



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:42 PM GMT

PDB ID : 1YBA
Title : The active form of phosphoglycerate dehydrogenase
Authors : Thompson, J.R.; Banaszak, L.J.
Deposited on : 2004-12-20
Resolution : 2.24 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

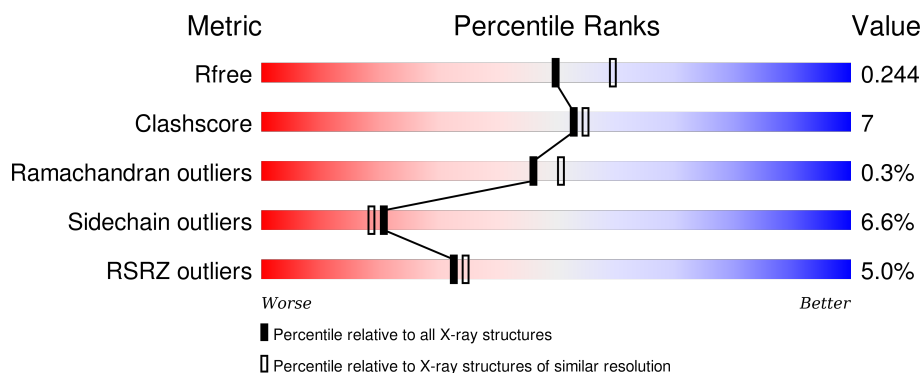
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	410	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	410	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
1	C	410	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	D	410	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>12%</div> <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	PO4	A	412	-	-	-	X
3	AKG	B	412	-	-	X	-
3	AKG	D	412	-	-	-	X
4	UNL	C	414	-	-	X	X
4	UNL	D	413	-	-	-	X
4	UNL	D	414	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14017 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 D-3-phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	Se	0	1	0
			3083	1950	535	586	4	8			
1	B	406	Total	C	N	O	S	Se	0	1	0
			3086	1952	535	587	4	8			
1	C	406	Total	C	N	O	S	Se	0	2	0
			3097	1958	540	587	4	8			
1	D	406	Total	C	N	O	S	Se	0	2	0
			3094	1956	536	590	4	8			

There are 32 discrepancies between the modelled and reference sequences:

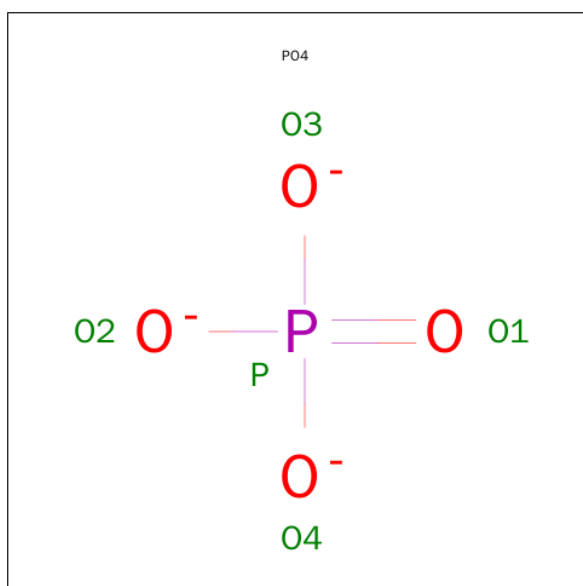
Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	229	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	397	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	229	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	397	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	229	MSE	MET	MODIFIED RESIDUE	UNP P08328

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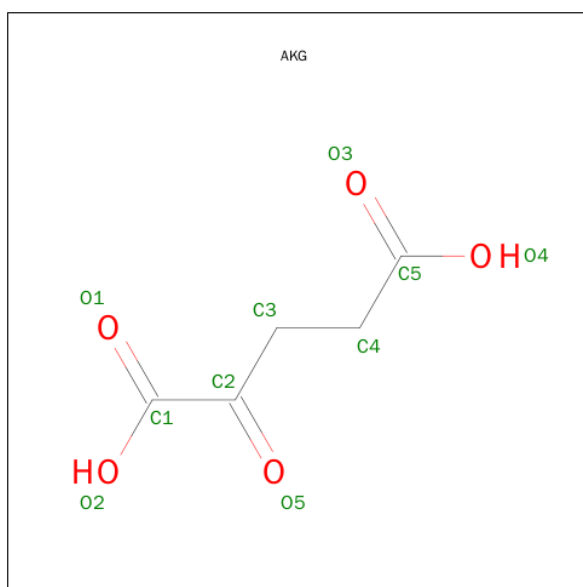
Chain	Residue	Modelled	Actual	Comment	Reference
C	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	397	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	229	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	397	MSE	MET	MODIFIED RESIDUE	UNP P08328

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).

