



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 02:35 PM EDT

PDB ID : 1EBF
Title : HOMOSERINE DEHYDROGENASE FROM S. CEREVISIAE COMPLEX
WITH NAD⁺
Authors : DeLaBarre, B.; Thompson, P.R.; Wright, G.D.; Berghuis, A.M.
Deposited on : unknown
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

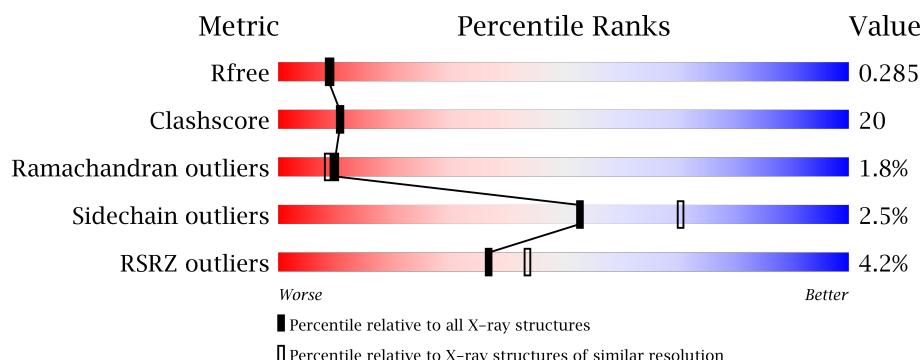
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	358	<div> <div>4%</div> <div>72%</div> <div>26%</div> <div>.</div> </div>
1	B	358	<div> <div>5%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	A	2104	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5719 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.

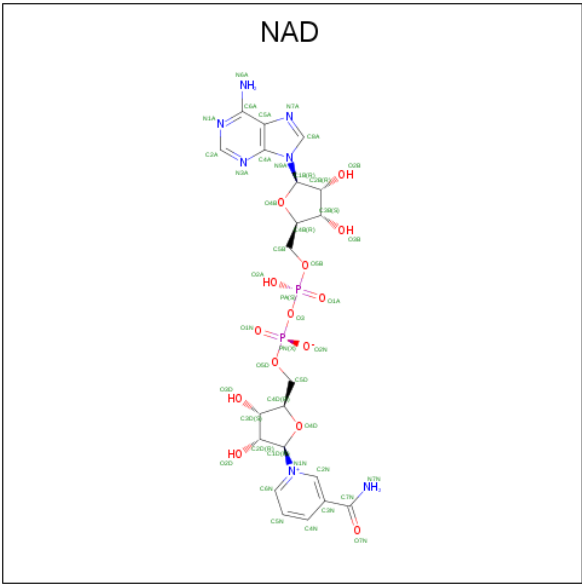
- Molecule 1 is a protein called HOMOSERINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2710	1737	443	529	1			
1	B	358	Total	C	N	O	S	0	0	0
			2710	1737	443	529	1			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

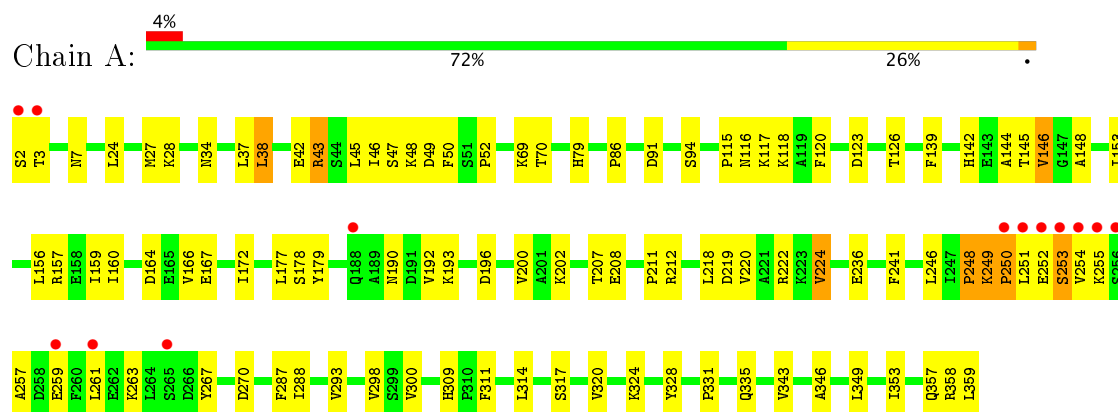
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	131	Total	O	0	0
			131	131		

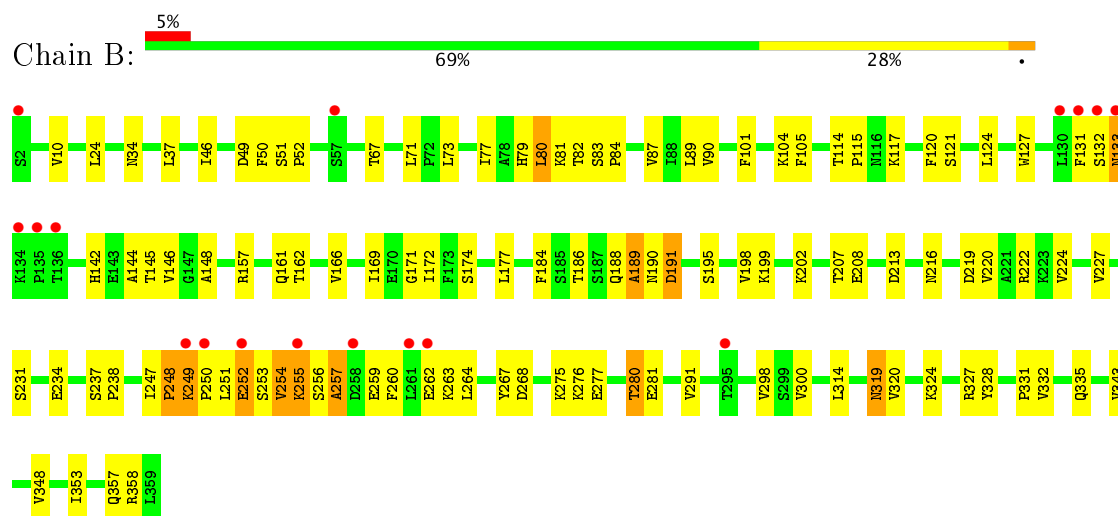
3 Residue-property plots

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 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: HOMOSERINE DEHYDROGENASE



• Molecule 1: HOMOSERINE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.40 Å 80.40 Å 250.16 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.96 – 2.30 39.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	85.7 (35.96-2.30) 91.3 (39.69-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.20 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.269 0.234 , 0.285	Depositor DCC
R_{free} test set	2505 reflections (7.01%)	DCC
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5719	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/2757	0.65	0/3741
1	B	0.37	0/2757	0.64	1/3741 (0.0%)
All	All	0.37	0/5514	0.64	1/7482 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	VAL	N-CA-C	-5.26	96.80	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2710	0	2782	114	0
1	B	2710	0	2782	119	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	44	0	26	0	0
4	A	122	0	0	1	0
4	B	131	0	0	0	0
All	All	5719	0	5590	226	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 20.

