



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:03 PM GMT

PDB ID : 1DTW  
Title : HUMAN BRANCHED-CHAIN ALPHA-KETO ACID DEHYDROGENASE  
Authors : AEvarsson, A.; Chuang, J.L.; Wynn, R.M.; Turley, S.; Chuang, D.T.; Hol, W.G.J.  
Deposited on : 2000-01-13  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

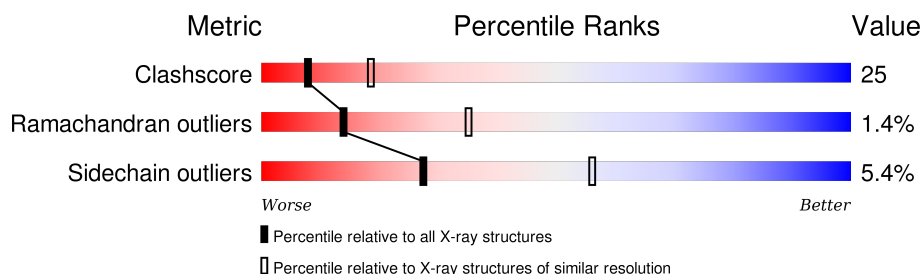
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	400	
2	B	342	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5670 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 BRANCHED-CHAIN ALPHA-KETO ACID DEHYDROGENASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3058	1927	547	568	16			

- Molecule 2 is a protein called BRANCHED-CHAIN ALPHA-KETO ACID DEHYDROGENASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	326	Total	C	N	O	S	0	0	0
			2535	1633	418	469	15			

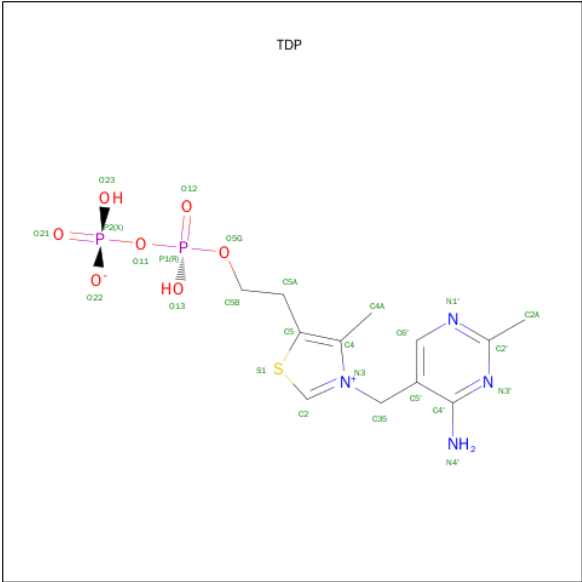
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		

- Molecule 5 is THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	19	Total O 19 19	0	0
6	B	29	Total O 29 29	0	0



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.76 Å   143.76 Å   69.16 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.8 (50.00-2.70)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.224 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, TDP, MG

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	0.41	0/3134	0.62	0/4233
2	B	0.43	0/2599	0.66	0/3532
All	All	0.42	0/5733	0.64	0/7765

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	3058	0	2953	153	0
2	B	2535	0	2509	128	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	26	0	16	3	0
6	A	19	0	0	3	0
6	B	29	0	0	8	0
All	All	5670	0	5478	276	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 25.