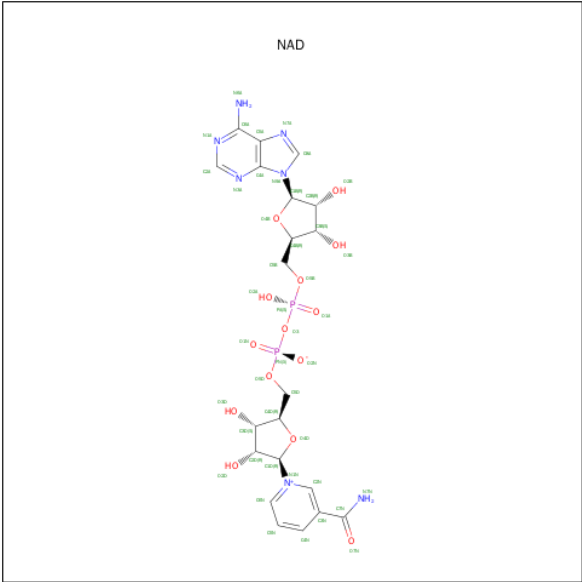


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	5	5		
4	A	2	Total	C	O	0	0
			20	10	10		
4	D	2	Total	C	O	0	0
			20	10	10		
4	C	2	Total	C	O	0	0
			20	10	10		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

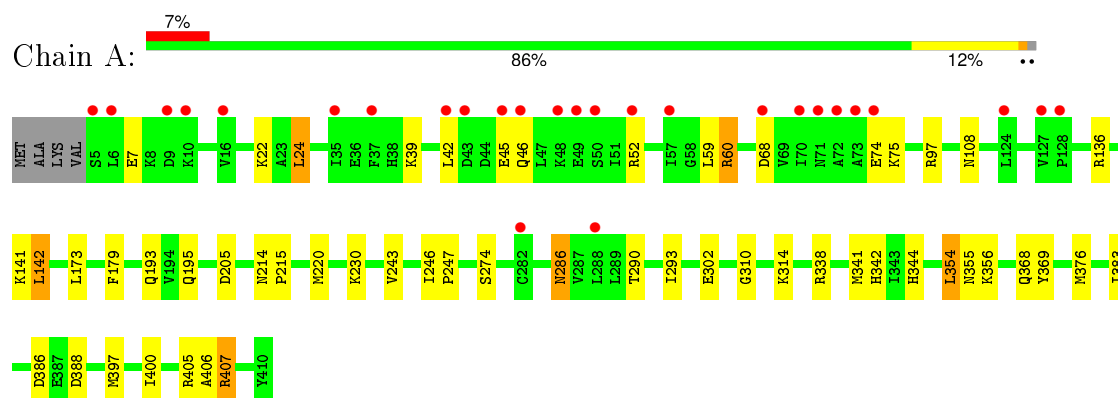
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	300	Total	O	0	0
			300	300		
6	B	330	Total	O	0	0
			330	330		
6	C	350	Total	O	0	0
			350	350		
6	D	366	Total	O	0	0
			366	366		

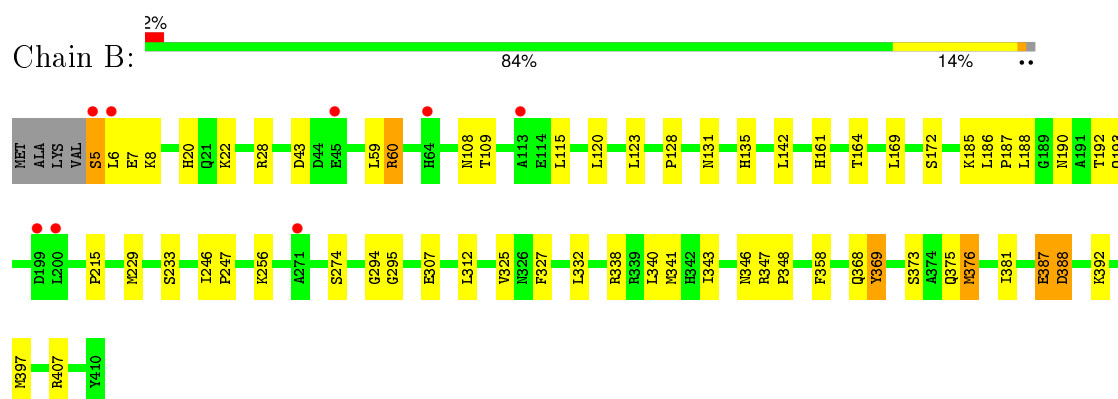
3 Residue-property plots [i](#)