All (226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LYS:HB3	1:A:250:PRO:HD2	1.17	1.07
1:B:172:ILE:O	1:B:319:ASN:HB2	1.53	1.05
1:B:291:VAL:HG22	1:B:298:VAL:HG22	1.42	1.01
1:A:249:LYS:HB3	1:A:250:PRO:CD	2.00	0.91
1:B:251:LEU:HD22	1:B:267:TYR:OH	1.72	0.89
1:A:314:LEU:HD21	1:A:320:VAL:HG21	1.53	0.88
1:B:142:HIS:HD2	1:B:145:THR:HG21	1.39	0.87
1:B:320:VAL:HG12	1:B:335:GLN:CB	2.03	0.87
1:A:142:HIS:HE1	1:A:157:ARG:HH21	1.22	0.86
1:B:255:LYS:HD3	1:B:259:GLU:HG3	1.56	0.86
1:A:255:LYS:HD2	1:A:259:GLU:HG3	1.59	0.82
1:B:145:THR:HG23	1:B:146:VAL:HG23	1.59	0.82
1:A:146:VAL:HG13	1:A:153:ILE:HD11	1.61	0.82
1:B:320:VAL:HG12	1:B:335:GLN:HB2	1.63	0.81
1:A:207:THR:HG21	1:A:211:PRO:HG3	1.63	0.80
1:B:220:VAL:O	1:B:224:VAL:HG23	1.82	0.79
1:A:249:LYS:CB	1:A:250:PRO:HD2	2.09	0.78
1:A:212:ARG:NH2	1:A:257:ALA:H	1.81	0.78
1:B:10:VAL:HG22	1:B:90:VAL:CG2	2.14	0.78
1:A:255:LYS:HD2	1:A:259:GLU:CG	2.14	0.77
1:B:255:LYS:HD3	1:B:259:GLU:CG	2.14	0.77
1:B:249:LYS:HB3	1:B:250:PRO:CD	2.13	0.77
1:A:220:VAL:O	1:A:224:VAL:HG12	1.85	0.76
1:B:117:LYS:HG2	1:B:145:THR:OG1	1.84	0.76
1:B:324:LYS:HG2	1:B:331:PRO:HG3	1.68	0.76
1:B:157:ARG:O	1:B:161:GLN:HG3	1.87	0.75
1:A:346:ALA:HB1	1:B:162:THR:HG21	1.69	0.75
1:A:346:ALA:CB	1:B:162:THR:HG21	2.16	0.74
1:A:27:MET:CE	1:A:353:ILE:HD11	2.18	0.74
1:B:249:LYS:HD2	1:B:249:LYS:H	1.53	0.73
1:B:10:VAL:HG22	1:B:90:VAL:HG21	1.68	0.72
1:A:190:ASN:HD22	1:A:192:VAL:HG23	1.54	0.71
1:A:320:VAL:HG22	1:A:335:GLN:HG2	1.72	0.71
1:A:142:HIS:CE1	1:A:157:ARG:HH21	2.08	0.71
1:A:218:LEU:O	1:A:222:ARG:HG3	1.90	0.70
1:B:249:LYS:HD2	1:B:249:LYS:N	2.09	0.68
1:B:142:HIS:O	1:B:145:THR:HG22	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LYS:HA	1:B:207:THR:HG22	1.76	0.67
1:B:248:PRO:O	1:B:249:LYS:O	2.12	0.66
1:A:37:LEU:HD12	1:A:46:ILE:HG22	1.76	0.66
1:A:42:GLU:H	1:A:42:GLU:CD	2.00	0.65
1:A:353:ILE:O	1:A:357:GLN:HG3	1.96	0.65
1:A:207:THR:HG22	1:A:208:GLU:O	1.98	0.64
1:B:314:LEU:HD21	1:B:320:VAL:HG11	1.79	0.64
1:A:27:MET:HE2	1:A:353:ILE:HD11	1.78	0.63
1:B:320:VAL:HG12	1:B:335:GLN:HB3	1.78	0.63
1:A:202:LYS:HD2	1:A:261:LEU:HD11	1.81	0.63
1:A:190:ASN:ND2	1:A:192:VAL:HG23	2.14	0.62
