



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:47 am BST

PDB ID : 2CVO  
Title : Crystal structure of putative N-acetyl-gamma-glutamyl-phosphate reductase (AK071544) from rice (*Oryza sativa*)  
Authors : Nonaka, T.; Kita, A.; Miura-Ohnuma, J.; Katoh, E.; Inagaki, N.; Yamazaki, T.; Miki, K.  
Deposited on : 2005-06-10  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

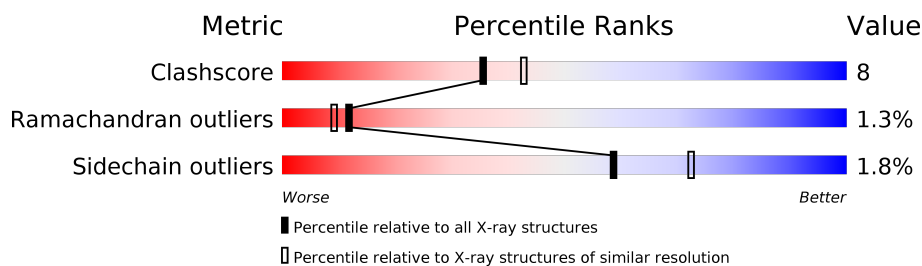
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	366	
1	B	366	
1	C	366	
1	D	366	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11554 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 putative Semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2685	1700	469	503	13			
1	B	348	Total	C	N	O	S	0	0	0
			2685	1700	469	503	13			
1	C	348	Total	C	N	O	S	0	0	0
			2685	1700	469	503	13			
1	D	345	Total	C	N	O	S	0	0	0
			2666	1689	465	499	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	CSO	CYS	MODIFIED RESIDUE	UNP Q6AV34
B	145	CSO	CYS	MODIFIED RESIDUE	UNP Q6AV34
C	145	CSO	CYS	MODIFIED RESIDUE	UNP Q6AV34
D	145	CSO	CYS	MODIFIED RESIDUE	UNP Q6AV34

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	186	Total	O	0	0
			186	186		
2	B	204	Total	O	0	0
			204	204		
2	C	245	Total	O	0	0
			245	245		
2	D	198	Total	O	0	0
			198	198		

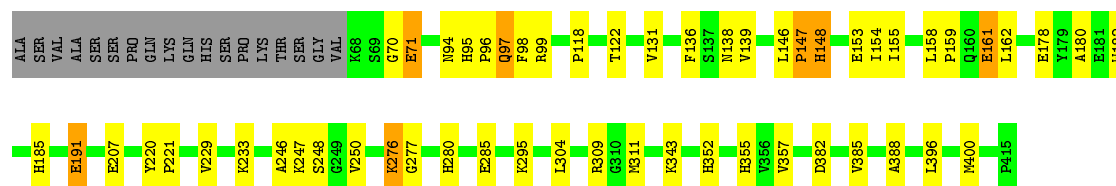
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.


Note EDS was not executed.

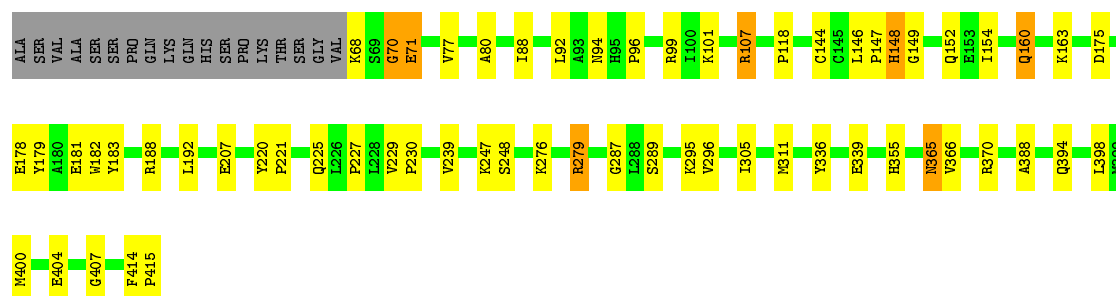
- Molecule 1: putative Semialdehyde dehydrogenase

Chain A: 