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.

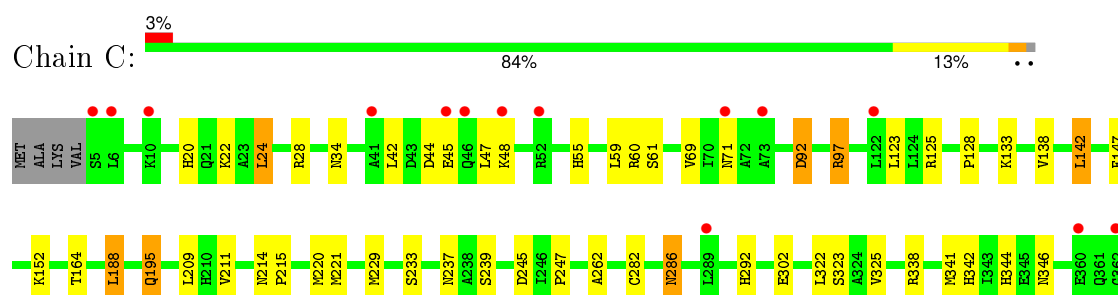
- Molecule 1: D-3-phosphoglycerate dehydrogenase

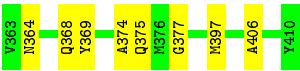


- Molecule 1: D-3-phosphoglycerate dehydrogenase

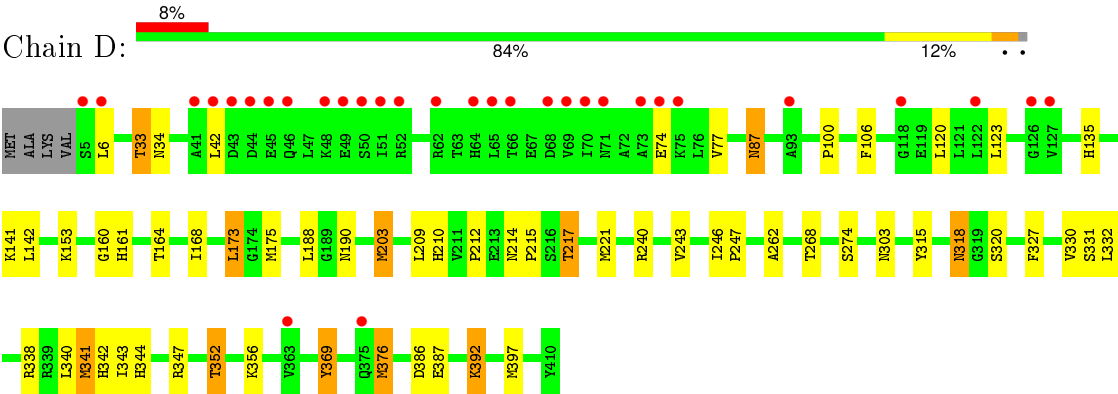


- Molecule 1: D-3-phosphoglycerate dehydrogenase





● Molecule 1: D-3-phosphoglycerate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	76.16 Å 76.16 Å 354.14 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.24 49.00 – 2.24	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-2.24) 94.2 (49.00-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	32.92 (at 2.24 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.235 0.204 , 0.244	Depositor DCC
R_{free} test set	4538 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.4	EDS
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 90530 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14017	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AKG, PO4, UNL, 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	0.74	0/3128	0.81	2/4224 (0.0%)
1	B	0.78	0/3131	0.81	4/4228 (0.1%)
1	C	0.75	0/3141	0.79	2/4239 (0.0%)
1	D	0.77	1/3139 (0.0%)	0.79	0/4239
All	All	0.76	1/12539 (0.0%)	0.80	8/16930 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	203	MSE	SE-CE	6.56	2.34	1.95

