-CA	-6.42	105.65	121.70
1	A	47	VAL	CG1-CB-CG2	6.42	121.17	110.90
1	A	143	ALA	N-CA-CB	-6.42	101.11	110.10
1	A	64	GLU	OE1-CD-OE2	-6.40	115.62	123.30
1	A	150	GLU	C-N-CA	-6.35	108.97	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	VAL	C-N-CA	-6.31	105.94	121.70
1	A	287	THR	CA-CB-CG2	6.26	121.17	112.40
1	A	309	TYR	CG-CD2-CE2	-6.22	116.33	121.30
1	A	189	TYR	CD1-CE1-CZ	-6.17	114.25	119.80
1	A	259	VAL	CG1-CB-CG2	6.03	120.54	110.90
1	A	65	GLN	N-CA-C	6.00	127.21	111.00
1	A	268	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	284	ASP	CB-CG-OD2	6.00	123.69	118.30
1	A	104	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	198	TYR	CG-CD2-CE2	-5.94	116.55	121.30
1	A	84	GLU	CB-CA-C	-5.90	98.60	110.40
1	A	104	LEU	N-CA-CB	-5.88	98.64	110.40
1	A	105	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	A	237	ALA	CB-CA-C	-5.85	101.33	110.10
1	A	114	GLY	C-N-CA	-5.85	107.08	121.70
1	A	189	TYR	N-CA-C	5.82	126.71	111.00
1	A	63	ARG	CB-CA-C	5.76	121.93	110.40
1	A	87	LEU	CB-CG-CD2	5.75	120.78	111.00
1	A	115	PHE	CD1-CG-CD2	5.74	125.77	118.30
1	A	177	TYR	CB-CG-CD1	-5.74	117.56	121.00
1	A	201	SER	CB-CA-C	-5.74	99.20	110.10
1	A	190	LEU	N-CA-CB	5.72	121.85	110.40
1	A	300	LEU	N-CA-C	5.71	126.41	111.00
1	A	264	VAL	CB-CA-C	-5.66	100.65	111.40
1	A	255	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	300	LEU	C-N-CA	-5.63	107.62	121.70
1	A	198	TYR	CB-CA-C	5.63	121.66	110.40
1	A	242	LYS	CB-CG-CD	5.63	126.23	111.60
1	A	161	PHE	N-CA-C	5.61	126.14	111.00
1	A	98	ASP	N-CA-CB	5.61	120.69	110.60
1	A	291	TYR	CG-CD2-CE2	-5.57	116.84	121.30
1	A	230	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	104	LEU	CB-CA-C	5.54	120.73	110.20
1	A	168	MET	CG-SD-CE	-5.54	91.34	100.20
1	A	203	GLY	N-CA-C	5.51	126.87	113.10
1	A	158	ILE	C-N-CA	-5.51	107.94	121.70
1	A	107	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	308	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	A	177	TYR	CG-CD2-CE2	-5.47	116.92	121.30
1	A	39	TYR	CB-CG-CD2	-5.44	117.73	121.00
1	A	129	ASN	N-CA-C	5.42	125.64	111.00
1	A	250	ARG	CD-NE-CZ	-5.39	116.06	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	THR	CA-C-N	-5.37	105.46	116.20
1	A	186	CYS	CA-CB-SG	5.37	123.66	114.00
1	A	33	VAL	CA-CB-CG2	-5.34	102.89	110.90
1	A	184	ILE	C-N-CA	-5.33	108.39	121.70
1	A	17	LEU	CD1-CG-CD2	-5.26	94.71	110.50
1	A	204	ILE	N-CA-CB	-5.26	98.70	110.80
1	A	198	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	A	159	SER	N-CA-CB	5.24	118.36	110.50
1	A	15	LEU	C-N-CA	-5.22	111.34	122.30
1	A	41	HIS	N-CA-CB	-5.22	101.21	110.60
1	A	80	CYS	C-N-CA	5.21	134.73	121.70
1	A	260	ILE	N-CA-C	5.20	125.04	111.00
1	A	39	TYR	CD1-CG-CD2	5.18	123.59	117.90
1	A	130	VAL	CA-CB-CG1	5.14	118.61	110.90
1	A	271	GLU	N-CA-C	5.14	124.88	111.00
1	A	39	TYR	CB-CA-C	-5.12	100.17	110.40
1	A	183	GLN	CA-CB-CG	-5.11	102.15	113.40
1	A	48	TYR	CG-CD1-CE1	-5.11	117.22	121.30
1	A	290	SER	N-CA-CB	5.11	118.16	110.50
1	A	93	GLN	N-CA-C	5.04	124.61	111.00
1	A	216	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	1	ALA	O-C-N	5.04	130.76	122.70
1	A	308	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	40	ARG	CD-NE-CZ	-5.03	116.56	123.60

