



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 08:05 AM GMT

PDB ID : 1EF3  
Title : FIDARESTAT BOUND TO HUMAN ALDOSE REDUCTASE  
Authors : Oka, M.; Matsumoto, Y.; Sugiyama, S.; Tsuruta, N.; Matsushima, M.  
Deposited on : 2000-02-06  
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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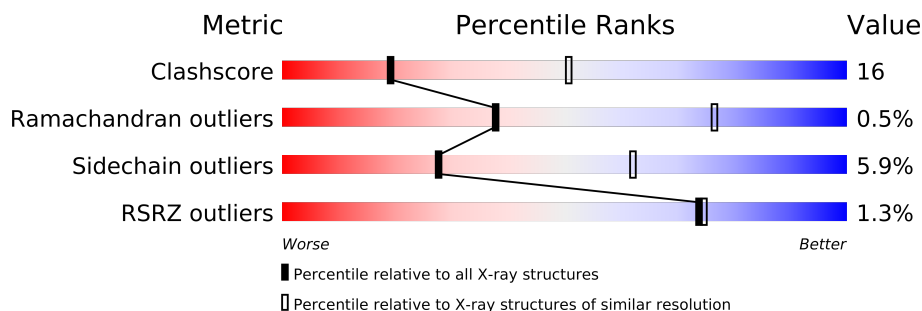
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	

## 2 Entry composition i

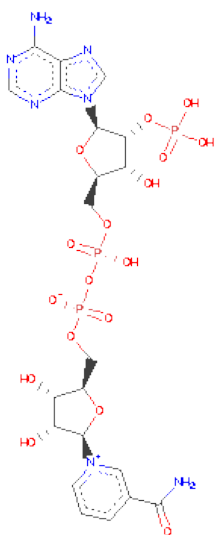
There are 4 unique types of molecules in this entry. The entry contains 5187 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

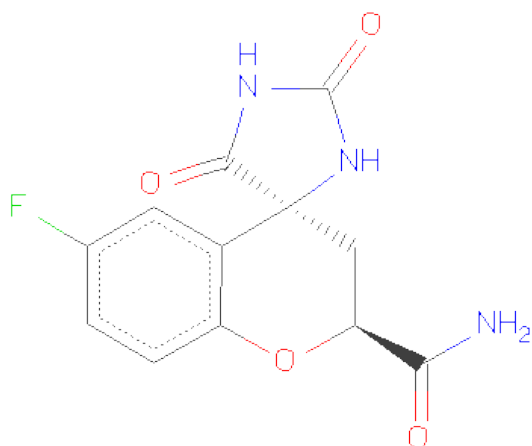
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2513	1615	424	462	12			
1	B	315	Total	C	N	O	S	0	0	0
			2513	1615	424	462	12			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (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		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is (2S,4S)-2-AMINOFORMYL-6-FLUORO-SPIRO[CHROMAN-4,4'-IMIDAZOLIDINE]-2',5'-DIONE (three-letter code: FID) (formula:  $C_{12}H_{10}FN_3O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			20	12	1	3	4		
3	B	1	Total	C	F	N	O	0	0
			20	12	1	3	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	16	Total	O	0	0
			16	16		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.14Å 62.56Å 118.99Å 90.00° 101.60° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 28.06 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 89.6 (28.06-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.94 (at 2.80Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.186 , 0.278 0.184 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 37.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 15476 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	4.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, FID