All (276) 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)
5:A:403:TDP:H2	5:A:403:TDP:C2	0.97	1.49
1:A:140:LEU:HD22	1:A:140:LEU:H	1.27	0.99
2:B:272:THR:HG22	2:B:274:ARG:H	1.27	0.98
2:B:242:LYS:HA	2:B:247:VAL:H	1.36	0.89
1:A:359:ASN:HD22	1:A:360:PRO:N	1.71	0.89
1:A:78:GLN:HG3	1:A:293:THR:HG21	1.56	0.85
1:A:371:MET:HG3	1:A:375:LEU:HD12	1.59	0.84
2:B:40:THR:CG2	2:B:92:THR:H	1.91	0.82
2:B:33:ASN:HB3	2:B:205:PRO:HG3	1.62	0.81
2:B:339:MET:O	2:B:342:TYR:HB2	1.80	0.81
2:B:139:VAL:HG13	2:B:191:LYS:HG3	1.63	0.79
1:A:38:ASP:OD2	1:A:42:GLN:HB2	1.83	0.78
2:B:22:ASN:H	2:B:25:GLN:NE2	1.82	0.77
2:B:258:ILE:HB	2:B:259:PRO:HD3	1.67	0.75
2:B:242:LYS:HG3	2:B:243:GLU:N	2.00	0.74
2:B:18:THR:HG21	2:B:200:GLU:HB3	1.71	0.73
1:A:198:GLU:HG3	6:A:422:HOH:O	1.89	0.71
2:B:218:GLU:HA	2:B:250:GLU:HG3	1.72	0.71
1:A:357:LYS:N	1:A:357:LYS:HD2	2.05	0.71
2:B:310:VAL:HG12	2:B:327:PRO:HB3	1.74	0.69
1:A:226:ILE:HG13	5:A:403:TDP:H5A2	1.74	0.69
2:B:22:ASN:H	2:B:25:GLN:HE21	1.40	0.68
1:A:80:GLN:OE1	1:A:82:ARG:NH1	2.27	0.67
1:A:168:ILE:HB	1:A:169:PRO:HD3	1.76	0.67
1:A:359:ASN:HD22	1:A:360:PRO:CD	2.07	0.67
2:B:139:VAL:CG1	2:B:191:LYS:HG3	2.25	0.67
2:B:18:THR:HG22	2:B:200:GLU:OE2	1.93	0.67
1:A:37:MET:HE2	1:A:318:ARG:HB3	1.75	0.67
2:B:77:GLN:HG2	6:B:346:HOH:O	1.93	0.66
1:A:140:LEU:CD2	1:A:140:LEU:H	2.07	0.66
1:A:37:MET:CE	1:A:318:ARG:HB3	2.26	0.66
1:A:267:GLU:OE1	1:A:271:ARG:HD2	1.96	0.66
1:A:359:ASN:C	1:A:359:ASN:HD22	1.96	0.66
1:A:82:ARG:HD3	1:A:353:GLU:OE2	1.94	0.65
2:B:46:GLU:HG3	6:B:365:HOH:O	1.94	0.65
1:A:152:CYS:SG	1:A:155:ARG:HG2	2.38	0.64
1:A:96:HIS:CE1	1:A:115:GLU:HA	2.32	0.64
1:A:269:ARG:O	1:A:273:VAL:HG23	1.98	0.63
2:B:23:LEU:HB3	2:B:194:TYR:HA	1.81	0.63
1:A:363:LEU:HD12	1:A:363:LEU:C	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:SER:HB2	2:B:310:VAL:O	1.99	0.63
1:A:358:PRO:HB3	1:A:362:LEU:HD12	1.79	0.62
1:A:177:ALA:HB1	2:B:89:THR:HG21	1.82	0.62
1:A:60:LEU:HD22	1:A:97:VAL:HG12	1.81	0.62
1:A:164:LEU:HD13	5:A:403:TDP:N4'	2.15	0.61
1:A:112:GLN:HE22	1:A:192:GLY:H	1.49	0.61
1:A:147:PRO:O	1:A:148:VAL:HB	2.00	0.61
2:B:40:THR:HG23	2:B:92:THR:H	1.65	0.61
1:A:113:TYR:HA	1:A:160:ILE:HD13	1.82	0.61
2:B:19:GLN:HB2	2:B:203:ILE:HD11	1.83	0.60
1:A:82:ARG:HH11	1:A:82:ARG:HG3	1.66	0.60
1:A:110:PHE:CZ	1:A:158:VAL:HG21	2.37	0.59
2:B:240:MET:HE1	2:B:329:LYS:HD2	1.85	0.59
1:A:60:LEU:HA	1:A:97:VAL:HG11	1.83	0.59
1:A:193:GLU:HB3	1:A:221:ASN:HA	1.84	0.59
1:A:40:GLN:O	1:A:42:GLN:HG2	2.03	0.59
2:B:163:VAL:HG21	2:B:210:LEU:HD22	1.84	0.59