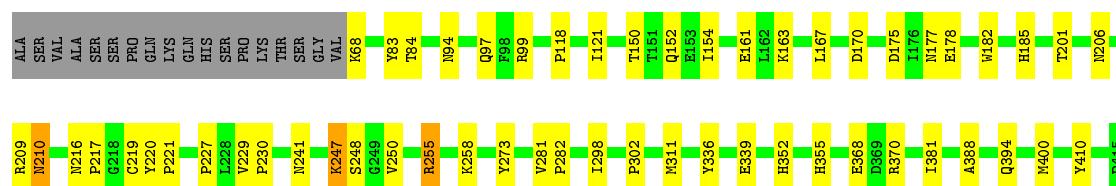
- Molecule 1: putative Semialdehyde dehydrogenase

Chain B: 



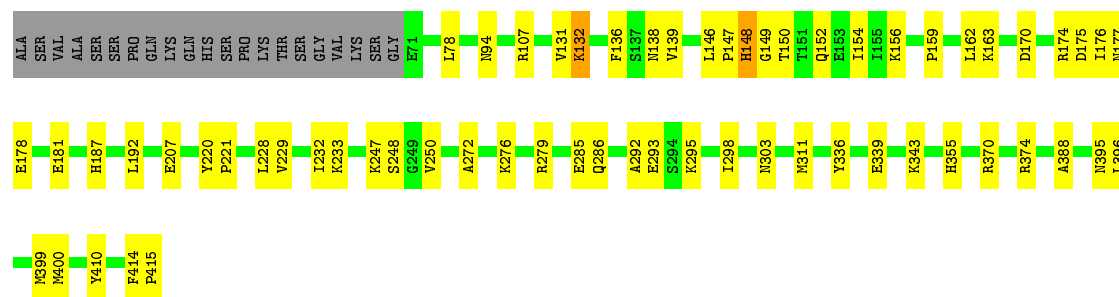
- Molecule 1: putative Semialdehyde dehydrogenase

Chain C: 



- Molecule 1: putative Semialdehyde dehydrogenase

Chain D: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.11Å 86.11Å 316.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.93 – 2.20	Depositor
% Data completeness (in resolution range)	98.2 (19.93-2.20)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.171 , 0.213	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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: CSO

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	0.30	0/2730	0.59	0/3697
1	B	0.31	0/2730	0.61	0/3697
1	C	0.31	0/2730	0.60	0/3697
1	D	0.31	0/2711	0.59	0/3673
All	All	0.31	0/10901	0.60	0/14764