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	0.65	0/2575	0.78	0/3496
1	B	0.67	1/2575 (0.0%)	0.80	2/3496 (0.1%)
All	All	0.66	1/5150 (0.0%)	0.79	2/6992 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	CYS	CB-SG	-5.80	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	LEU	CA-CB-CG	5.76	128.55	115.30
1	B	109	ILE	N-CA-C	-5.08	97.29	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	TYR	Sidechain
1	A	209	TYR	Sidechain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2513	0	2528	92	0
1	B	2513	0	2528	74	0
2	A	48	0	25	10	0
2	B	48	0	25	6	0
3	A	20	0	10	2	0
3	B	20	0	10	0	0
4	A	9	0	0	0	0
4	B	16	0	0	1	0
All	All	5187	0	5126	169	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (169) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:GLU:HA	1:A:274:LYS:HE2	1.47	0.95
1:B:45:ALA:HB2	1:B:77:LYS:HE3	1.49	0.92
1:A:77:LYS:HG2	1:A:108:LEU:HB2	1.56	0.87
1:B:215:PRO:HD2	2:B:330:NAP:H4B	1.56	0.87
1:A:3:ARG:HG2	1:A:11:LYS:HB3	1.66	0.76
1:A:158:ILE:HG13	1:A:182:ASN:ND2	2.03	0.74
1:A:116:LYS:HD2	1:A:131:VAL:HG11	1.70	0.74
1:A:28:THR:O	1:A:32:LYS:HD3	1.89	0.72
1:A:130:VAL:HG11	1:A:303:CYS:SG	2.29	0.72
1:A:251:PHE:HB3	1:A:252:PRO:HD3	1.71	0.71
1:A:189:TYR:HE1	1:A:225:PRO:HB2	1.54	0.71
1:B:262:LYS:O	2:B:330:NAP:H8A	1.91	0.70
1:A:4:LEU:O	1:A:11:LYS:HA	1.90	0.70
1:A:183:GLN:OE1	2:A:320:NAP:H2N	1.92	0.69
1:B:163:HIS:HB2	1:B:198:TYR:CD2	2.29	0.68
1:A:32:LYS:HG2	1:A:61:LYS:HD3	1.76	0.68
1:B:96:LEU:HD23	1:B:104:LEU:HD13	1.75	0.67
1:B:115:PHE:O	1:B:133:SER:HB2	1.97	0.65
1:A:124:LEU:HD22	1:A:128:GLY:O	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:215:PRO:HG2	2:A:320:NAP:H4B	1.79	0.64
1:A:228:LEU:HA	1:A:244:THR:HG21	1.78	0.64
1:B:221:LYS:HE3	1:B:223:GLU:OE2	1.97	0.63
1:B:215:PRO:HD2	2:B:330:NAP:C4B	2.27	0.63
1:A:79:TRP:HD1	1:A:81:THR:HG1	1.45	0.62
1:B:7:ASN:HB2	4:B:418:HOH:O	1.98	0.62
1:A:240:HIS:O	1:A:242:LYS:HG2	1.99	0.62
1:A:13:PRO:HB2	1:A:41:HIS:HB2	1.82	0.62
1:B:56:VAL:O	1:B:60:GLU:HG3	2.00	0.61
1:A:242:LYS:HE2	1:A:278:PHE:CD1	2.37	0.60
1:A:158:ILE:HG13	1:A:182:ASN:HD22	1.65	0.60
1:A:213:GLY:O	1:A:297:VAL:HG21	2.02	0.60
1:A:189:TYR:CE1	1:A:225:PRO:HB2	2.34	0.59
1:B:59:GLN:HG2	1:B:63:ARG:NH1	2.17	0.59
1:A:31:VAL:HG21	1:A:54:VAL:HG13	1.85	0.59
1:A:307:LYS:H	1:A:307:LYS:HD3	1.68	0.59
1:B:67:VAL:HG11	1:B:72:LEU:HG	1.86	0.57
1:B:84:GLU:H	1:B:84:GLU:CD	2.08	0.57
1:B:185:GLU:OE1	1:B:297:VAL:HB	2.05	0.56
1:B:229:GLU:HA	1:B:234:LYS:NZ	2.19	0.56
1:B:23:PRO:HG2	1:B:26:GLN:HB2	1.87	0.56
1:B:77:LYS:HG2	1:B:108:LEU:HB2	1.88	0.56
1:A:271:GLU:HA	1:A:274:LYS:CE	2.30	0.56
1:A:136:ASN:O	1:A:139:ASP:HB2	2.06	0.56
1:A:307:LYS:H	1:A:307:LYS:CD	2.19	0.56
1:A:138:LEU:H	1:A:138:LEU:HD22	1.70	0.56
1:A:130:VAL:CG1	1:A:303:CYS:SG	2.93	0.55
1:A:89:LYS:HD3	1:A:93:GLN:HE22	1.70	0.55