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Peptide
1	A	112	PRO	Peptide
1	A	121	PHE	Sidechain
1	A	126	GLU	Peptide
1	A	160	ASN	Peptide
1	A	163	HIS	Peptide
1	A	189	TYR	Sidechain,Peptide
1	A	195	LEU	Peptide
1	A	198	TYR	Sidechain
1	A	199	CYS	Peptide
1	A	201	SER	Peptide
1	A	202	LYS	Peptide
1	A	209	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	221	LYS	Peptide
1	A	222	PRO	Peptide
1	A	224	ASP	Peptide
1	A	291	TYR	Sidechain
1	A	298	CYS	Peptide
1	A	3	ARG	Sidechain
1	A	309	TYR	Sidechain
1	A	63	ARG	Sidechain
1	A	82	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	2513	0	2528	144	0
2	A	48	0	25	7	0
3	A	26	0	11	3	0
4	A	186	0	0	20	0
All	All	2773	0	2564	147	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 29.

All (147) 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:58:ILE:HG21	4:A:502:HOH:O	1.63	0.98
1:A:27:VAL:HG23	4:A:524:HOH:O	1.71	0.89
1:A:85:LYS:HB2	1:A:143:ALA:HB2	1.59	0.84
1:A:115:PHE:HZ	1:A:121:PHE:O	1.64	0.81
1:A:81:THR:HG23	1:A:115:PHE:HE2	1.46	0.79
1:A:60:GLU:O	1:A:64:GLU:HB2	1.86	0.74
1:A:106:LEU:HD21	1:A:181:VAL:HG11	1.70	0.73
1:A:98:ASP:HA	4:A:505:HOH:O	1.90	0.71
1:A:58:ILE:CG2	4:A:502:HOH:O	2.31	0.71
1:A:35:ILE:HG23	1:A:40:ARG:HH12	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LYS:HA	1:A:88:VAL:HG23	1.75	0.68
1:A:83:HIS:O	1:A:140:THR:HG22	1.93	0.68
1:A:8:ASN:ND2	1:A:155:ALA:HB2	2.09	0.67
1:A:15:LEU:HD12	1:A:276:PHE:CZ	2.29	0.66
1:A:190:LEU:HA	1:A:292:ASN:OD1	1.94	0.66
1:A:115:PHE:CZ	1:A:121:PHE:O	2.49	0.66
1:A:96:LEU:HD21	1:A:104:LEU:HB2	1.78	0.65
1:A:81:THR:HG23	1:A:115:PHE:CE2	2.30	0.64
1:A:48:TYR:O	4:A:518:HOH:O	2.14	0.64
1:A:104:LEU:HD11	1:A:107:TYR:CD1	2.33	0.63
1:A:17:LEU:O	1:A:42:ILE:HG22	2.01	0.61
1:A:179:PRO:O	1:A:204:ILE:HG12	2.00	0.61
1:A:161:PHE:CE2	1:A:165:GLN:HB3	2.36	0.60
1:A:77:LYS:HD2	1:A:110:HIS:CD2	2.36	0.60
1:A:291:TYR:CD1	1:A:291:TYR:N	2.69	0.59
1:A:167:GLU:HA	1:A:170:LEU:HD11	1.85	0.59
1:A:185:GLU:HB3	1:A:209:TYR:CE1	2.38	0.59
1:A:184:ILE:HD13	1:A:195:LEU:HD21	1.85	0.58
1:A:110:HIS:O	1:A:159:SER:HB3	2.04	0.58
1:A:195:LEU:HB3	1:A:315:PHE:HB2	1.85	0.58
1:A:160:ASN:HB3	1:A:183:GLN:O	2.04	0.57
1:A:255:ARG:HD3	4:A:392:HOH:O	2.04	0.57
1:A:217:ARG:O	1:A:219:TRP:N	2.38	0.56
1:A:230:ASP:O	1:A:233:ILE:HG22	2.05	0.56
1:A:189:TYR:OH	1:A:230:ASP:OD1	2.24	0.55
1:A:136:ASN:HB3	1:A:139:ASP:HB2	1.87	0.55
1:A:82:TYR:HA	4:A:416:HOH:O	2.06	0.55