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	2685	0	2697	41	0
1	B	2685	0	2697	51	0
1	C	2685	0	2697	42	0
1	D	2666	0	2676	53	0
2	A	186	0	0	6	0
2	B	204	0	0	7	0
2	C	245	0	0	3	0
2	D	198	0	0	4	0
All	All	11554	0	10767	174	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 8.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:VAL:HG21	1:B:296:VAL:HG22	1.54	0.89
1:D:107:ARG:NH1	1:D:107:ARG:HB2	1.89	0.88
1:B:146:LEU:HD13	1:B:154:ILE:HD12	1.60	0.83
1:C:241:ASN:HD22	1:D:374:ARG:HE	1.24	0.81
1:A:146:LEU:HB3	1:A:147:PRO:HD2	1.64	0.80
1:D:131:VAL:HG13	1:D:132:LYS:HD2	1.62	0.80
1:B:398:LEU:HD21	1:B:404:GLU:HG3	1.64	0.77
1:A:309:ARG:HD2	1:A:357:VAL:HG13	1.66	0.77
1:C:83:TYR:CZ	1:C:255:ARG:HG2	2.20	0.77
1:D:146:LEU:HD13	1:D:154:ILE:HD12	1.67	0.76
1:B:365:ASN:HD22	1:B:366:VAL:H	1.34	0.73
1:D:107:ARG:HH11	1:D:107:ARG:HB2	1.54	0.72
1:C:241:ASN:ND2	1:D:374:ARG:HE	1.88	0.70
1:D:174:ARG:H	1:D:286:GLN:HE22	1.38	0.69
1:B:239:VAL:HG22	1:B:296:VAL:HG13	1.74	0.67
1:A:285:GLU:HB3	2:A:1407:HOH:O	1.95	0.66
1:C:281:VAL:HB	1:C:282:PRO:HD3	1.78	0.65
1:A:147:PRO:O	1:A:148:HIS:HB2	1.96	0.65
1:A:161:GLU:H	1:A:161:GLU:CD	1.99	0.65
1:A:146:LEU:HD13	1:A:154:ILE:HD12	1.80	0.64
1:C:163:LYS:HG3	1:C:400:MET:CE	2.28	0.64
1:A:247:LYS:HE3	1:B:247:LYS:HE3	1.81	0.63
1:D:220:TYR:HB2	1:D:221:PRO:HD3	1.80	0.63
1:B:225:GLN:HE21	1:B:287:GLY:HA3	1.64	0.62
1:C:336:TYR:HD1	1:C:339:GLU:HG3	1.63	0.62
1:B:68:LYS:HB2	1:B:96:PRO:O	2.00	0.62
1:A:153:GLU:HB2	2:A:1584:HOH:O	2.00	0.62
1:D:147:PRO:HD2	1:D:150:THR:HG21	1.82	0.61
1:B:398:LEU:CD2	1:B:404:GLU:HG3	2.31	0.61
1:A:248:SER:HB2	1:A:311:MET:HE2	1.82	0.61
1:B:160:GLN:O	1:B:160:GLN:HG3	2.00	0.61
1:B:239:VAL:HG21	1:B:296:VAL:CG2	2.27	0.61
1:C:220:TYR:HB2	1:C:221:PRO:HD3	1.83	0.59
1:B:365:ASN:ND2	1:B:366:VAL:H	2.00	0.59
1:A:220:TYR:HB2	1:A:221:PRO:HD3	1.85	0.59
1:B:225:GLN:NE2	1:B:287:GLY:HA3	2.18	0.59
1:B:107:ARG:NE	1:B:107:ARG:HA	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:THR:O	1:C:154:ILE:HD13	2.03	0.58
1:B:175:ASP:OD2	1:B:178:GLU:HG3	2.04	0.58
1:C:381:ILE:HG23	2:C:1754:HOH:O	2.03	0.58
1:B:279:ARG:HD3	2:B:1703:HOH:O	2.03	0.58
1:D:174:ARG:H	1:D:286:GLN:NE2	2.01	0.58
1:D:94:ASN:HB3	1:D:410:TYR:OH	2.04	0.58
1:B:207:GLU:HG3	2:B:5003:HOH:O	2.03	0.58
1:A:178:GLU:O	1:A:182:TRP:HD1	1.87	0.57
1:D:159:PRO:HG2	1:D:162:LEU:HD12	1.85	0.57
1:B:99:ARG:HG2	1:B:101:LYS:NZ	2.20	0.57
1:B:220:TYR:HB2	1:B:221:PRO:HD3	1.87	0.57
1:D:177:ASN:O	1:D:181:GLU:HG3	2.05	0.57
1:C:68:LYS:HB2	1:C:99:ARG:HH12	1.70	0.57
1:B:88:ILE:O	1:B:92:LEU:HG	2.05	0.57
1:A:180:ALA:HA	1:A:185:HIS:O	2.05	0.56
1:A:147:PRO:O	1:A:148:HIS:CB	2.53	0.56
1:C:230:PRO:HG3	2:C:1209:HOH:O	2.05	0.56
1:A:146:LEU:HB3	1:A:147:PRO:CD	2.34	0.56