1:A:112:GLN:NE2	1:A:192:GLY:H	1.99	0.59
2:B:30:ALA:HB2	2:B:172:LYS:HG3	1.84	0.58
2:B:86:ILE:O	2:B:89:THR:HB	2.04	0.58
1:A:329:TRP:HE1	1:A:334:GLU:HB2	1.68	0.58
2:B:247:VAL:HG21	2:B:340:ILE:HD13	1.85	0.57
1:A:234:TYR:CE1	1:A:238:GLY:HA2	2.39	0.57
2:B:41:ALA:HA	2:B:92:THR:HB	1.86	0.57
2:B:222:VAL:HA	2:B:272:THR:CG2	2.35	0.57
1:A:371:MET:CG	1:A:375:LEU:HD12	2.33	0.57
1:A:73:ILE:HD12	1:A:345:VAL:CG1	2.34	0.57
1:A:140:LEU:HD22	1:A:140:LEU:N	2.10	0.57
2:B:339:MET:HE2	6:B:347:HOH:O	2.04	0.56
1:A:104:ASP:OD2	1:A:106:THR:HG22	2.05	0.56
2:B:240:MET:CE	2:B:329:LYS:HB2	2.35	0.56
2:B:258:ILE:CB	2:B:259:PRO:HD3	2.35	0.56
1:A:222:ASN:ND2	1:A:287:ARG:HB2	2.21	0.56
2:B:38:ASP:OD2	2:B:40:THR:HG22	2.05	0.56
2:B:198:ALA:O	2:B:199:GLU:HB3	2.06	0.56
2:B:340:ILE:C	2:B:342:TYR:H	2.08	0.56
1:A:314:HIS:ND1	1:A:315:PRO:HD2	2.21	0.56
1:A:226:ILE:HG12	1:A:291:HIS:CD2	2.42	0.55
1:A:7:PRO:HA	1:A:16:PHE:CZ	2.41	0.55
1:A:136:ASN:HD22	1:A:136:ASN:C	2.10	0.55
2:B:242:LYS:CG	2:B:243:GLU:N	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:PRO:HG3	1:A:276:ASN:OD1	2.07	0.55
1:A:62:LYS:O	1:A:66:LEU:HB2	2.06	0.54
2:B:136:TRP:HE1	2:B:151:GLU:HG2	1.72	0.54
2:B:136:TRP:CE3	2:B:190:PRO:HG3	2.42	0.54
1:A:370:GLU:HB3	6:A:418:HOH:O	2.07	0.54
1:A:351:GLN:O	1:A:355:LYS:HG3	2.08	0.53
2:B:33:ASN:HD21	2:B:172:LYS:HZ1	1.56	0.53
2:B:270:ILE:HG23	2:B:302:ASN:OD1	2.09	0.53
2:B:99:PHE:HB2	2:B:102:TYR:CD1	2.43	0.53
1:A:346:MET:O	1:A:350:GLU:HG3	2.09	0.53
1:A:359:ASN:C	1:A:359:ASN:ND2	2.62	0.53
1:A:125:PRO:HD3	1:A:155:ARG:NH2	2.24	0.53
1:A:73:ILE:HD12	1:A:345:VAL:HG11	1.89	0.53
2:B:247:VAL:HG11	2:B:340:ILE:HD11	1.91	0.53
2:B:258:ILE:O	2:B:260:TRP:N	2.42	0.53
1:A:60:LEU:CD2	1:A:97:VAL:HG12	2.39	0.52
1:A:86:TYR:O	1:A:293:THR:HG23	2.08	0.52
2:B:57:THR:HA	2:B:60:LEU:HD12	1.91	0.52
1:A:64:MET:CE	1:A:319:LEU:HD23	2.40	0.52
1:A:120:MET:CE	1:A:120:MET:HA	2.39	0.52
1:A:334:GLU:HG3	1:A:338:ARG:HE	1.74	0.52
2:B:52:GLY:HA3	6:B:357:HOH:O	2.08	0.52
2:B:211:SER:OG	2:B:259:PRO:HB2	2.10	0.52
1:A:7:PRO:O	1:A:8:GLN:HB2	2.10	0.52
2:B:160:ILE:HG13	2:B:258:ILE:CD1	2.40	0.52
1:A:86:TYR:HB3	1:A:293:THR:CG2	2.40	0.51
2:B:155:ALA:HA	2:B:258:ILE:HG12	1.92	0.51
1:A:55:GLU:CD	1:A:55:GLU:H	2.13	0.51
1:A:50:PRO:HG3	1:A:263:ASN:OD1	2.10	0.51
2:B:161:LYS:HB2	2:B:185:CYS:SG	2.50	0.51
2:B:33:ASN:HD21	2:B:172:LYS:NZ	2.09	0.51
2:B:240:MET:HE3	2:B:329:LYS:HB2	1.93	0.51
1:A:380:GLU:O	1:A:383:ALA:HB3	2.11	0.50
1:A:76:GLU:OE2	1:A:80:GLN:NE2	2.44	0.50