1:A:159:ILE:CG2	1:A:164:ASP:HB3	2.29	0.62
1:A:252:GLU:HG3	1:A:253:SER:H	1.64	0.62
1:A:34:ASN:OD1	1:A:52:PRO:HG3	2.00	0.62
1:A:49:ASP:O	1:A:50:PHE:HB2	1.99	0.62
1:B:222:ARG:HG3	1:B:222:ARG:HH11	1.65	0.62
1:A:314:LEU:CD2	1:A:320:VAL:HG21	2.29	0.62
1:B:115:PRO:HG3	1:B:348:VAL:HG21	1.83	0.61
1:A:357:GLN:HB3	1:B:358:ARG:HG3	1.82	0.61
1:B:190:ASN:HD22	1:B:275:LYS:NZ	1.99	0.60
1:B:34:ASN:OD1	1:B:52:PRO:HG3	2.01	0.60
1:B:121:SER:OG	1:B:222:ARG:HD2	2.02	0.60
1:B:142:HIS:CD2	1:B:145:THR:HG21	2.28	0.60
1:A:27:MET:HE3	1:A:349:LEU:HD21	1.84	0.60
1:B:247:ILE:HG23	1:B:260:PHE:CE1	2.36	0.60
1:A:190:ASN:HD22	1:A:192:VAL:H	1.49	0.60
1:B:90:VAL:O	1:B:90:VAL:HG23	2.02	0.60
1:A:156:LEU:O	1:A:160:ILE:HG12	2.02	0.59
1:A:255:LYS:HE3	1:A:263:LYS:HG2	1.83	0.59
1:A:328:TYR:OH	1:B:343:VAL:HG13	2.01	0.59
1:B:314:LEU:HD21	1:B:320:VAL:CG1	2.32	0.59
1:A:160:ILE:HD11	1:A:166:VAL:HG23	1.82	0.59
1:A:167:GLU:HA	1:A:293:VAL:HG22	1.83	0.59
1:A:69:LYS:HD2	1:A:70:THR:N	2.18	0.58
1:B:249:LYS:HB2	1:B:251:LEU:CD1	2.33	0.58
1:A:166:VAL:O	1:A:293:VAL:HG21	2.04	0.58
1:B:256:SER:O	1:B:257:ALA:HB3	2.02	0.58
1:A:193:LYS:HB2	1:A:196:ASP:OD2	2.04	0.57
1:B:247:ILE:HG21	1:B:252:GLU:HB2	1.85	0.57
1:B:319:ASN:HD22	1:B:319:ASN:C	2.08	0.57
1:A:248:PRO:O	1:A:249:LYS:O	2.23	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HG23	1:A:164:ASP:HB3	1.87	0.56
1:A:207:THR:CG2	1:A:211:PRO:HA	2.35	0.56
1:A:69:LYS:HE3	1:A:70:THR:O	2.06	0.56
1:A:251:LEU:HD22	1:A:267:TYR:OH	2.06	0.56
1:B:190:ASN:O	1:B:191:ASP:HB2	2.04	0.56
1:A:27:MET:HE1	1:A:353:ILE:HD11	1.88	0.56
1:A:27:MET:HE1	1:A:349:LEU:HG	1.88	0.56
1:A:172:ILE:HD12	1:A:314:LEU:HD11	1.87	0.56
1:A:37:LEU:CD1	1:A:46:ILE:HG22	2.36	0.56
1:B:280:THR:HG22	1:B:281:GLU:HG3	1.87	0.55
1:A:252:GLU:O	1:A:254:VAL:N	2.31	0.55
1:A:250:PRO:C	1:A:252:GLU:H	2.10	0.55
1:A:123:ASP:HB2	1:A:126:THR:OG1	2.06	0.55
1:A:167:GLU:HA	1:A:293:VAL:CG2	2.37	0.55
1:B:79:HIS:O	1:B:82:THR:HB	2.05	0.55
1:A:324:LYS:CE	1:A:331:PRO:HG3	2.36	0.55
1:A:212:ARG:HH22	1:A:257:ALA:H	1.56	0.54
1:A:86:PRO:CB	1:A:359:LEU:HD13	2.38	0.54
1:A:343:VAL:HG13	1:B:328:TYR:OH	2.06	0.54
1:A:86:PRO:HB3	1:A:359:LEU:HD13	1.90	0.53
1:B:73:LEU:HD12	1:B:101:PHE:CD1	2.43	0.53