1:B:239:VAL:CG2	1:B:296:VAL:HG22	2.32	0.56
1:A:94:ASN:HB2	2:D:1090:HOH:O	2.05	0.56
1:C:152:GLN:HG3	1:C:170:ASP:OD2	2.05	0.56
1:B:365:ASN:HD22	1:B:366:VAL:N	2.03	0.55
1:C:241:ASN:HD22	1:D:374:ARG:NE	2.01	0.55
1:C:247:LYS:NZ	1:D:247:LYS:HE3	2.22	0.54
1:B:148:HIS:HE1	1:B:183:TYR:HD2	1.54	0.54
1:D:159:PRO:HG2	1:D:162:LEU:CD1	2.37	0.54
1:B:163:LYS:HG3	1:B:400:MET:SD	2.48	0.54
1:C:368:GLU:HG3	1:D:276:LYS:CE	2.37	0.53
1:D:229:VAL:O	1:D:233:LYS:HG3	2.08	0.53
1:B:295:LYS:HE3	2:B:1239:HOH:O	2.08	0.53
1:C:229:VAL:HB	1:C:230:PRO:HD3	1.90	0.53
1:C:175:ASP:HB3	1:C:178:GLU:HB2	1.89	0.53
1:C:161:GLU:H	1:C:161:GLU:CD	2.12	0.53
1:A:207:GLU:HG2	2:A:1489:HOH:O	2.09	0.53
1:D:248:SER:HB2	1:D:311:MET:HE2	1.90	0.53
1:D:152:GLN:HG3	1:D:170:ASP:OD2	2.08	0.52
1:A:191:GLU:CD	1:A:191:GLU:H	2.11	0.52
1:D:132:LYS:HD2	1:D:132:LYS:N	2.25	0.52
1:C:400:MET:CE	1:C:400:MET:HA	2.40	0.51
1:D:395:ASN:O	1:D:399:MET:HG2	2.10	0.51
1:D:107:ARG:CZ	1:D:107:ARG:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:LYS:HA	1:D:192:LEU:HD11	1.92	0.51
1:A:146:LEU:CD1	1:A:154:ILE:HD12	2.40	0.51
1:B:149:GLY:CA	1:B:188:ARG:HH21	2.24	0.51
1:B:152:GLN:HG3	2:B:1159:HOH:O	2.10	0.51
1:D:295:LYS:HD2	2:D:1651:HOH:O	2.10	0.50
1:C:83:TYR:CE1	1:C:255:ARG:HG2	2.47	0.50
1:C:210:ASN:HD22	1:C:210:ASN:C	2.14	0.50
1:B:148:HIS:CE1	1:B:183:TYR:HD2	2.30	0.50
1:D:207:GLU:N	1:D:207:GLU:OE1	2.41	0.50
1:B:394:GLN:O	1:B:398:LEU:HD23	2.12	0.49
1:D:396:LEU:HA	1:D:399:MET:HG2	1.94	0.49
1:D:175:ASP:OD1	1:D:177:ASN:HB2	2.12	0.49
1:D:139:VAL:O	1:D:162:LEU:HD21	2.12	0.49
1:B:144:CYS:SG	2:B:1003:HOH:O	2.45	0.49
1:C:118:PRO:O	1:C:121:ILE:HG23	2.13	0.49
1:C:248:SER:HB2	1:C:311:MET:HE2	1.95	0.49
1:A:309:ARG:HD3	1:A:382:ASP:OD1	2.13	0.48
1:A:155:ILE:HA	1:A:158:LEU:HD12	1.95	0.48
1:B:248:SER:HB2	1:B:311:MET:HE2	1.95	0.48
1:B:94:ASN:OD1	1:B:407:GLY:HA2	2.14	0.48
1:D:414:PHE:CD1	1:D:415:PRO:HA	2.49	0.48
1:B:148:HIS:CE1	1:B:183:TYR:CD2	3.02	0.47
1:D:396:LEU:HD12	1:D:399:MET:HG3	1.96	0.47
1:D:410:TYR:HD1	2:D:1090:HOH:O	1.96	0.47
1:A:161:GLU:OE1	1:A:161:GLU:N	2.38	0.47
1:A:136:PHE:HA	1:A:139:VAL:CG2	2.45	0.47
1:B:355:HIS:CE1	1:C:118:PRO:HB2	2.49	0.47
1:A:295:LYS:HG3	2:A:1518:HOH:O	2.14	0.47
1:B:229:VAL:HB	1:B:230:PRO:HD3	1.96	0.47
1:D:396:LEU:HA	1:D:399:MET:CG	2.45	0.46
1:C:250:VAL:HG22	1:C:250:VAL:O	2.15	0.46
1:A:343:LYS:HB2	2:A:3019:HOH:O	2.16	0.46
1:A:159:PRO:HD2	1:A:162:LEU:HD12	1.97	0.46
1:B:414:PHE:CD1	1:B:415:PRO:HA	2.50	0.46
1:C:163:LYS:HG3	1:C:400:MET:HE1	1.96	0.46
1:A:396:LEU:O	1:A:400:MET:HG2	2.16	0.46
1:C:206:ASN:O	1:C:209:ARG:HG2	2.15	0.46
1:C:400:MET:HE2	1:C:400:MET:HA	1.97	0.46
1:D:285:GLU:HB3	2:D:1651:HOH:O	2.15	0.46
1:D:78:LEU:HD21	1:D:136:PHE:CE1	2.50	0.46