2:B:19:GLN:CB	2:B:203:ILE:HD11	2.42	0.50
1:A:359:ASN:HD22	1:A:360:PRO:HD2	1.76	0.50
1:A:161:SER:HB3	2:B:120:ARG:CZ	2.42	0.50
2:B:33:ASN:O	2:B:37:LYS:HG3	2.11	0.50
1:A:60:LEU:O	1:A:64:MET:HG3	2.11	0.50
1:A:144:ARG:HH12	1:A:366:ASP:HB2	1.77	0.50
2:B:221:ASP:HB2	2:B:247:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:H	1:A:44:ILE:HD12	1.76	0.50
2:B:258:ILE:HB	2:B:259:PRO:CD	2.40	0.49
2:B:46:GLU:OE1	2:B:74:LEU:HA	2.13	0.49
2:B:226:ALA:HB1	2:B:230:GLN:HB3	1.95	0.49
1:A:96:HIS:CD2	1:A:117:GLY:H	2.29	0.49
1:A:101:ALA:HA	1:A:121:TYR:CE2	2.48	0.49
1:A:329:TRP:NE1	1:A:334:GLU:HB2	2.28	0.49
1:A:170:GLN:O	2:B:85:GLY:HA3	2.12	0.49
2:B:204:GLU:HB3	2:B:205:PRO:HD2	1.93	0.49
2:B:322:GLU:HB3	2:B:323:PRO:HD3	1.93	0.49
2:B:55:ARG:HA	2:B:55:ARG:HE	1.76	0.49
1:A:338:ARG:O	1:A:342:ARG:HB2	2.12	0.49
1:A:65:THR:HG22	1:A:316:ILE:HD13	1.94	0.49
1:A:96:HIS:CE1	1:A:114:ARG:O	2.67	0.48
1:A:377:LYS:O	1:A:380:GLU:HG2	2.12	0.48
2:B:129:SER:C	6:B:364:HOH:O	2.51	0.48
1:A:122:ARG:NH1	1:A:155:ARG:O	2.44	0.48
2:B:109:GLN:O	2:B:113:GLU:HB2	2.13	0.48
1:A:66:LEU:HD13	1:A:120:MET:SD	2.53	0.48
1:A:82:ARG:HG3	1:A:82:ARG:NH1	2.27	0.48
1:A:136:ASN:HA	1:A:357:LYS:HA	1.95	0.48
2:B:143:ALA:O	2:B:317:PHE:HB3	2.14	0.48
1:A:367:VAL:HG12	1:A:368:TYR:CD1	2.48	0.48
2:B:222:VAL:HA	2:B:272:THR:HG21	1.96	0.48
1:A:167:GLN:N	1:A:167:GLN:OE1	2.40	0.48
2:B:18:THR:CG2	2:B:200:GLU:HB3	2.41	0.48
2:B:48:VAL:HG22	2:B:57:THR:HG21	1.95	0.48
1:A:320:ARG:O	1:A:323:LEU:HB2	2.14	0.48
1:A:78:GLN:CG	1:A:293:THR:HG21	2.37	0.48
1:A:130:MET:HG2	1:A:349:PHE:HA	1.94	0.48
1:A:357:LYS:O	1:A:399:ASP:N	2.46	0.48
1:A:77:SER:O	1:A:82:ARG:HB2	2.14	0.48
2:B:165:PRO:HD2	2:B:188:PHE:O	2.14	0.47
2:B:177:SER:HA	2:B:207:ASN:HD22	1.79	0.47
1:A:168:ILE:HG22	1:A:204:GLY:HA3	1.96	0.47
2:B:37:LYS:O	2:B:39:PRO:HD3	2.14	0.47
2:B:160:ILE:HG13	2:B:258:ILE:HD12	1.95	0.47
2:B:275:LEU:HD12	2:B:295:VAL:HG11	1.96	0.47
2:B:177:SER:HA	2:B:207:ASN:ND2	2.29	0.47
1:A:112:GLN:HG2	1:A:113:TYR:CE2	2.49	0.47
1:A:237:ASP:HB3	1:A:241:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:ASN:HD22	2:B:205:PRO:HA	1.79	0.47
2:B:82:PHE:CE2	2:B:86:ILE:HD11	2.50	0.47
1:A:110:PHE:CE1	1:A:158:VAL:HG21	2.50	0.47
1:A:324:LEU:HD23	1:A:329:TRP:O	2.15	0.47
2:B:222:VAL:HA	2:B:272:THR:HG23	1.95	0.46
2:B:204:GLU:HB3	2:B:205:PRO:CD	2.45	0.46
2:B:288:ALA:HB3	6:B:348:HOH:O	2.14	0.46
1:A:114:ARG:HB3	1:A:220:ARG:NH2	2.31	0.46
1:A:335:LYS:HA	1:A:338:ARG:HD2	1.97	0.46
2:B:302:ASN:HD22	2:B:302:ASN:H	1.64	0.46