1:A:233:ILE:HD11	1:A:248:LEU:CD1	2.37	0.55
1:A:296:ARG:HD3	1:A:311:PHE:CD2	2.42	0.54
1:A:290:SER:N	4:A:515:HOH:O	2.41	0.54
1:A:291:TYR:HD1	1:A:291:TYR:N	2.04	0.54
1:A:189:TYR:HD1	1:A:291:TYR:O	1.90	0.54
1:A:188:PRO:HD2	1:A:227:LEU:HD11	1.88	0.54
1:A:250:ARG:O	1:A:253:MET:HG2	2.07	0.54
1:A:108:LEU:N	1:A:108:LEU:HD22	2.24	0.53
1:A:172:LYS:O	1:A:175:LEU:HB2	2.09	0.53
1:A:231:PRO:HA	1:A:234:LYS:CE	2.38	0.53
1:A:295:TRP:HB2	4:A:514:HOH:O	2.08	0.53
1:A:161:PHE:HE2	1:A:165:GLN:HB3	1.74	0.52
1:A:259:VAL:O	1:A:261:PRO:HD2	2.10	0.52
1:A:183:GLN:HG3	1:A:207:THR:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:THR:HG21	3:A:351:ZES:BR3	2.65	0.52
1:A:164:LEU:O	1:A:168:MET:HG3	2.10	0.52
1:A:244:THR:O	1:A:248:LEU:HB2	2.10	0.52
1:A:57:ALA:O	1:A:61:LYS:HG2	2.09	0.52
1:A:309:TYR:HE2	4:A:376:HOH:O	1.92	0.52
1:A:306:HIS:CG	4:A:517:HOH:O	2.62	0.51
1:A:275:VAL:HG23	1:A:278:PHE:CE1	2.46	0.51
1:A:156:ILE:HD11	1:A:177:TYR:HB3	1.93	0.51
1:A:219:TRP:HZ2	1:A:298:CYS:HA	1.76	0.51
1:A:85:LYS:NZ	1:A:139:ASP:HB3	2.25	0.51
1:A:141:TRP:HA	1:A:141:TRP:CE3	2.47	0.50
1:A:85:LYS:HB2	1:A:143:ALA:CB	2.38	0.50
1:A:85:LYS:HE3	1:A:139:ASP:O	2.11	0.49
1:A:233:ILE:HD11	1:A:248:LEU:HD13	1.93	0.49
1:A:161:PHE:H	1:A:310:PRO:HB3	1.77	0.49
1:A:146:GLU:O	1:A:150:GLU:HG3	2.13	0.49
1:A:14:ILE:HA	4:A:357:HOH:O	2.13	0.48
1:A:64:GLU:O	1:A:65:GLN:HB2	2.12	0.48
1:A:193:GLU:O	1:A:196:ILE:HB	2.12	0.48
1:A:3:ARG:HG3	1:A:13:PRO:HA	1.95	0.48
1:A:115:PHE:HZ	1:A:121:PHE:C	2.16	0.48
1:A:217:ARG:HD2	1:A:219:TRP:NE1	2.28	0.48
1:A:103:TYR:CE2	1:A:154:LYS:HE2	2.48	0.48
1:A:20:TRP:HB2	2:A:350:NAP:H2D	1.96	0.48
1:A:147:LEU:HD23	1:A:152:LEU:HD13	1.94	0.48
1:A:132:PRO:HB3	1:A:306:HIS:HD2	1.77	0.48
1:A:231:PRO:HA	1:A:234:LYS:HE2	1.95	0.48
1:A:209:TYR:CD1	2:A:350:NAP:C5N	2.97	0.47
1:A:275:VAL:HG23	1:A:278:PHE:HE1	1.78	0.47
1:A:233:ILE:HA	1:A:236:ILE:HG12	1.96	0.47
1:A:192:GLN:HG3	4:A:493:HOH:O	2.14	0.47
1:A:178:LYS:HG2	1:A:179:PRO:HD2	1.96	0.47
1:A:252:PRO:O	1:A:257:LEU:HB2	2.15	0.47
1:A:197:GLN:O	1:A:201:SER:HB3	2.15	0.47
1:A:65:GLN:HG3	1:A:65:GLN:O	2.15	0.47
1:A:180:ALA:O	1:A:204:ILE:HG23	2.15	0.46
1:A:252:PRO:HG3	1:A:259:VAL:HG13	1.98	0.46
1:A:251:PHE:HZ	1:A:289:LEU:HD23	1.81	0.46
1:A:99:LEU:HD12	4:A:490:HOH:O	2.16	0.46
2:A:350:NAP:O3X	2:A:350:NAP:H3B	2.15	0.46
1:A:115:PHE:CE2	1:A:123:PRO:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:O	1:A:58:ILE:HD12	2.16	0.45