1:A:179:TYR:HB2	1:A:317:SER:HB3	1.91	0.53
1:A:255:LYS:HD2	1:A:259:GLU:HG2	1.92	0.52
1:A:69:LYS:HD2	1:A:70:THR:H	1.74	0.52
1:B:314:LEU:HD11	1:B:320:VAL:HG13	1.90	0.52
1:B:115:PRO:HG3	1:B:348:VAL:CG2	2.39	0.52
1:A:116:ASN:OD1	1:A:118:LYS:HG2	2.09	0.52
1:B:219:ASP:O	1:B:222:ARG:HB2	2.08	0.52
1:A:207:THR:HG21	1:A:211:PRO:CG	2.37	0.52
1:A:349:LEU:HD23	1:B:162:THR:HG23	1.91	0.52
1:A:224:VAL:CG2	1:A:298:VAL:HG13	2.40	0.51
1:B:254:VAL:HB	1:B:255:LYS:HE3	1.91	0.51
1:B:89:LEU:HD22	1:B:105:PHE:CE2	2.45	0.51
1:B:171:GLY:HA3	1:B:320:VAL:O	2.09	0.51
1:B:174:SER:HB3	1:B:177:LEU:HB2	1.92	0.51
1:B:131:PHE:O	1:B:133:ASN:N	2.41	0.51
1:B:256:SER:O	1:B:257:ALA:CB	2.59	0.51
1:A:196:ASP:O	1:A:200:VAL:HG23	2.11	0.50
1:B:188:GLN:O	1:B:188:GLN:HG2	2.12	0.50
1:B:249:LYS:HB3	1:B:250:PRO:HD3	1.92	0.50
1:B:324:LYS:HE3	1:B:331:PRO:HG3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ARG:NH1	1:B:222:ARG:HG3	2.25	0.50
1:A:328:TYR:CZ	1:B:343:VAL:HG13	2.46	0.49
1:A:159:ILE:HG23	1:A:164:ASP:CB	2.42	0.49
1:A:42:GLU:N	1:A:42:GLU:CD	2.64	0.49
1:B:198:VAL:HG21	1:B:264:LEU:HD23	1.95	0.49
1:B:186:THR:HB	1:B:188:GLN:NE2	2.28	0.49
1:A:324:LYS:HE3	1:A:331:PRO:HG3	1.94	0.49
1:B:162:THR:CG2	1:B:327:ARG:HH12	2.26	0.49
1:B:249:LYS:HB3	1:B:250:PRO:HD2	1.93	0.49
1:A:34:ASN:CG	1:A:52:PRO:HG3	2.33	0.48
1:B:198:VAL:HG23	1:B:199:LYS:N	2.29	0.48
1:A:207:THR:HG22	1:A:208:GLU:N	2.28	0.48
1:B:247:ILE:HG21	1:B:252:GLU:CB	2.43	0.48
1:B:77:ILE:O	1:B:81:LYS:HG3	2.13	0.48
1:B:46:ILE:HD11	1:B:71:LEU:HD13	1.96	0.48
1:A:177:LEU:HD13	1:A:287:PHE:CD2	2.49	0.47
1:A:159:ILE:HG22	1:A:164:ASP:HB3	1.96	0.47
1:B:207:THR:HG23	1:B:208:GLU:O	2.15	0.47
1:B:213:ASP:HA	1:B:216:ASN:ND2	2.29	0.47
1:B:252:GLU:HG2	1:B:253:SER:N	2.29	0.47
1:B:162:THR:HG22	1:B:327:ARG:HH12	1.78	0.47
1:B:50:PHE:CE2	1:B:83:SER:HB2	2.50	0.46
1:B:10:VAL:HA	1:B:90:VAL:HG22	1.98	0.46
1:B:166:VAL:HG11	1:B:231:SER:CB	2.45	0.46
1:B:195:SER:O	1:B:198:VAL:HG22	2.15	0.46
1:B:169:ILE:HG21	1:B:227:VAL:HG11	1.97	0.46
1:A:120:PHE:CZ	1:A:142:HIS:HB3	2.51	0.46
1:B:120:PHE:CZ	1:B:142:HIS:HB3	2.50	0.46
1:A:202:LYS:CD	1:A:261:LEU:HD11	2.45	0.46
1:A:241:PHE:HE1	1:A:300:VAL:HG23	1.80	0.46