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	60	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	A	60	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	B	28	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	C	322	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	B	60	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	28	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	60	ARG	NE-CZ-NH2	-5.21	117.69	120.30

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	3083	0	3120	34	0
1	B	3086	0	3121	36	0
1	C	3097	0	3135	57	0
1	D	3094	0	3124	42	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	4	0
3	C	10	0	4	2	0
3	D	10	0	4	0	0
4	A	20	0	0	0	0
4	B	10	0	0	1	0
4	C	20	0	0	2	0
4	D	20	0	0	2	0
5	A	44	0	26	0	0
5	B	44	0	26	1	0
5	C	44	0	26	0	0
5	D	44	0	26	0	0
6	A	300	0	0	5	0
6	B	330	0	0	6	0
6	C	350	0	0	7	0
6	D	366	0	0	7	0
All	All	14017	0	12620	168	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 7.

All (168) 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:D:175:MSE:SE	1:D:175:MSE:CE	2.16	1.42
1:A:376:MSE:SE	1:A:376:MSE:CE	2.18	1.41
1:D:376:MSE:SE	1:D:376:MSE:CE	2.21	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:MSE:CE	1:D:203:MSE:SE	2.34	1.25
1:D:212:PRO:O	1:D:217:THR:HG21	1.66	0.96
1:C:97:ARG:HD3	6:C:671:HOH:O	1.66	0.95
1:C:375[B]:GLN:NE2	1:C:375[B]:GLN:H	1.66	0.92
1:A:355:ASN:HD21	1:A:368:GLN:HE22	1.12	0.92
1:C:375[B]:GLN:H	1:C:375[B]:GLN:HE21	0.94	0.91
1:B:348:PRO:HB3	1:C:364:ASN:ND2	1.88	0.88
1:B:343:ILE:HG23	1:B:376:MSE:HE3	1.59	0.84
1:B:190:ASN:HD21	1:D:190:ASN:HD21	1.27	0.82
1:B:348:PRO:HB3	1:C:364:ASN:HD21	1.41	0.81
1:C:375[B]:GLN:N	1:C:375[B]:GLN:HE21	1.77	0.80
1:C:342:HIS:HD2	1:C:344:HIS:HD2	1.26	0.80
1:B:387:GLU:HB2	6:B:674:HOH:O	1.81	0.78
1:B:340:LEU:HD13	1:B:397:MSE:HE1	1.72	0.70
1:C:214:ASN:HB2	1:C:215:PRO:HD2	1.73	0.70
1:A:342:HIS:HD2	1:A:344:HIS:HD2	1.39	0.70
1:C:342:HIS:HD2	1:C:344:HIS:CD2	2.10	0.69
1:D:341:MSE:HE3	1:D:343:ILE:HG13	1.73	0.69
1:A:24:LEU:H	1:A:24:LEU:HD23	1.57	0.69
3:B:412:AKG:O4	3:B:412:AKG:C2	2.41	0.68
1:B:164:THR:HG23	1:B:188:LEU:CD1	2.25	0.67
1:C:142:LEU:O	1:C:142:LEU:HD22	1.95	0.66
1:A:286:ASN:HD22	1:A:286:ASN:H	1.43	0.66
1:D:303:ASN:HB3	6:D:718:HOH:O	1.95	0.65
1:A:355:ASN:ND2	1:A:368:GLN:HE22	1.92	0.65
1:A:22:LYS:HE2	1:A:302:GLU:OE2	1.97	0.65
1:C:375[B]:GLN:HG2	6:C:500:HOH:O	1.96	0.64
4:D:414:UNL:O4	4:D:414:UNL:C2	2.44	0.64