1:A:151:GLY:HA2	4:A:535:HOH:O	2.15	0.45
1:A:248:LEU:O	1:A:252:PRO:HD2	2.17	0.45
1:A:160:ASN:N	1:A:161:PHE:HB2	2.32	0.45
1:A:151:GLY:C	4:A:535:HOH:O	2.54	0.45
1:A:28:THR:HA	1:A:57:ALA:HB2	1.99	0.45
2:A:350:NAP:C7N	3:A:351:ZES:O32	2.65	0.45
1:A:137:ILE:O	1:A:140:THR:OG1	2.34	0.45
1:A:198:TYR:CD2	1:A:198:TYR:O	2.69	0.45
1:A:214:SER:O	1:A:217:ARG:HG2	2.17	0.44
1:A:189:TYR:HB2	1:A:295:TRP:HE3	1.83	0.44
1:A:231:PRO:HA	1:A:234:LYS:HE3	1.99	0.44
1:A:109:ILE:HD11	1:A:144:MET:SD	2.58	0.44
1:A:188:PRO:HG3	1:A:251:PHE:CE2	2.53	0.44
1:A:79:TRP:CE3	1:A:79:TRP:HA	2.53	0.44
1:A:189:TYR:CE1	1:A:291:TYR:HB3	2.53	0.43
1:A:189:TYR:HE1	1:A:291:TYR:HB3	1.83	0.43
1:A:80:CYS:SG	1:A:111:TRP:HB2	2.58	0.43
1:A:61:LYS:HA	1:A:61:LYS:HD2	1.72	0.43
1:A:250:ARG:NH1	1:A:275:VAL:O	2.52	0.43
1:A:48:TYR:HE2	2:A:350:NAP:HO2N	1.65	0.43
1:A:132:PRO:HB3	1:A:306:HIS:CD2	2.53	0.43
1:A:130:VAL:HB	4:A:475:HOH:O	2.17	0.43
1:A:289:LEU:HB2	4:A:515:HOH:O	2.17	0.43
1:A:116:LYS:HA	1:A:117:PRO:HD2	1.62	0.43
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.85	0.43
1:A:249:ILE:HD11	1:A:272:ASN:OD1	2.19	0.43
1:A:31:VAL:HG21	1:A:54:VAL:HG13	2.01	0.43
1:A:141:TRP:O	1:A:145:GLU:HG3	2.19	0.43
1:A:22:SER:HA	1:A:23:PRO:HD3	1.91	0.42
1:A:306:HIS:CB	4:A:517:HOH:O	2.68	0.42
1:A:259:VAL:HG12	1:A:261:PRO:HD3	2.01	0.42
1:A:75:VAL:HG13	1:A:108:LEU:HD21	2.02	0.42
1:A:72:LEU:HA	1:A:72:LEU:HD12	1.85	0.42
1:A:300:LEU:HD23	1:A:301:LEU:N	2.35	0.42
1:A:189:TYR:CD1	1:A:291:TYR:O	2.72	0.42
1:A:243:THR:O	1:A:247:VAL:HG23	2.20	0.42
1:A:138:LEU:O	1:A:141:TRP:HB3	2.20	0.41
1:A:306:HIS:O	1:A:309:TYR:HB2	2.21	0.41
1:A:141:TRP:CE3	1:A:144:MET:SD	3.14	0.41
1:A:99:LEU:HB3	1:A:101:LEU:HG	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:MET:CB	1:A:147:LEU:HD12	2.51	0.41
1:A:262:LYS:O	2:A:350:NAP:H8A	2.20	0.41
1:A:255:ARG:HD2	1:A:289:LEU:HD21	2.02	0.41
1:A:300:LEU:HB2	3:A:351:ZES:C18	2.50	0.41
1:A:187:HIS:HD2	1:A:189:TYR:N	2.18	0.41
1:A:136:ASN:OD1	1:A:138:LEU:HD12	2.20	0.41
1:A:144:MET:HG3	4:A:389:HOH:O	2.20	0.41
1:A:233:ILE:HD13	1:A:233:ILE:HG21	1.59	0.41
1:A:82:TYR:N	1:A:82:TYR:CD2	2.89	0.41
1:A:185:GLU:HB3	1:A:209:TYR:CD1	2.55	0.40
1:A:85:LYS:HZ1	1:A:139:ASP:HB3	1.84	0.40
1:A:230:ASP:HA	1:A:231:PRO:HD3	1.79	0.40
1:A:306:HIS:ND1	1:A:308:ASP:N	2.70	0.40
2:A:350:NAP:C3B	2:A:350:NAP:O3X	2.68	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	313/316 (99%)	243 (78%)	40 (13%)	30 (10%)	1 0