1:A:252:GLU:C	1:A:254:VAL:H	2.15	0.46
1:B:49:ASP:OD1	1:B:51:SER:HB3	2.15	0.46
1:A:142:HIS:HB2	1:A:145:THR:CG2	2.46	0.46
1:A:48:LYS:HD2	1:A:79:HIS:CE1	2.50	0.46
1:B:255:LYS:N	1:B:255:LYS:HE2	2.30	0.46
1:A:94:SER:O	1:A:118:LYS:HE3	2.16	0.45
1:B:67:THR:O	1:B:67:THR:HG22	2.17	0.45
1:A:224:VAL:HG21	1:A:298:VAL:HG13	1.98	0.45
1:A:38:LEU:HB3	1:A:45:LEU:HB2	1.97	0.45
1:A:251:LEU:HD21	1:A:263:LYS:CE	2.46	0.45
1:B:195:SER:HB2	1:B:268:ASP:OD2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LEU:C	1:B:37:LEU:HD23	2.37	0.45
1:B:144:ALA:HA	1:B:148:ALA:O	2.16	0.45
1:B:255:LYS:CA	1:B:255:LYS:HE2	2.47	0.45
1:B:277:GLU:HG2	1:B:281:GLU:OE2	2.16	0.45
1:A:91:ASP:O	1:A:115:PRO:HD2	2.17	0.45
1:B:188:GLN:O	1:B:189:ALA:C	2.54	0.45
1:B:263:LYS:O	1:B:263:LYS:HD3	2.17	0.45
1:A:117:LYS:HE3	1:A:219:ASP:OD2	2.16	0.44
1:A:190:ASN:ND2	1:A:192:VAL:CG2	2.80	0.44
1:B:237:SER:HB2	1:B:238:PRO:HD2	1.99	0.44
1:A:146:VAL:O	1:A:146:VAL:HG22	2.18	0.44
1:A:159:ILE:HD12	4:A:2113:HOH:O	2.15	0.44
1:A:251:LEU:HD21	1:A:263:LYS:CG	2.48	0.44
1:B:255:LYS:HA	1:B:255:LYS:HE2	1.99	0.44
1:B:251:LEU:HD22	1:B:267:TYR:HH	1.80	0.44
1:A:314:LEU:CD2	1:A:335:GLN:HE21	2.31	0.43
1:B:124:LEU:HD21	1:B:234:GLU:HB3	2.01	0.43
1:B:83:SER:HA	1:B:84:PRO:HD3	1.76	0.43
1:B:353:ILE:O	1:B:357:GLN:HG3	2.18	0.43
1:B:80:LEU:HG	1:B:87:VAL:HG11	2.00	0.43
1:A:172:ILE:CG2	1:A:178:SER:HB2	2.49	0.43
1:A:139:PHE:CE1	1:A:358:ARG:HG2	2.54	0.43
1:A:249:LYS:CB	1:A:250:PRO:CD	2.80	0.43
1:B:251:LEU:HD22	1:B:267:TYR:CZ	2.54	0.43
1:B:49:ASP:O	1:B:50:PHE:HB2	2.19	0.43
1:B:184:PHE:CE1	1:B:275:LYS:HD2	2.54	0.43
1:A:250:PRO:HA	1:A:252:GLU:HG2	2.00	0.42
1:A:47:SER:OG	1:A:50:PHE:N	2.48	0.42
1:A:48:LYS:HD2	1:A:48:LYS:HA	1.85	0.42
1:B:249:LYS:C	1:B:251:LEU:HD12	2.39	0.42
1:B:77:ILE:HD13	1:B:104:LYS:HB3	2.00	0.42
1:B:202:LYS:HA	1:B:207:THR:CG2	2.47	0.42
1:B:247:ILE:CG2	1:B:252:GLU:HB3	2.50	0.42
1:B:249:LYS:HB2	1:B:251:LEU:HD11	2.01	0.42
1:B:255:LYS:HD3	1:B:259:GLU:HG2	1.98	0.42
1:A:142:HIS:HB2	1:A:145:THR:HG23	2.01	0.42
1:A:251:LEU:HG	1:A:251:LEU:O	2.20	0.42
1:B:324:LYS:CG	1:B:331:PRO:HG3	2.42	0.42
1:A:42:GLU:HG3	1:A:43:ARG:CZ	2.50	0.42
1:A:288:ILE:HD12	1:A:288:ILE:C	2.41	0.42
