



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:33 PM GMT

PDB ID : 3BCX
Title : E1 Dehydrase
Authors : Tsai, S-C.; Smith, P.
Deposited on : 2007-11-13
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

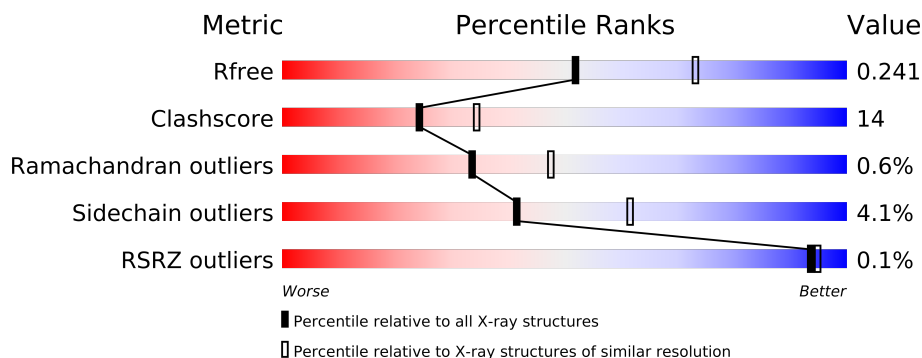
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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))
R_{free}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. 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	437	<div><div></div><div></div></div>
1	B	437	<div><div></div><div></div></div>

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	BEN	A	502[A]	-	X
3	BEN	A	503[B]	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6771 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 CDP-6-deoxy-L-threo-D-glycero-4-hexulose-3-dehydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3284	2108	535	628	13			
1	B	419	Total	C	N	O	S	0	0	0
			3266	2096	533	625	12			

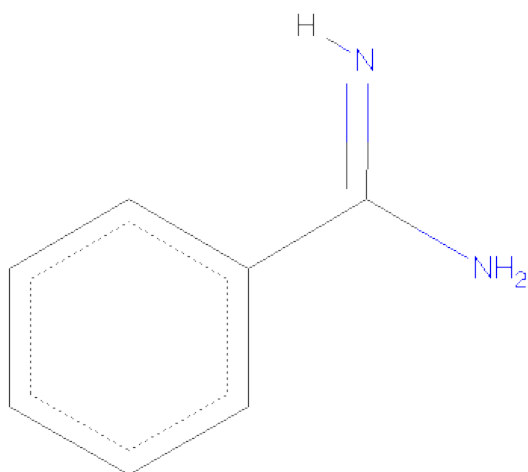
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	ARG	PRO	SEE REMARK 999	UNP Q57174
B	305	ARG	PRO	SEE REMARK 999	UNP Q57174

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			9	7	2		
3	A	1	Total	C	N	0	1
			9	7	2		
3	A	1	Total	C	N	0	1
			9	7	2		

- Molecule 4 is water.

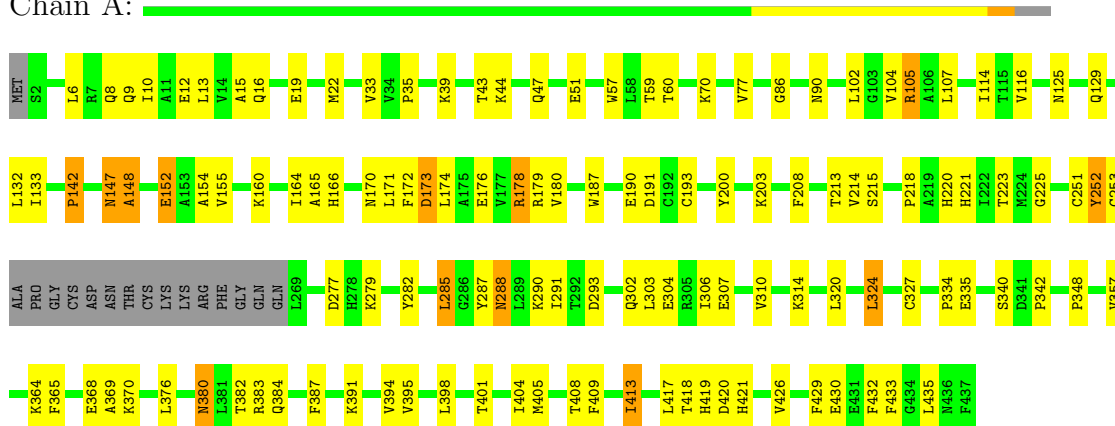
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		
4	B	92	Total	O	0	0
			92	92		

3 Residue-property plots

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.