2:B:63:LYS:HG2	2:B:64:TYR:CE1	2.51	0.46
1:A:170:GLN:HA	2:B:81:GLY:O	2.16	0.46
2:B:139:VAL:O	2:B:140:GLY:C	2.54	0.46
1:A:149:HIS:HE1	1:A:162:SER:OG	1.98	0.46
2:B:299:CYS:O	2:B:303:LEU:HD23	2.16	0.46
1:A:172:VAL:HG21	1:A:204:GLY:O	2.16	0.46
1:A:183:ALA:C	1:A:185:ARG:N	2.70	0.46
1:A:95:THR:HG22	1:A:96:HIS:ND1	2.31	0.45
1:A:359:ASN:ND2	1:A:360:PRO:HD2	2.31	0.45
2:B:211:SER:HG	2:B:259:PRO:HB2	1.80	0.45
2:B:52:GLY:HA2	6:B:370:HOH:O	2.16	0.45
2:B:55:ARG:HE	2:B:55:ARG:CA	2.30	0.45
1:A:52:LEU:HD22	1:A:56:LYS:CD	2.47	0.45
2:B:22:ASN:HB2	2:B:25:GLN:CD	2.37	0.45
1:A:130:MET:HB3	1:A:352:ALA:CB	2.47	0.45
1:A:226:ILE:HG22	1:A:227:SER:N	2.31	0.45
1:A:185:ARG:NH2	6:A:416:HOH:O	2.48	0.45
1:A:184:ASN:CG	1:A:184:ASN:O	2.55	0.45
1:A:166:THR:O	1:A:169:PRO:HD2	2.17	0.45
1:A:253:VAL:HG12	1:A:254:ASP:N	2.32	0.45
2:B:30:ALA:HB1	2:B:176:LEU:HG	1.98	0.45
2:B:272:THR:HG22	2:B:274:ARG:N	2.12	0.44
2:B:240:MET:HE1	2:B:329:LYS:HB2	1.98	0.44
2:B:61:ARG:NH2	2:B:66:LYS:HG2	2.32	0.44
1:A:180:ARG:NH2	2:B:68:ARG:HD3	2.31	0.44
1:A:114:ARG:HB3	1:A:220:ARG:CZ	2.48	0.44
1:A:186:VAL:HG22	1:A:187:VAL:H	1.82	0.44
2:B:210:LEU:O	2:B:211:SER:HB2	2.18	0.44
2:B:237:VAL:HA	2:B:240:MET:CE	2.48	0.44
1:A:43:ILE:HD12	1:A:43:ILE:N	2.32	0.44
2:B:88:VAL:HA	2:B:126:ASN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ASP:OD1	1:A:333:GLN:HB2	2.17	0.44
2:B:51:GLY:HA2	2:B:58:VAL:HA	1.98	0.44
2:B:23:LEU:HD23	2:B:194:TYR:CD2	2.53	0.44
1:A:373:ALA:HA	1:A:376:ARG:NH1	2.33	0.43
1:A:50:PRO:HB2	1:A:52:LEU:HG	2.00	0.43
1:A:108:LEU:HD13	1:A:110:PHE:HE1	1.82	0.43
1:A:144:ARG:NH1	1:A:366:ASP:HB2	2.33	0.43
1:A:285:THR:OG1	1:A:286:TYR:N	2.50	0.43
2:B:221:ASP:CB	2:B:247:VAL:HG13	2.49	0.43
1:A:168:ILE:HA	1:A:189:CYS:SG	2.58	0.43
1:A:359:ASN:ND2	1:A:361:ASN:H	2.16	0.43
1:A:37:MET:CE	1:A:41:GLY:HA2	2.47	0.43
1:A:228:THR:HA	1:A:229:PRO:HD3	1.80	0.43
1:A:149:HIS:CE1	1:A:162:SER:OG	2.72	0.43
2:B:296:GLN:HE21	2:B:297:GLU:N	2.16	0.43
2:B:89:THR:CG2	2:B:89:THR:O	2.66	0.43
1:A:184:ASN:OD1	1:A:184:ASN:O	2.37	0.43
2:B:173:GLY:HA3	2:B:208:ILE:HG13	2.01	0.43
1:A:389:TYR:O	1:A:391:GLU:N	2.52	0.43
2:B:40:THR:HG21	2:B:91:ALA:HA	2.01	0.43
1:A:107:ASP:HA	1:A:185:ARG:HG3	2.01	0.43
2:B:18:THR:HG23	2:B:201:VAL:C	2.39	0.42
2:B:236:GLU:OE1	2:B:236:GLU:HA	2.20	0.42
1:A:9:PHE:HA	1:A:10:PRO:HD3	1.81	0.42
2:B:164:ILE:HG12	2:B:188:PHE:HB2	2.02	0.42
1:A:102:ALA:HB3	1:A:265:THR:CG2	2.48	0.42
1:A:100:ALA:O	1:A:103:LEU:HB2	2.19	0.42
2:B:242:LYS:O	2:B:246:GLY:N	2.50	0.42