1:A:42:GLU:HG2	1:A:43:ARG:H	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:VAL:HG22	1:B:90:VAL:HG22	2.01	0.41
1:B:213:ASP:HA	1:B:216:ASN:HD21	1.84	0.41
1:A:252:GLU:H	1:A:252:GLU:HG2	1.71	0.41
1:B:276:LYS:HB2	1:B:276:LYS:HE3	1.90	0.41
1:B:73:LEU:HD12	1:B:101:PHE:CE1	2.55	0.41
1:A:172:ILE:HG21	1:A:178:SER:HB2	2.03	0.41
1:A:324:LYS:HE2	1:A:331:PRO:HG3	2.02	0.41
1:B:262:GLU:OE1	1:B:262:GLU:HA	2.20	0.41
1:B:10:VAL:HG13	1:B:90:VAL:HG23	2.03	0.41
1:B:120:PHE:HB3	1:B:127:TRP:HZ3	1.85	0.41
1:B:114:THR:HA	1:B:115:PRO:HD3	1.83	0.41
1:A:146:VAL:CG1	1:A:153:ILE:HD11	2.42	0.41
1:B:220:VAL:CG2	1:B:300:VAL:HG21	2.51	0.41
1:A:249:LYS:O	1:A:251:LEU:N	2.54	0.41
1:A:241:PHE:CD1	1:A:298:VAL:HG12	2.56	0.41
1:A:309:HIS:HD2	1:A:311:PHE:HB2	1.86	0.41
1:B:267:TYR:CD1	1:B:267:TYR:N	2.89	0.40
1:A:212:ARG:NH2	1:A:257:ALA:N	2.61	0.40
1:A:2:SER:HB3	1:A:359:LEU:OXT	2.21	0.40
1:B:133:ASN:O	1:B:133:ASN:ND2	2.55	0.40
1:B:224:VAL:CG1	1:B:298:VAL:HG13	2.51	0.40
1:B:314:LEU:HD23	1:B:314:LEU:N	2.35	0.40
1:A:144:ALA:HA	1:A:148:ALA:O	2.21	0.40
1:A:7:ASN:HD22	1:A:34:ASN:HB2	1.86	0.40
1:B:73:LEU:HA	1:B:73:LEU:HD23	1.89	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	356/358 (99%)	325 (91%)	26 (7%)	5 (1%)	13 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	356/358 (99%)	330 (93%)	18 (5%)	8 (2%)	8	6
All	All	712/716 (99%)	655 (92%)	44 (6%)	13 (2%)	10	9

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	LYS
1	B	191	ASP
1	B	249	LYS
1	B	257	ALA
1	A	3	THR
1	A	253	SER
1	B	132	SER
1	B	189	ALA
1	B	254	VAL
1	B	255	LYS
1	A	250	PRO
1	B	248	PRO
1	A	248	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	300/300 (100%)	291 (97%)	9 (3%)	46	63
1	B	300/300 (100%)	294 (98%)	6 (2%)	60	77
All	All	600/600 (100%)	585 (98%)	15 (2%)	53	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	28	LYS
1	A	38	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	43	ARG
1	A	146	VAL
1	A	224	VAL
1	A	236	GLU
1	A	246	LEU
1	A	270	ASP
1	B	24	LEU
1	B	80	LEU
1	B	133	ASN
1	B	252	GLU
1	B	280	THR
1	B	319	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	133	ASN
1	A	137	ASN
1	A	142	HIS
1	A	190	ASN
1	A	309	HIS
1	A	319	ASN