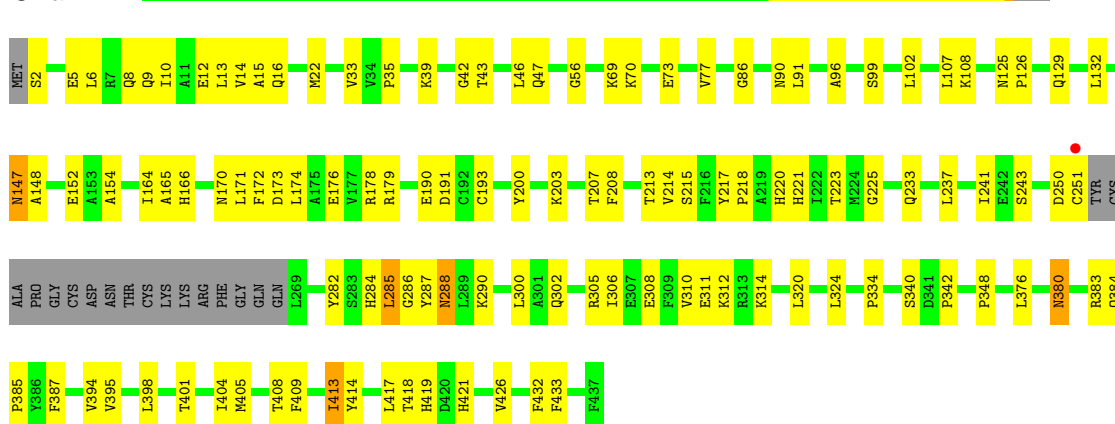
- Molecule 1: CDP-6-deoxy-L-threo-D-glycero-4-hexulose-3-dehydrase

Chain A:



- Molecule 1: CDP-6-deoxy-L-threo-D-glycero-4-hexulose-3-dehydrase

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	97.31Å 97.31Å 142.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.40 48.66 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.40) 98.5 (48.66-2.38)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.231 0.219 , 0.241	Depositor DCC
R_{free} test set	5719 reflections (9.79%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.3	EDS
Estimated twinning fraction	0.014 for -h,-k,l 0.447 for h,-h-k,-l 0.014 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 119744 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6771	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: BEN, FE

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	0.35	0/3359	0.59	0/4558
1	B	0.36	0/3340	0.59	0/4532
All	All	0.36	0/6699	0.59	0/9090

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	LEU	Peptide
1	B	285	LEU	Peptide

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	3284	0	3229	106	0
1	B	3266	0	3215	94	0
2	A	1	0	0	0	0
3	A	18	0	16	2	0
3	B	9	0	8	2	0
4	A	101	0	0	15	0
4	B	92	0	0	6	0
All	All	6771	0	6468	184	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 14.