1:B:164:LEU:HD12	1:B:313:GLU:HG3	1.88	0.55
1:A:106:LEU:HD21	1:A:181:VAL:HB	1.89	0.55
1:B:3:ARG:HG2	1:B:13:PRO:HA	1.87	0.55
1:B:252:PRO:HG2	1:B:259:VAL:CG2	2.37	0.55
1:A:7:ASN:C	1:A:7:ASN:HD22	2.10	0.55
2:A:320:NAP:H3D	2:A:320:NAP:H6N	1.89	0.54
1:A:172:LYS:HB3	1:A:175:LEU:HD13	1.89	0.54
1:B:21:LYS:HB2	1:B:21:LYS:NZ	2.23	0.54
1:B:67:VAL:HG13	1:B:71:GLU:HB2	1.88	0.54
1:A:146:GLU:O	1:A:150:GLU:HB2	2.07	0.54
1:A:266:PRO:HG2	1:A:267:GLU:OE2	2.07	0.54
1:A:32:LYS:CG	1:A:61:LYS:HD3	2.37	0.53
1:A:262:LYS:O	2:A:320:NAP:H8A	2.08	0.53
1:A:262:LYS:HB2	2:A:320:NAP:O3D	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:183:GLN:OE1	2:B:330:NAP:H2N	2.08	0.53
1:A:89:LYS:CD	1:A:93:GLN:HE22	2.22	0.52
1:B:94:LYS:HZ3	1:B:94:LYS:HB3	1.74	0.52
1:A:132:PRO:HB3	1:A:306:HIS:CD2	2.44	0.52
1:A:272:ASN:HD21	2:A:320:NAP:H61A	1.56	0.52
1:B:242:LYS:HE3	1:B:278:PHE:CD1	2.44	0.51
1:A:96:LEU:HD21	1:A:104:LEU:HG	1.92	0.51
1:B:27:VAL:O	1:B:31:VAL:HG23	2.09	0.51
1:A:231:PRO:HA	1:A:234:LYS:HE2	1.91	0.51
1:A:45:ALA:HB3	1:A:48:TYR:CD1	2.46	0.51
1:A:172:LYS:HD3	1:A:175:LEU:HD12	1.92	0.51
1:B:196:ILE:O	1:B:200:GLN:HG3	2.10	0.51
1:B:20:TRP:O	1:B:21:LYS:HB2	2.10	0.51
1:A:162:ASN:OD1	1:A:165:GLN:HG3	2.10	0.51
1:B:189:TYR:HD1	1:B:295:TRP:CE3	2.27	0.51
1:B:232:ARG:NH2	1:B:291:TYR:CD1	2.79	0.51
1:B:252:PRO:HG2	1:B:259:VAL:HG22	1.93	0.50
1:B:277:ASP:O	1:B:278:PHE:HB3	2.11	0.50
1:A:44:CYS:O	1:A:76:SER:HA	2.12	0.49
1:B:217:ARG:CD	1:B:297:VAL:HG13	2.42	0.49
1:A:210:SER:N	1:A:211:PRO:CD	2.76	0.48
1:A:190:LEU:HA	1:A:292:ASN:HD22	1.78	0.48
1:B:217:ARG:HD3	1:B:297:VAL:HG13	1.95	0.48
1:A:92:CYS:SG	1:A:147:LEU:HD13	2.53	0.48
1:B:112:PRO:HG3	1:B:310:PRO:HB3	1.96	0.48
1:A:89:LYS:HD3	1:A:93:GLN:NE2	2.29	0.47
1:B:196:ILE:HD12	1:B:255:ARG:NH2	2.29	0.47
1:B:126:GLU:N	1:B:126:GLU:CD	2.66	0.47
1:A:272:ASN:ND2	2:A:320:NAP:H61A	2.13	0.47
1:A:57:ALA:O	1:A:61:LYS:HG2	2.15	0.47
1:B:40:ARG:NH1	1:B:67:VAL:HG22	2.30	0.47
1:B:243:THR:OG1	1:B:246:GLN:HG3	2.14	0.47
1:B:187:HIS:HB2	1:B:227:LEU:HD11	1.96	0.47
1:B:229:GLU:HA	1:B:234:LYS:HZ1	1.80	0.47
1:A:78:LEU:HD11	1:A:82:TYR:HB2	1.96	0.47
1:B:141:TRP:O	1:B:145:GLU:HG3	2.14	0.46
1:B:84:GLU:HG3	1:B:135:THR:CG2	2.45	0.46
1:A:20:TRP:O	1:A:21:LYS:HB2	2.15	0.46
1:B:158:ILE:HD12	1:B:166:VAL:HG22	1.97	0.46
1:A:260:ILE:O	2:A:320:NAP:H51N	2.16	0.46
1:B:98:ASP:O	1:B:100:LYS:HD2	2.15	0.46
1:B:210:SER:N	1:B:211:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:20:TRP:CE3	1:B:21:LYS:HE3	2.50	0.46
1:A:186:CYS:HB3	1:A:208:ALA:HB1	1.98	0.46
1:B:209:TYR:HB2	2:B:330:NAP:O4D	2.16	0.45
1:A:3:ARG:HG2	1:A:11:LYS:CB	2.43	0.45
1:A:232:ARG:HB3	1:A:291:TYR:OH	2.16	0.45
1:B:268:ARG:HD3	2:B:330:NAP:C5A	2.47	0.45
1:A:69:ARG:HE	1:A:101:LEU:HD22	1.82	0.45
1:B:85:LYS:HG2	1:B:143:ALA:HB2	1.97	0.45