1	A	330	ASN
1	A	335	GLN
1	B	7	ASN
1	B	54	ASN
1	B	133	ASN
1	B	142	HIS
1	B	188	GLN
1	B	190	ASN
1	B	319	ASN
1	B	330	ASN

5.3.3 RNA ⓘ

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 3 ligands modelled in this entry, 2 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	$\# Z > 2$
3	NAD	A	2109	-	41,48,48	2.38	9 (21%)	43,73,73	1.66	5 (11%)

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	NAD	A	2109	-	-	0/22/62/62	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2109	NAD	C2D-C1D	-3.33	1.48	1.53
3	A	2109	NAD	C2B-C1B	-2.00	1.50	1.53
3	A	2109	NAD	C2A-N1A	2.07	1.37	1.33
3	A	2109	NAD	O7N-C7N	2.27	1.28	1.24
3	A	2109	NAD	C7N-N7N	2.90	1.38	1.33
3	A	2109	NAD	C6N-N1N	3.27	1.43	1.35
3	A	2109	NAD	C5N-C4N	5.90	1.50	1.38
3	A	2109	NAD	C2N-C3N	7.40	1.50	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2109	NAD	C4N-C3N	8.66	1.53	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2109	NAD	C5N-C4N-C3N	-6.69	112.48	120.35
3	A	2109	NAD	O2N-PN-O5D	2.22	118.64	108.14
3	A	2109	NAD	C5A-C6A-N6A	2.64	125.86	120.47
3	A	2109	NAD	C6N-C5N-C4N	3.43	124.62	119.44
3	A	2109	NAD	C3N-C7N-N7N	3.88	122.20	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	358/358 (100%)	-0.09	13 (3%)	43	50	10, 22, 59, 80	0
1	B	358/358 (100%)	0.00	17 (4%)	32	39	11, 24, 57, 72	0
All	All	716/716 (100%)	-0.05	30 (4%)	37	44	10, 23, 59, 80	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	PRO	7.6
1	A	250	PRO	7.1
1	A	253	SER	7.0
1	B	133	ASN	6.1
1	A	3	THR	5.7
1	A	251	LEU	4.7
1	B	130	LEU	4.6
1	A	255	LYS	4.4
1	A	254	VAL	4.2
1	B	249	LYS	4.2
1	B	132	SER	4.1
1	B	262	GLU	4.0
1	B	252	GLU	3.3
1	B	136	THR	3.0
1	B	131	PHE	3.0
1	B	134	LYS	2.9
1	A	259	GLU	2.8
1	B	295	THR	2.7
1	A	256	SER	2.6
1	A	252	GLU	2.5
1	B	261	LEU	2.5
1	B	135	PRO	2.4
1	A	188	GLN	2.4
1	B	2	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	265	SER	2.4
1	A	2	SER	2.3
1	B	255	LYS	2.3
1	A	261	LEU	2.2
1	B	57	SER	2.1
1	B	258	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NA	A	2104	1/1	0.95	0.31	7.19	29,29,29,29	0
3	NAD	A	2109	44/44	0.91	0.15	1.22	18,28,42,47	0
2	NA	B	2114	1/1	0.88	0.15	0.19	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.