All (184) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:430:GLU:HA	4:A:589:HOH:O	1.66	0.95
1:B:171:LEU:HD13	1:B:340:SER:HB2	1.59	0.85
1:A:171:LEU:HD13	1:A:340:SER:HB2	1.63	0.81
1:A:164:ILE:HG12	4:A:578:HOH:O	1.83	0.79
1:A:287:TYR:HB3	4:A:506:HOH:O	1.82	0.78
1:A:171:LEU:HD22	1:A:200:TYR:HB2	1.66	0.78
1:A:435:LEU:HD12	4:A:589:HOH:O	1.84	0.76
1:A:223:THR:H	1:A:302:GLN:HE21	1.31	0.76
1:B:223:THR:H	1:B:302:GLN:HE21	1.34	0.76
1:B:171:LEU:HD22	1:B:200:TYR:HB2	1.66	0.75
1:A:324:LEU:HD13	1:A:426:VAL:HG22	1.70	0.74
1:A:174:LEU:O	1:A:178:ARG:HB2	1.90	0.72
1:B:203:LYS:HE2	1:B:207:THR:OG1	1.90	0.71
1:B:10:ILE:O	1:B:14:VAL:HG13	1.91	0.71
1:B:380:ASN:HD22	1:B:380:ASN:C	1.93	0.70
1:A:327:CYS:SG	4:A:589:HOH:O	2.49	0.70
1:B:418:THR:H	1:B:421:HIS:HD2	1.40	0.70
1:A:418:THR:H	1:A:421:HIS:CD2	2.10	0.69
1:A:114:ILE:HD11	4:A:574:HOH:O	1.93	0.69
1:B:174:LEU:O	1:B:178:ARG:HG2	1.94	0.68
1:A:116:VAL:HG22	4:A:578:HOH:O	1.94	0.67
1:A:418:THR:H	1:A:421:HIS:HD2	1.40	0.66
1:B:166:HIS:HD2	1:B:172:PHE:H	1.43	0.66
1:A:193:CYS:O	1:A:220:HIS:HD2	1.78	0.66
1:A:166:HIS:HD2	1:A:172:PHE:H	1.43	0.66
1:B:418:THR:H	1:B:421:HIS:CD2	2.14	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:9:GLN:HG2	1:B:13:LEU:HD13	1.76	0.66
1:A:380:ASN:HD22	1:A:380:ASN:C	2.00	0.64
1:A:15:ALA:HA	1:A:43:THR:HG23	1.79	0.64
1:A:282:TYR:H	1:B:384:GLN:NE2	1.96	0.64
1:A:365:PHE:CE2	1:A:432:PHE:HB2	2.34	0.63
1:A:252:TYR:O	1:A:253:CYS:SG	2.56	0.63
1:A:154:ALA:HA	1:A:395:VAL:HG21	1.82	0.62
1:B:287:TYR:HB3	4:B:504:HOH:O	2.00	0.62
1:B:8:GLN:O	1:B:12:GLU:HG2	2.00	0.62
1:A:429:PHE:O	1:A:433:PHE:HD2	1.84	0.61
1:B:433:PHE:HA	3:B:502:BEN:C3	2.31	0.61
1:A:104:VAL:HG12	3:A:502[A]:BEN:H5	1.83	0.61
1:A:105:ARG:HG3	1:A:187:TRP:NE1	2.16	0.60
1:B:170:ASN:HA	1:B:342:PRO:HB3	1.83	0.59
1:A:8:GLN:O	1:A:12:GLU:HG2	2.03	0.59
1:A:384:GLN:NE2	1:B:282:TYR:H	2.01	0.59
1:A:166:HIS:HE1	1:A:190:GLU:OE2	1.85	0.59
1:A:105:ARG:HG3	1:A:187:TRP:HE1	1.68	0.58
1:A:105:ARG:O	1:A:105:ARG:HG3	2.04	0.58
1:B:193:CYS:O	1:B:220:HIS:HD2	1.87	0.58
1:B:237:LEU:O	1:B:241:ILE:HG12	2.04	0.57
1:A:51:GLU:HG2	4:A:601:HOH:O	2.03	0.57
1:A:15:ALA:O	1:A:19:GLU:HG2	2.04	0.57
1:B:218:PRO:HD3	1:B:225:GLY:O	2.05	0.57
1:A:6:LEU:O	1:A:10:ILE:HG13	2.05	0.56
1:B:6:LEU:O	1:B:10:ILE:HG13	2.05	0.56
1:A:334:PRO:HB3	1:A:348:PRO:HG2	1.87	0.56
1:B:432:PHE:O	3:B:502:BEN:H3	2.05	0.56
1:A:164:ILE:HB	4:A:579:HOH:O	2.06	0.56
1:A:164:ILE:HD12	4:A:579:HOH:O	2.05	0.56
1:B:69:LYS:O	1:B:73:GLU:HG3	2.06	0.55
1:B:77:VAL:HA	4:B:576:HOH:O	2.06	0.54
1:B:203:LYS:HB3	1:B:208:PHE:CZ	2.42	0.54
1:A:176:GLU:O	1:A:180:VAL:HG23	2.07	0.54
1:B:166:HIS:HE1	1:B:190:GLU:OE2	1.91	0.54
1:A:310:VAL:HG12	1:A:314:LYS:HE3	1.90	0.54
1:A:218:PRO:HD3	1:A:225:GLY:O	2.09	0.52