1:A:103:TYR:CD2	1:A:154:LYS:HE3	2.51	0.45
1:A:185:GLU:O	1:A:192:GLN:HG3	2.16	0.45
1:A:122:PHE:O	1:A:124:LEU:HG	2.17	0.44
1:A:260:ILE:HG13	1:A:260:ILE:O	2.18	0.44
1:A:132:PRO:HB3	1:A:306:HIS:NE2	2.32	0.44
1:A:190:LEU:HA	1:A:292:ASN:ND2	2.33	0.44
1:A:45:ALA:HB2	1:A:77:LYS:HE3	1.99	0.44
1:A:231:PRO:HA	1:A:234:LYS:CE	2.48	0.44
1:B:63:ARG:HH11	1:B:63:ARG:HG3	1.82	0.44
1:B:230:ASP:OD1	1:B:232:ARG:HD3	2.17	0.44
1:A:84:GLU:HG3	1:A:117:PRO:HG3	1.98	0.44
1:B:181:VAL:HG12	1:B:182:ASN:N	2.33	0.44
1:A:240:HIS:C	1:A:242:LYS:H	2.21	0.44
1:B:181:VAL:HA	1:B:205:VAL:O	2.18	0.43
1:A:249:ILE:HG22	1:A:253:MET:HE3	1.98	0.43
1:A:49:GLN:HE21	1:A:49:GLN:HB2	1.66	0.43
1:B:163:HIS:HB2	1:B:198:TYR:CE2	2.52	0.43
1:B:62:LEU:HD23	1:B:67:VAL:O	2.18	0.43
1:B:6:LEU:HD21	1:B:12:MET:SD	2.58	0.43
1:A:22:SER:HB3	1:A:264:VAL:CG1	2.48	0.43
1:A:197:GLN:HB2	1:A:197:GLN:HE21	1.59	0.43
1:B:23:PRO:HA	1:B:24:PRO:HD3	1.75	0.43
1:A:198:TYR:O	1:A:201:SER:HB2	2.19	0.43
2:A:320:NAP:C4N	3:A:340:FID:C2I	2.97	0.43
1:B:163:HIS:ND1	1:B:315:PHE:O	2.52	0.42
1:B:7:ASN:OD1	1:B:7:ASN:N	2.52	0.42
1:A:103:TYR:HA	1:A:152:LEU:O	2.19	0.42
1:B:15:LEU:HD12	1:B:259:VAL:HB	2.00	0.42
1:A:75:VAL:HG13	1:A:106:LEU:O	2.19	0.42
1:B:69:ARG:NE	1:B:101:LEU:HD22	2.35	0.42
1:B:146:GLU:O	1:B:150:GLU:HG3	2.20	0.42
1:A:95:THR:HG21	1:A:104:LEU:HD11	2.01	0.42
1:A:74:ILE:HG21	1:A:101:LEU:HD11	2.00	0.42
1:B:134:ASP:CG	1:B:135:THR:N	2.73	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:262:LYS:HD3	1:A:262:LYS:C	2.41	0.41
1:B:217:ARG:HD2	1:B:219:TRP:HE1	1.85	0.41
1:B:158:ILE:O	1:B:182:ASN:HA	2.20	0.41
1:A:5:LEU:HD12	1:A:10:ALA:O	2.20	0.41
1:A:217:ARG:HA	1:A:218:PRO:HD3	1.86	0.41
1:A:293:ARG:HG3	1:A:295:TRP:HB2	2.02	0.41
1:B:67:VAL:HG11	1:B:72:LEU:CG	2.49	0.41
1:A:77:LYS:HD3	1:A:108:LEU:HD12	2.03	0.41
2:A:320:NAP:C5N	3:A:340:FID:O3I	2.69	0.41
1:A:190:LEU:CA	1:A:292:ASN:HD22	2.34	0.41
1:A:27:VAL:HG11	1:A:50:ASN:HB2	2.03	0.41
1:A:271:GLU:CA	1:A:274:LYS:HE2	2.35	0.41
1:B:265:THR:HB	1:B:268:ARG:HB2	2.03	0.41
1:A:186:CYS:HB3	1:A:208:ALA:CB	2.51	0.41
1:B:204:ILE:N	1:B:204:ILE:HD12	2.36	0.41
1:B:252:PRO:HG2	1:B:259:VAL:HG21	2.02	0.41
1:B:16:GLY:HA2	1:B:41:HIS:HB3	2.02	0.41
1:A:284:ASP:O	1:A:287:THR:HB	2.21	0.41
1:B:255:ARG:O	1:B:256:ASN:HB2	2.20	0.40
1:A:80:CYS:SG	1:A:111:TRP:HB2	2.61	0.40
1:A:139:ASP:O	1:A:142:ALA:HB3	2.22	0.40
1:A:270:ALA:O	1:A:274:LYS:HG3	2.21	0.40
1:B:217:ARG:HD2	1:B:219:TRP:NE1	2.36	0.40
1:B:80:CYS:SG	1:B:111:TRP:HB2	2.61	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	313/315 (99%)	290 (93%)	22 (7%)	1 (0%)	50	84
1	B	313/315 (99%)	288 (92%)	23 (7%)	2 (1%)	33	72
All	All	626/630 (99%)	578 (92%)	45 (7%)	3 (0%)	38	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	B	80	CYS
1	B	85	LYS