1:C:201:THR:HG21	1:C:394:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:HD13	1:B:154:ILE:CD1	2.41	0.45
1:B:295:LYS:CE	2:B:1239:HOH:O	2.64	0.45
1:C:68:LYS:HB2	1:C:99:ARG:NH1	2.31	0.45
1:D:176:ILE:HG23	1:D:187:HIS:CB	2.47	0.45
1:C:94:ASN:HB2	1:C:410:TYR:OH	2.17	0.45
1:B:148:HIS:HE1	1:B:183:TYR:CD2	2.33	0.44
1:A:131:VAL:HG12	2:A:1431:HOH:O	2.17	0.44
1:B:398:LEU:HD21	1:B:404:GLU:CG	2.40	0.44
1:C:370:ARG:HD3	1:D:298:ILE:O	2.18	0.44
1:D:228:LEU:O	1:D:232:ILE:HG13	2.18	0.44
1:D:336:TYR:HD1	1:D:339:GLU:HG3	1.82	0.44
1:A:118:PRO:HB2	1:D:355:HIS:CE1	2.53	0.44
1:C:298:ILE:O	1:D:370:ARG:HD3	2.18	0.44
1:A:95:HIS:HA	1:A:96:PRO:HD2	1.91	0.44
1:C:273:TYR:O	1:C:302:PRO:HG2	2.18	0.44
1:A:122:THR:HG22	1:D:343:LYS:HD2	1.98	0.44
1:A:229:VAL:CG1	1:A:233:LYS:HE3	2.48	0.43
1:D:163:LYS:HG3	1:D:400:MET:SD	2.58	0.43
1:A:71:GLU:OE1	1:A:71:GLU:HA	2.18	0.43
1:B:295:LYS:NZ	2:B:1239:HOH:O	2.47	0.43
1:A:220:TYR:HB2	1:A:280:HIS:HD2	1.84	0.43
1:D:146:LEU:HD13	1:D:154:ILE:CD1	2.43	0.43
1:B:70:GLY:O	1:B:71:GLU:O	2.35	0.43
1:D:147:PRO:HD2	1:D:150:THR:CG2	2.48	0.43
2:C:1476:HOH:O	1:D:276:LYS:HG2	2.18	0.43
1:B:77:VAL:HG12	1:B:80:ALA:HB2	2.01	0.43
1:D:78:LEU:HD21	1:D:136:PHE:HE1	1.83	0.43
1:B:179:TYR:O	1:B:183:TYR:HD1	2.02	0.42
1:C:182:TRP:CE2	1:C:282:PRO:HG3	2.55	0.42
1:C:216:ASN:HA	1:C:217:PRO:HD3	1.86	0.42
1:B:336:TYR:HD1	1:B:339:GLU:HG3	1.83	0.42
1:A:221:PRO:HD3	1:A:280:HIS:CD2	2.55	0.42
1:B:227:PRO:O	1:B:230:PRO:HD2	2.19	0.42
1:C:247:LYS:CD	1:C:247:LYS:N	2.83	0.42
1:B:181:GLU:OE2	1:B:182:TRP:HD1	2.02	0.42
1:A:352:HIS:HB2	1:A:355:HIS:ND1	2.35	0.42
1:C:84:THR:CG2	1:C:167:LEU:HD22	2.50	0.42
1:D:250:VAL:HG22	1:D:250:VAL:O	2.20	0.41
1:D:176:ILE:HG23	1:D:187:HIS:HB2	2.01	0.41
1:D:178:GLU:HA	1:D:181:GLU:CD	2.41	0.41
1:C:352:HIS:HB2	1:C:355:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:O	1:A:158:LEU:HG	2.20	0.41
1:A:220:TYR:CE1	1:A:246:ALA:HB1	2.56	0.41
1:A:250:VAL:HA	1:A:304:LEU:HD11	2.02	0.41
1:D:292:ALA:O	1:D:293:GLU:HB2	2.20	0.41
1:B:118:PRO:HB2	1:C:355:HIS:CE1	2.55	0.41
1:A:97:GLN:HE21	1:A:97:GLN:HB2	1.64	0.41
1:C:258:LYS:HB3	1:C:258:LYS:NZ	2.36	0.41
1:B:247:LYS:HB3	1:B:305:ILE:HG13	2.02	0.41
1:A:276:LYS:HE3	1:B:370:ARG:HA	2.01	0.41
1:D:279:ARG:HG2	1:D:279:ARG:HH11	1.85	0.40
1:A:98:PHE:CE2	1:A:396:LEU:HD23	2.57	0.40
1:C:247:LYS:HD3	1:C:247:LYS:N	2.36	0.40
1:D:272:ALA:HA	1:D:303:ASN:HA	2.03	0.40
1:B:289:SER:HA	1:B:296:VAL:HG23	2.03	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	345/366 (94%)	323 (94%)	16 (5%)	6 (2%)	9	6
1	B	345/366 (94%)	329 (95%)	9 (3%)	7 (2%)	7	4
1	C	345/366 (94%)	333 (96%)	10 (3%)	2 (1%)	25	26
1	D	342/366 (93%)	325 (95%)	14 (4%)	3 (1%)	17	16
All	All	1377/1464 (94%)	1310 (95%)	49 (4%)	18 (1%)	12	9