1:A:285:LEU:HD21	1:B:129:GLN:CG	2.40	0.52
1:B:164:ILE:HG13	1:B:172:PHE:CE2	2.44	0.52
1:A:376:LEU:HD23	1:A:404:ILE:HG21	1.91	0.51
1:B:250:ASP:O	1:B:251:CYS:CB	2.58	0.51
1:A:252:TYR:O	1:A:253:CYS:CB	2.58	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:324:LEU:HD13	1:B:426:VAL:HG22	1.92	0.51
1:A:10:ILE:HD13	1:B:14:VAL:HG12	1.93	0.51
1:A:6:LEU:HD21	1:B:16:GLN:NE2	2.26	0.51
1:A:39:LYS:HE3	1:B:56:GLY:O	2.11	0.51
1:A:285:LEU:HD21	1:B:129:GLN:HG3	1.92	0.50
1:B:408:THR:HG22	1:B:409:PHE:N	2.27	0.50
1:B:42:GLY:O	1:B:46:LEU:HD13	2.12	0.50
1:B:154:ALA:HA	1:B:395:VAL:HG21	1.93	0.50
1:A:277:ASP:OD1	1:A:279:LYS:HB2	2.11	0.50
1:A:6:LEU:HD11	1:B:16:GLN:HE21	1.75	0.50
1:B:306:ILE:O	1:B:310:VAL:HG23	2.12	0.50
1:B:288:ASN:HD21	1:B:290:LYS:NZ	2.10	0.50
1:A:107:LEU:HG	1:A:132:LEU:HD21	1.94	0.50
1:B:33:VAL:HG23	1:B:35:PRO:HD3	1.93	0.50
1:A:147:ASN:HD22	1:A:147:ASN:C	2.14	0.50
1:A:306:ILE:HG23	1:A:307:GLU:N	2.27	0.49
1:A:142:PRO:HG2	1:A:335:GLU:HB2	1.94	0.49
1:A:77:VAL:HA	4:A:604:HOH:O	2.12	0.49
1:B:380:ASN:C	1:B:380:ASN:ND2	2.63	0.49
1:A:105:ARG:O	1:A:105:ARG:CG	2.60	0.49
1:A:90:ASN:HD22	1:A:213:THR:HG21	1.78	0.49
1:A:44:LYS:HE2	1:A:304:GLU:OE2	2.13	0.49
1:B:376:LEU:HD23	1:B:404:ILE:HG21	1.94	0.49
1:A:408:THR:HG22	1:A:409:PHE:N	2.28	0.49
1:A:166:HIS:CD2	1:A:172:PHE:H	2.28	0.49
1:B:334:PRO:HB3	1:B:348:PRO:HG2	1.95	0.48
1:A:16:GLN:HA	1:A:19:GLU:HG3	1.95	0.48
1:A:282:TYR:H	1:B:384:GLN:HE22	1.60	0.48
1:B:86:GLY:HA3	1:B:215:SER:HB2	1.95	0.48
1:B:91:LEU:HA	1:B:126:PRO:HB3	1.95	0.48
1:A:172:PHE:O	1:A:174:LEU:N	2.47	0.48
1:B:288:ASN:HD21	1:B:290:LYS:HZ2	1.61	0.48
1:A:105:ARG:HA	1:A:160:LYS:NZ	2.28	0.48
1:A:398:LEU:HB3	1:A:401:THR:HB	1.95	0.48
1:A:193:CYS:HA	1:A:214:VAL:HA	1.94	0.47
1:B:243:SER:OG	1:B:284:HIS:HD2	1.97	0.47
1:B:320:LEU:O	1:B:324:LEU:HB2	2.14	0.47
1:A:86:GLY:HA3	1:A:215:SER:HB2	1.95	0.47
1:B:35:PRO:HG2	1:B:414:TYR:OH	2.14	0.47
1:B:165:ALA:HB2	1:B:191:ASP:HB3	1.97	0.47
1:B:193:CYS:HA	1:B:214:VAL:HA	1.97	0.46
1:A:13:LEU:HD11	1:B:9:GLN:HE21	1.81	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:15:ALA:HA	1:B:43:THR:HG23	1.96	0.46
1:A:288:ASN:HD21	1:A:290:LYS:NZ	2.13	0.46
1:B:96:ALA:CB	1:B:241:ILE:HD13	2.46	0.46
1:B:165:ALA:HA	1:B:191:ASP:HB3	1.98	0.46
1:A:102:LEU:O	3:A:502[A]:BEN:H6	2.16	0.46
1:B:384:GLN:NE2	1:B:385:PRO:HD2	2.31	0.46
1:B:99:SER:OG	1:B:284:HIS:HE1	1.98	0.46
1:A:221:HIS:HD2	4:A:511:HOH:O	1.99	0.46
1:B:221:HIS:HD2	4:B:507:HOH:O	1.99	0.46
1:A:364:LYS:O	1:A:368:GLU:HG3	2.16	0.45
1:B:398:LEU:HB3	1:B:401:THR:HB	1.98	0.45
1:B:310:VAL:HG12	1:B:314:LYS:HE3	1.99	0.45
1:A:60:THR:HG23	1:A:291:ILE:O	2.17	0.45
1:A:164:ILE:HG22	1:A:165:ALA:N	2.31	0.45
1:B:96:ALA:HB2	1:B:241:ILE:HD13	1.99	0.45
1:A:152:GLU:OE1	1:A:179:ARG:NH2	2.49	0.45