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	121	PHE
1	A	135	THR
1	A	161	PHE
1	A	200	GLN
1	A	201	SER
1	A	218	PRO

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Mol	Chain	Res	Type
1	A	224	ASP
1	A	241	ASN
1	A	299	ALA
1	A	300	LEU
1	A	125	ASP
1	A	137	ILE
1	A	164	LEU
1	A	282	SER
1	A	21	LYS
1	A	89	LYS
1	A	126	GLU
1	A	202	LYS
1	A	234	LYS
1	A	267	GLU
1	A	292	ASN
1	A	62	LEU
1	A	223	GLU
1	A	120	GLU
1	A	160	ASN
1	A	112	PRO
1	A	221	LYS
1	A	222	PRO
1	A	236	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	279/281 (99%)	214 (77%)	65 (23%)	1 1

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	LEU
1	A	7	ASN

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Mol	Chain	Res	Type
1	A	21	LYS
1	A	22	SER
1	A	26	GLN
1	A	39	TYR
1	A	41	HIS
1	A	42	ILE
1	A	63	ARG
1	A	65	GLN
1	A	69	ARG
1	A	72	LEU
1	A	74	ILE
1	A	77	LYS
1	A	78	LEU
1	A	82	TYR
1	A	85	LYS
1	A	93	GLN
1	A	94	LYS
1	A	99	LEU
1	A	101	LEU
1	A	104	LEU
1	A	105	ASP
1	A	108	LEU
1	A	113	THR
1	A	115	PHE
1	A	116	LYS
1	A	119	LYS
1	A	123	PRO
1	A	125	ASP
1	A	134	ASP
1	A	138	LEU
1	A	144	MET
1	A	146	GLU
1	A	154	LYS
1	A	160	ASN
1	A	164	LEU
1	A	167	GLU
1	A	170	LEU
1	A	175	LEU
1	A	178	LYS
1	A	181	VAL
1	A	182	ASN
1	A	186	CYS