### 5.3.2 Protein sidechains ⓘ

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	279/280 (100%)	261 (94%)	18 (6%)	24	57
1	B	279/280 (100%)	264 (95%)	15 (5%)	31	66
All	All	558/560 (100%)	525 (94%)	33 (6%)	28	62

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	41	HIS
1	A	62	LEU
1	A	65	GLN
1	A	70	GLU
1	A	84	GLU
1	A	93	GLN
1	A	102	ASP
1	A	150	GLU
1	A	179	PRO
1	A	181	VAL
1	A	197	GLN
1	A	229	GLU
1	A	257	LEU
1	A	258	VAL
1	A	264	VAL
1	A	283	GLN
1	A	307	LYS
1	B	7	ASN
1	B	32	LYS
1	B	40	ARG

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Mol	Chain	Res	Type
1	B	41	HIS
1	B	83	HIS
1	B	94	LYS
1	B	104	LEU
1	B	126	GLU
1	B	130	VAL
1	B	134	ASP
1	B	170	LEU
1	B	188	PRO
1	B	193	GLU
1	B	197	GLN
1	B	307	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	93	GLN
1	A	182	ASN
1	A	187	HIS
1	A	197	GLN
1	A	272	ASN
1	A	292	ASN
1	B	83	HIS
1	B	182	ASN
1	B	197	GLN
1	B	292	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	320	-	52,52,52	1.51	11 (21%)	80,80,80	1.32	10 (12%)
3	FID	A	340	-	22,22,22	1.39	2 (9%)	34,34,34	1.31	2 (5%)
2	NAP	B	330	-	52,52,52	1.55	11 (21%)	80,80,80	1.29	9 (11%)
3	FID	B	350	-	22,22,22	1.19	2 (9%)	34,34,34	1.50	2 (5%)