1:A:148:ALA:HB2	1:A:173:ASP:HB3	1.99	0.45
1:A:223:THR:HG22	1:A:302:GLN:NE2	2.32	0.45
1:A:70:LYS:HB3	1:A:303:LEU:HD13	1.99	0.45
1:B:43:THR:O	1:B:47:GLN:HG3	2.17	0.44
1:A:170:ASN:HA	1:A:342:PRO:HB3	1.99	0.44
1:A:33:VAL:HG23	1:A:35:PRO:HD3	1.99	0.44
1:A:125:ASN:ND2	1:B:286:GLY:H	2.14	0.44
1:B:223:THR:N	1:B:302:GLN:HE21	2.07	0.44
1:B:147:ASN:C	1:B:147:ASN:HD22	2.20	0.44
1:B:152:GLU:OE1	1:B:179:ARG:NH2	2.51	0.44
1:B:77:VAL:HG12	4:B:576:HOH:O	2.16	0.44
1:B:148:ALA:HB1	1:B:176:GLU:CG	2.47	0.44
1:B:2:SER:O	1:B:5:GLU:HB2	2.17	0.44
1:A:288:ASN:HD21	1:A:290:LYS:HZ2	1.66	0.43
1:A:282:TYR:O	1:B:385:PRO:HG2	2.18	0.43
1:A:384:GLN:HE22	1:B:282:TYR:H	1.65	0.43
1:B:193:CYS:O	1:B:220:HIS:CD2	2.70	0.43
1:B:310:VAL:O	1:B:314:LYS:HG3	2.19	0.43
1:B:305:ARG:HH21	1:B:308:GLU:CD	2.22	0.43
1:A:155:VAL:HA	4:A:574:HOH:O	2.17	0.43
1:A:133:ILE:HD12	1:A:391:LYS:HG2	2.00	0.43
1:A:203:LYS:HB3	1:A:208:PHE:CZ	2.54	0.43
1:A:129:GLN:HG3	1:B:285:LEU:HD21	2.01	0.43
1:A:178:ARG:NH1	1:A:178:ARG:HG3	2.33	0.43
1:B:70:LYS:HE2	1:B:300:LEU:HD12	2.01	0.43
1:B:107:LEU:HB3	1:B:132:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:429:PHE:O	1:A:433:PHE:CD2	2.69	0.42
1:B:165:ALA:CB	1:B:191:ASP:HB3	2.49	0.42
1:A:164:ILE:HG23	4:A:578:HOH:O	2.19	0.42
1:A:13:LEU:HD11	1:B:9:GLN:NE2	2.35	0.42
1:A:57:TRP:HD1	1:A:59:THR:O	2.03	0.42
1:A:383:ARG:HD2	1:A:405:MET:SD	2.59	0.42
1:A:165:ALA:HA	1:A:191:ASP:HB3	2.01	0.42
1:B:383:ARG:HD2	1:B:405:MET:SD	2.59	0.42
1:A:320:LEU:O	1:A:324:LEU:HB2	2.20	0.41
1:B:172:PHE:O	1:B:174:LEU:N	2.53	0.41
1:A:43:THR:O	1:A:47:GLN:HG3	2.20	0.41
1:B:413:ILE:C	1:B:413:ILE:HD12	2.41	0.41
1:A:380:ASN:ND2	1:A:380:ASN:C	2.71	0.41
1:A:105:ARG:HA	1:A:160:LYS:HZ2	1.85	0.41
1:B:217:TYR:O	1:B:220:HIS:HB2	2.20	0.41
1:A:369:ALA:O	1:A:370:LYS:HB2	2.20	0.41
1:B:312:LYS:HE3	1:B:312:LYS:HB2	1.92	0.41
1:B:166:HIS:CD2	1:B:171:LEU:HA	2.55	0.41
1:B:126:PRO:HG2	4:B:535:HOH:O	2.21	0.41
1:B:90:ASN:HD22	1:B:213:THR:HG21	1.85	0.41
1:A:404:ILE:HA	1:A:408:THR:OG1	2.20	0.41
1:B:250:ASP:O	1:B:251:CYS:HB3	2.20	0.41
1:B:125:ASN:N	1:B:126:PRO:HD2	2.35	0.41
1:B:165:ALA:CA	1:B:191:ASP:HB3	2.50	0.41
1:A:413:ILE:HD12	1:A:413:ILE:C	2.41	0.41
1:A:171:LEU:N	1:A:171:LEU:HD12	2.36	0.41
1:B:108:LYS:HB3	1:B:108:LYS:HE2	1.84	0.41
1:B:233:GLN:HG2	4:B:576:HOH:O	2.21	0.40
1:A:380:ASN:ND2	1:A:382:THR:OG1	2.54	0.40
1:A:421:HIS:HE1	4:A:596:HOH:O	2.05	0.40
1:A:287:TYR:N	1:A:287:TYR:CD1	2.89	0.40
1:A:147:ASN:C	1:A:147:ASN:ND2	2.74	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	417/437 (95%)	395 (95%)	19 (5%)	3 (1%)	30	43
1	B	415/437 (95%)	397 (96%)	16 (4%)	2 (0%)	38	53
All	All	832/874 (95%)	792 (95%)	35 (4%)	5 (1%)	33	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASP
1	B	173	ASP
1	A	148	ALA
1	A	413	ILE
1	B	413	ILE