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Mol	Chain	Res	Type
1	A	189	TYR
1	A	190	LEU
1	A	194	LYS
1	A	195	LEU
1	A	196	ILE
1	A	197	GLN
1	A	199	CYS
1	A	202	LYS
1	A	218	PRO
1	A	229	GLU
1	A	248	LEU
1	A	253	MET
1	A	271	GLU
1	A	279	GLU
1	A	280	LEU
1	A	301	LEU
1	A	307	LYS
1	A	309	TYR
1	A	313	GLU
1	A	315	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	93	GLN
1	A	182	ASN
1	A	187	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	NAP	A	350	-	42,52,52	2.62	12 (28%)	54,80,80	2.34	18 (33%)
3	ZES	A	351	-	22,28,28	2.18	8 (36%)	26,41,41	3.01	8 (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
2	NAP	A	350	-	-	0/27/67/67	0/5/5/5
3	ZES	A	351	-	-	0/6/8/8	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	351	ZES	C3-C4	-3.78	1.38	1.41
3	A	351	ZES	C27-N13	-3.71	1.41	1.48
3	A	351	ZES	C19-C18	-3.52	1.31	1.37
2	A	350	NAP	O2B-C2B	-3.49	1.33	1.44
2	A	350	NAP	C3N-C7N	-3.44	1.45	1.50
3	A	351	ZES	C6-CL6	-3.30	1.67	1.74
2	A	350	NAP	P2B-O2B	-3.24	1.50	1.60
3	A	351	ZES	C14-N11	-2.96	1.43	1.48
2	A	350	NAP	O4D-C4D	-2.95	1.38	1.45
3	A	351	ZES	C4-N13	-2.95	1.36	1.40
3	A	351	ZES	C10-N11	-2.84	1.34	1.38
2	A	350	NAP	C2N-C3N	-2.37	1.35	1.39
3	A	351	ZES	C14-C15	2.42	1.56	1.51
2	A	350	NAP	C5B-C4B	2.60	1.60	1.51
2	A	350	NAP	O2D-C2D	2.75	1.49	1.43
2	A	350	NAP	C5D-C4D	3.64	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	NAP	O3D-C3D	3.69	1.51	1.43
2	A	350	NAP	C5N-C4N	4.75	1.48	1.38
2	A	350	NAP	C6N-N1N	6.21	1.52	1.35
2	A	350	NAP	C4N-C3N	10.11	1.56	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	350	NAP	N3A-C2A-N1A	-5.73	124.51	128.89
2	A	350	NAP	C5N-C4N-C3N	-4.80	114.30	120.33
3	A	351	ZES	C28-C27-N13	-3.81	108.97	114.15
2	A	350	NAP	O2N-PN-O5D	-3.76	89.49	108.46
3	A	351	ZES	C14-C15-C18	-3.45	116.41	121.09
2	A	350	NAP	N6A-C6A-N1A	-3.39	111.92	119.20
2	A	350	NAP	O2B-P2B-O1X	-3.27	98.93	107.11
2	A	350	NAP	C4N-C3N-C7N	-3.07	112.97	121.09
2	A	350	NAP	O7N-C7N-C3N	-3.00	116.31	119.59
2	A	350	NAP	O7N-C7N-N7N	-2.98	118.40	122.59
3	A	351	ZES	BR3-C20-C19	-2.95	114.98	119.28
2	A	350	NAP	P2B-O2B-C2B	-2.51	115.54	121.56
3	A	351	ZES	C21-C22-C15	-2.25	118.29	121.41
3	A	351	ZES	C1-C2-C3	-2.14	118.26	121.49
2	A	350	NAP	C4A-C5A-N7A	-2.06	107.58	109.48
3	A	351	ZES	C5-C4-C3	-2.02	117.65	120.69
2	A	350	NAP	O2A-PA-O3	2.04	114.33	105.09
2	A	350	NAP	O2D-C2D-C3D	2.59	120.24	111.83
2	A	350	NAP	C3B-C2B-C1B	2.91	108.36	102.73
2	A	350	NAP	C6N-C5N-C4N	3.09	124.11	119.44
2	A	350	NAP	C2N-C3N-C4N	3.49	122.17	118.29
2	A	350	NAP	O3B-C3B-C2B	4.46	124.05	111.16
2	A	350	NAP	O3-PN-O5D	4.79	115.65	102.94
3	A	351	ZES	C3-C10-N11	6.52	121.47	116.09
2	A	350	NAP	C3N-C7N-N7N	6.82	125.28	117.82
3	A	351	ZES	C2-C3-C4	11.46	123.33	118.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	NAP	7	0
3	A	351	ZES	3	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

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	315/316 (99%)	-1.04	0 100 100	3, 11, 20, 27	0

There are no RSRZ outliers to report.

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	NAP	A	350	48/48	0.97	0.10	0.01	2,11,21,23	0
3	ZES	A	351	26/26	0.98	0.08	-0.90	2,8,13,19	0

6.5 Other polymers

There are no such residues in this entry.