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	320	-	-	0/35/67/67	0/3/5/5
3	FID	A	340	-	-	0/4/34/34	0/1/3/3
2	NAP	B	330	-	-	0/35/67/67	0/3/5/5
3	FID	B	350	-	-	0/4/34/34	0/1/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	330	NAP	C3N-C7N	-3.86	1.43	1.50
2	B	330	NAP	C2N-N1N	3.80	1.40	1.35
2	A	320	NAP	C2N-C3N	3.73	1.44	1.38
2	B	330	NAP	C2N-C3N	3.61	1.44	1.38
3	A	340	FID	C2I-N4	-3.44	1.32	1.39
2	A	320	NAP	C3N-C7N	-3.36	1.44	1.50
2	A	320	NAP	C2N-N1N	3.30	1.39	1.35
2	A	320	NAP	PA-O2A	-2.94	1.41	1.55
2	B	330	NAP	P2B-O3X	-2.86	1.44	1.54
3	A	340	FID	C8I-C9	2.85	1.57	1.52
3	B	350	FID	C2I-N4	-2.79	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	330	NAP	P2B-O2X	-2.68	1.44	1.54
2	A	320	NAP	C2D-C1D	2.56	1.57	1.53
2	B	330	NAP	C8A-N7A	-2.47	1.29	1.34
2	A	320	NAP	P2B-O3X	-2.44	1.45	1.54
2	B	330	NAP	C5A-C4A	-2.40	1.35	1.40
2	A	320	NAP	P2B-O2X	-2.33	1.46	1.54
2	B	330	NAP	C2B-C1B	-2.29	1.48	1.52
2	A	320	NAP	PN-O2N	2.28	1.54	1.48
2	B	330	NAP	C2D-C1D	2.27	1.56	1.53
3	B	350	FID	C8I-C9	2.27	1.56	1.52
2	B	330	NAP	PA-O2A	-2.26	1.44	1.55
2	A	320	NAP	C8A-N7A	-2.26	1.30	1.34
2	A	320	NAP	C5A-C4A	-2.23	1.35	1.40
2	B	330	NAP	C3B-C4B	-2.15	1.47	1.53
2	A	320	NAP	C8A-N9A	2.13	1.39	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	350	FID	C7I-N1I-C2I	-6.22	109.99	113.38
3	A	340	FID	C7I-N1I-C2I	-4.71	110.81	113.38
2	A	320	NAP	N3A-C2A-N1A	-4.09	125.29	128.71
2	A	320	NAP	O7N-C7N-N7N	-3.94	116.91	122.59
3	B	350	FID	N4-C2I-N1I	3.45	111.47	107.64
2	B	330	NAP	O7N-C7N-N7N	-3.36	117.74	122.59
2	B	330	NAP	N3A-C2A-N1A	-3.18	126.05	128.71
2	B	330	NAP	O4B-C1B-C2B	-3.08	104.07	106.95
2	A	320	NAP	O4B-C1B-C2B	-2.91	104.23	106.95
2	A	320	NAP	C2D-C1D-N1N	-2.77	109.17	113.86
3	A	340	FID	N4-C2I-N1I	2.75	110.69	107.64
2	B	330	NAP	O7N-C7N-C3N	2.67	122.59	119.58
2	A	320	NAP	O2X-P2B-O2B	-2.60	99.60	107.09
2	B	330	NAP	O3-PN-O5D	2.57	111.66	101.36
2	A	320	NAP	C3N-C7N-N7N	2.47	120.59	117.77
2	A	320	NAP	C8A-N9A-C4A	-2.47	105.02	106.90
2	A	320	NAP	O7N-C7N-C3N	2.36	122.24	119.58
2	B	330	NAP	O2X-P2B-O2B	-2.34	100.34	107.09
2	A	320	NAP	C4A-C5A-N7A	2.15	111.36	109.52
2	B	330	NAP	C8A-N9A-C4A	-2.13	105.28	106.90
2	B	330	NAP	O3B-C3B-C4B	-2.10	104.89	111.08
2	B	330	NAP	C3N-C2N-N1N	-2.05	116.90	120.36
2	A	320	NAP	O3-PN-O5D	2.02	109.48	101.36



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	315/315 (100%)	-0.31	4 (1%) 74 75	5, 5, 5, 5	0
1	B	315/315 (100%)	-0.38	3 (0%) 79 79	5, 5, 5, 5	0
All	All	630/630 (100%)	-0.34	7 (1%) 74 78	5, 5, 5, 5	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	ASN	4.0
1	A	283	GLN	2.8
1	A	128	GLY	2.6
1	A	126	GLU	2.5
1	B	134	ASP	2.4
1	B	260	ILE	2.0
1	B	198	TYR	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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	B	330	48/48	0.14	-0.55	4,4,4,4	0
3	FID	B	350	20/20	0.13	-	4,4,4,4	0
3	FID	A	340	20/20	0.12	-	4,4,4,4	0
2	NAP	A	320	48/48	0.12	-	4,4,4,4	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.