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	352/365 (96%)	334 (95%)	18 (5%)	33	50
1	B	350/365 (96%)	339 (97%)	11 (3%)	52	74
All	All	702/730 (96%)	673 (96%)	29 (4%)	41	61

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	105	ARG
1	A	142	PRO
1	A	147	ASN
1	A	152	GLU
1	A	178	ARG
1	A	251	CYS
1	A	252	TYR
1	A	288	ASN
1	A	293	ASP

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Mol	Chain	Res	Type
1	A	324	LEU
1	A	357	VAL
1	A	380	ASN
1	A	387	PHE
1	A	394	VAL
1	A	417	LEU
1	A	419	HIS
1	A	420	ASP
1	B	22	MET
1	B	39	LYS
1	B	102	LEU
1	B	147	ASN
1	B	288	ASN
1	B	311	GLU
1	B	380	ASN
1	B	387	PHE
1	B	394	VAL
1	B	417	LEU
1	B	419	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	8	GLN
1	A	16	GLN
1	A	90	ASN
1	A	130	ASN
1	A	145	ASN
1	A	147	ASN
1	A	166	HIS
1	A	220	HIS
1	A	221	HIS
1	A	284	HIS
1	A	288	ASN
1	A	302	GLN
1	A	316	ASN
1	A	325	GLN
1	A	380	ASN
1	A	384	GLN
1	A	400	ASN
1	A	407	GLN