1:A:54:LYS:HG3	1:A:328:TRP:CD2	2.55	0.42
2:B:37:LYS:HD3	2:B:205:PRO:HG2	2.00	0.42
1:A:124:TYR:HA	1:A:125:PRO:HD3	1.88	0.42
2:B:317:PHE:HA	2:B:318:PRO:HD3	1.85	0.42
1:A:277:GLN:HA	1:A:278:PRO:HD3	1.90	0.42
1:A:130:MET:HE3	1:A:349:PHE:HB2	2.01	0.42
1:A:226:ILE:HG12	1:A:291:HIS:CG	2.55	0.42
1:A:134:TYR:CZ	1:A:353:GLU:HG2	2.55	0.42
2:B:54:PHE:HB2	6:B:363:HOH:O	2.20	0.42
1:A:131:ALA:HB1	1:A:136:ASN:HD21	1.85	0.41
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.92	0.41
2:B:302:ASN:H	2:B:302:ASN:ND2	2.18	0.41
1:A:44:ILE:HD12	1:A:44:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD23	1:A:93:GLU:HG3	2.02	0.41
2:B:258:ILE:CB	2:B:259:PRO:CD	2.98	0.41
1:A:363:LEU:CD1	1:A:363:LEU:C	2.88	0.41
1:A:112:GLN:O	1:A:113:TYR:HB3	2.21	0.41
2:B:318:PRO:HB2	2:B:321:PHE:HB2	2.02	0.41
2:B:42:VAL:HG12	2:B:92:THR:O	2.20	0.41
2:B:267:LYS:NZ	2:B:267:LYS:HB2	2.36	0.41
2:B:275:LEU:O	2:B:339:MET:HE1	2.21	0.41
2:B:276:LEU:HD23	2:B:276:LEU:C	2.40	0.41
2:B:182:LYS:HA	2:B:182:LYS:HD3	1.85	0.41
2:B:61:ARG:CZ	2:B:66:LYS:HG2	2.51	0.41
2:B:247:VAL:HG11	2:B:340:ILE:CD1	2.51	0.41
2:B:276:LEU:HD23	2:B:276:LEU:O	2.21	0.41
1:A:109:VAL:HG22	1:A:188:ILE:CG2	2.51	0.41
1:A:235:ARG:HA	1:A:235:ARG:HD3	1.85	0.41
1:A:27:VAL:O	1:A:27:VAL:HG12	2.21	0.41
2:B:115:ALA:HB2	2:B:160:ILE:HG23	2.03	0.41
2:B:318:PRO:CB	2:B:321:PHE:HB2	2.51	0.41
2:B:223:THR:N	2:B:272:THR:HG21	2.36	0.40
1:A:213:CYS:HA	1:A:214:PRO:HD3	1.77	0.40
2:B:244:LYS:O	2:B:245:LEU:HD23	2.21	0.40
1:A:74:LEU:O	1:A:77:SER:HB3	2.21	0.40
1:A:173:GLY:HA2	2:B:82:PHE:CE1	2.56	0.40
2:B:136:TRP:CG	2:B:137:GLY:N	2.89	0.40
1:A:130:MET:HB3	1:A:352:ALA:HB2	2.02	0.40
1:A:78:GLN:C	1:A:80:GLN:H	2.25	0.40
1:A:92:GLU:OE1	1:A:220:ARG:HD2	2.21	0.40
1:A:31:ILE:HA	1:A:32:PRO:HD3	1.91	0.40
2:B:38:ASP:HA	2:B:39:PRO:HD3	1.89	0.40
1:A:121:TYR:C	1:A:123:ASP:H	2.25	0.40
1:A:183:ALA:C	1:A:185:ARG:H	2.24	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	378/400 (94%)	342 (90%)	29 (8%)	7 (2%)	10	25
2	B	324/342 (95%)	287 (89%)	34 (10%)	3 (1%)	21	49
All	All	702/742 (95%)	629 (90%)	63 (9%)	10 (1%)	14	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	TYR
1	A	148	VAL
1	A	51	HIS
1	A	390	GLY
2	B	341	ASN
1	A	226	ILE
2	B	196	ALA
1	A	52	LEU
2	B	258	ILE
1	A	44	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	318/336 (95%)	303 (95%)	15 (5%)	32	63
2	B	275/289 (95%)	258 (94%)	17 (6%)	23	49
All	All	593/625 (95%)	561 (95%)	32 (5%)	27	56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	66	LEU
1	A	76	GLU