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	HIS

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Mol	Chain	Res	Type
1	B	71	GLU
1	B	147	PRO
1	A	70	GLY
1	B	70	GLY
1	D	148	HIS
1	B	148	HIS
1	C	388	ALA
1	A	276	LYS
1	B	276	LYS
1	B	388	ALA
1	D	149	GLY
1	D	388	ALA
1	A	388	ALA
1	B	160	GLN
1	A	277	GLY
1	A	385	VAL
1	C	227	PRO

### 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	289/304 (95%)	282 (98%)	7 (2%)	49	62
1	B	289/304 (95%)	285 (99%)	4 (1%)	67	80
1	C	289/304 (95%)	282 (98%)	7 (2%)	49	62
1	D	287/304 (94%)	284 (99%)	3 (1%)	76	86
All	All	1154/1216 (95%)	1133 (98%)	21 (2%)	59	72

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	97	GLN
1	A	99	ARG
1	A	138	ASN

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Mol	Chain	Res	Type
1	A	147	PRO
1	A	161	GLU
1	A	191	GLU
1	B	107	ARG
1	B	192	LEU
1	B	279	ARG
1	B	365	ASN
1	C	97	GLN
1	C	177	ASN
1	C	185	HIS
1	C	210	ASN
1	C	219	CYS
1	C	247	LYS
1	C	255	ARG
1	D	132	LYS
1	D	138	ASN
1	D	148	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	97	GLN
1	A	123	GLN
1	A	138	ASN
1	A	280	HIS
1	A	312	GLN
1	A	346	ASN
1	B	97	GLN
1	B	123	GLN
1	B	127	ASN
1	B	148	HIS
1	B	225	GLN
1	B	241	ASN
1	B	280	HIS
1	B	312	GLN
1	B	365	ASN
1	B	411	GLN
1	C	97	GLN
1	C	123	GLN
1	C	148	HIS
1	C	177	ASN

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Mol	Chain	Res	Type
1	C	210	ASN
1	C	241	ASN
1	C	312	GLN
1	C	411	GLN
1	D	127	ASN
1	D	138	ASN
1	D	286	GLN
1	D	312	GLN
1	D	346	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSO	D	145	1	3,6,7	1.20	0	0,6,8	0.00	-
1	CSO	C	145	1	3,6,7	1.35	1 (33%)	0,6,8	0.00	-
1	CSO	B	145	1	3,6,7	1.30	1 (33%)	0,6,8	0.00	-
1	CSO	A	145	1	3,6,7	1.36	1 (33%)	0,6,8	0.00	-

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
1	CSO	D	145	1	-	0/1/5/7	-
1	CSO	C	145	1	-	0/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	B	145	1	-	0/1/5/7	-
1	CSO	A	145	1	-	0/1/5/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	145	CSO	CB-CA	2.13	1.58	1.53
1	A	145	CSO	CB-CA	2.12	1.58	1.53
1	B	145	CSO	CB-CA	2.00	1.58	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.