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Mol	Chain	Res	Type
1	A	421	HIS
1	B	8	GLN
1	B	9	GLN
1	B	16	GLN
1	B	90	ASN
1	B	130	ASN
1	B	145	ASN
1	B	147	ASN
1	B	166	HIS
1	B	220	HIS
1	B	221	HIS
1	B	284	HIS
1	B	288	ASN
1	B	302	GLN
1	B	316	ASN
1	B	325	GLN
1	B	380	ASN
1	B	384	GLN
1	B	400	ASN
1	B	407	GLN
1	B	421	HIS

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 ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	BEN	A	502[A]	-	9,9,9	3.62	8 (88%)	11,11,11	1.05	1 (9%)
3	BEN	A	503[B]	-	9,9,9	3.57	8 (88%)	11,11,11	0.97	1 (9%)
3	BEN	B	502	-	9,9,9	3.58	8 (88%)	11,11,11	0.97	1 (9%)

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	BEN	A	502[A]	-	-	0/4/4/4	0/1/1/1
3	BEN	A	503[B]	-	-	0/4/4/4	0/1/1/1
3	BEN	B	502	-	-	0/4/4/4	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502[A]	BEN	C-N1	6.04	1.46	1.27
3	A	503[B]	BEN	C-N1	6.00	1.46	1.27
3	B	502	BEN	C-N1	5.97	1.46	1.27
3	A	502[A]	BEN	C1-C	4.52	1.53	1.49
3	B	502	BEN	C1-C	4.18	1.53	1.49
3	A	503[B]	BEN	C1-C	4.08	1.53	1.49
3	A	503[B]	BEN	C6-C1	4.07	1.46	1.39
3	A	502[A]	BEN	C2-C1	4.07	1.46	1.39
3	B	502	BEN	C6-C1	4.06	1.46	1.39
3	A	502[A]	BEN	C6-C1	3.98	1.46	1.39
3	A	503[B]	BEN	C2-C1	3.95	1.46	1.39
3	B	502	BEN	C2-C1	3.94	1.46	1.39
3	B	502	BEN	C5-C6	2.99	1.45	1.39
3	A	503[B]	BEN	C5-C6	2.96	1.45	1.39
3	B	502	BEN	C3-C2	2.95	1.45	1.39
3	A	503[B]	BEN	C3-C2	2.92	1.45	1.39
3	A	502[A]	BEN	C3-C2	2.88	1.45	1.39
3	A	502[A]	BEN	C5-C6	2.83	1.45	1.39
3	A	502[A]	BEN	C4-C3	2.51	1.45	1.37
3	B	502	BEN	C5-C4	2.51	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	BEN	C4-C3	2.48	1.45	1.37
3	A	503[B]	BEN	C5-C4	2.47	1.45	1.37
3	A	503[B]	BEN	C4-C3	2.47	1.45	1.37
3	A	502[A]	BEN	C5-C4	2.45	1.45	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502[A]	BEN	C1-C-N2	2.62	122.12	117.99
3	A	503[B]	BEN	C1-C-N2	2.40	121.77	117.99
3	B	502	BEN	C1-C-N2	2.38	121.75	117.99

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, 95th 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	421/437 (96%)	-0.18	0 100 100	20, 46, 77, 99	0
1	B	419/437 (95%)	-0.15	1 (0%) 93 94	28, 47, 76, 98	0
All	All	840/874 (96%)	-0.16	1 (0%) 93 95	20, 47, 77, 99	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	CYS	3.7

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, 95th 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(Å ²)	Q<0.9
3	BEN	A	503[B]	9/9	0.22	4.59	37,39,43,44	9
3	BEN	A	502[A]	9/9	0.18	2.55	47,48,50,52	9

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BEN	B	502	9/9	0.19	1.86	37,39,43,44	0
2	FE	A	501	1/1	0.17	-0.40	127,127,127,127	0

6.5 Other polymers ⓘ

There are no such residues in this entry.