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Mol	Chain	Res	Type
1	A	95	THR
1	A	108	LEU
1	A	130	MET
1	A	136	ASN
1	A	140	LEU
1	A	182	ASN
1	A	271	ARG
1	A	333	GLN
1	A	347	GLU
1	A	357	LYS
1	A	359	ASN
1	A	363	LEU
2	B	22	ASN
2	B	40	THR
2	B	46	GLU
2	B	48	VAL
2	B	50	PHE
2	B	55	ARG
2	B	117	TYR
2	B	139	VAL
2	B	141	HIS
2	B	151	GLU
2	B	224	LEU
2	B	236	GLU
2	B	239	SER
2	B	243	GLU
2	B	275	LEU
2	B	296	GLN
2	B	303	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	112	GLN
1	A	136	ASN
1	A	149	HIS
1	A	156	HIS
1	A	333	GLN
1	A	359	ASN
1	A	361	ASN
1	A	379	GLN

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Mol	Chain	Res	Type
1	A	387	GLN
2	B	19	GLN
2	B	22	ASN
2	B	25	GLN
2	B	33	ASN
2	B	77	GLN
2	B	141	HIS
2	B	146	HIS
2	B	296	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	TDP	A	403	3	21,27,27	1.35	3 (14%)	31,40,40	1.34	5 (16%)

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
5	TDP	A	403	3	-	0/16/17/17	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	TDP	C35-N3	2.28	1.53	1.48
5	A	403	TDP	C2'-N1'	2.75	1.39	1.34
5	A	403	TDP	C4'-N3'	2.98	1.39	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403	TDP	N1'-C2'-N3'	-2.33	121.30	125.60
5	A	403	TDP	C4A-C4-C5	-2.00	124.40	128.90
5	A	403	TDP	P1-O5G-C5B	2.40	135.20	121.50
5	A	403	TDP	C5A-C5-C4	2.76	130.03	127.56
5	A	403	TDP	C2A-C2'-N1'	3.47	121.20	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	TDP	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.