1:C:71:ASN:HD21	1:C:97:ARG:NH2	1.96	0.63
1:C:397:MSE:HE2	1:C:406:ALA:HB1	1.80	0.63
1:C:342:HIS:CD2	1:C:344:HIS:HD2	2.13	0.63
1:C:22:LYS:HG3	1:C:302:GLU:HG3	1.80	0.62
1:A:342:HIS:HD2	1:A:344:HIS:CD2	2.17	0.62
1:B:186:LEU:HD12	1:B:187:PRO:HD2	1.81	0.62
4:C:414:UNL:O2	4:C:414:UNL:O4	2.18	0.62
1:B:190:ASN:ND2	1:D:190:ASN:HD21	1.95	0.62
1:B:340:LEU:HD22	1:B:397:MSE:HE1	1.81	0.62
1:D:153:LYS:HE2	1:D:203:MSE:HE2	1.81	0.61
1:B:340:LEU:HD22	1:B:397:MSE:CE	2.30	0.61
1:A:24:LEU:N	1:A:24:LEU:HD23	2.15	0.60
1:C:20:HIS:HD2	1:C:22:LYS:H	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:HD22	1:B:295:GLY:HA3	1.66	0.60
1:C:47:LEU:HB3	1:C:48:LYS:HE3	1.84	0.60
1:B:20:HIS:HD2	1:B:22:LYS:H	1.50	0.60
1:D:33:THR:HG22	6:D:762:HOH:O	2.01	0.59
1:C:71:ASN:HD21	1:C:97:ARG:HH21	1.51	0.59
1:A:214:ASN:HB2	1:A:215:PRO:HD2	1.83	0.59
1:B:332:LEU:HD13	1:B:369:TYR:HB2	1.85	0.59
1:C:375[B]:GLN:CG	6:C:500:HOH:O	2.51	0.58
1:B:161:HIS:HD2	5:B:414:NAD:O2A	1.86	0.58
1:D:217:THR:HG22	6:D:531:HOH:O	2.03	0.58
1:B:164:THR:HG23	1:B:188:LEU:HD12	1.86	0.58
1:D:341:MSE:C	1:D:341:MSE:HE2	2.24	0.58
1:A:405:ARG:HD3	6:A:707:HOH:O	2.04	0.57
1:C:286:ASN:H	1:C:286:ASN:HD22	1.50	0.57
1:A:60:ARG:HD3	6:A:507:HOH:O	2.03	0.57
1:D:217:THR:HG23	1:D:243:VAL:HG22	1.86	0.57
4:B:413:UNL:C2	4:B:413:UNL:O3	2.52	0.56
1:D:341:MSE:HE2	1:D:342:HIS:N	2.20	0.56
1:D:318:ASN:HD22	1:D:318:ASN:C	2.08	0.56
1:C:44:ASP:O	1:C:48:LYS:HG2	2.06	0.55
1:B:185:LYS:H	1:B:193:GLN:HE22	1.54	0.55
1:C:92:ASP:OD2	1:C:92:ASP:N	2.40	0.55
1:B:387:GLU:OE2	1:B:387:GLU:HA	2.06	0.55
1:C:61:SER:HG	3:C:412:AKG:C5	2.19	0.54
4:C:414:UNL:C2	4:C:414:UNL:O4	2.55	0.54
1:C:209:LEU:HD22	1:C:220:MSE:HE3	1.89	0.54
1:C:209:LEU:CD2	1:C:220:MSE:HE3	2.38	0.54
1:C:211:VAL:HG21	1:C:220:MSE:HE2	1.90	0.54
1:C:142:LEU:C	1:C:142:LEU:CD2	2.76	0.54
1:D:210:HIS:HD2	6:D:482:HOH:O	1.91	0.53
1:A:142:LEU:HD23	1:A:142:LEU:O	2.09	0.53
3:B:412:AKG:H42	6:B:559:HOH:O	2.09	0.53
1:A:290:THR:HB	1:A:293:ILE:HD11	1.91	0.53
1:A:141:LYS:HZ1	3:B:412:AKG:H31	1.74	0.52
1:D:164:THR:HG23	1:D:188:LEU:HD22	1.91	0.52
1:B:388:ASP:OD2	1:B:388:ASP:N	2.40	0.51
1:D:87:ASN:N	1:D:87:ASN:OD1	2.43	0.51
1:A:59:LEU:N	1:A:59:LEU:HD23	2.25	0.51
1:C:20:HIS:HE1	6:C:681:HOH:O	1.92	0.51
1:C:142:LEU:O	1:C:142:LEU:CD2	2.59	0.51
4:D:414:UNL:C5	4:D:414:UNL:O2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD22	1:B:294:GLY:HA2	1.93	0.51
1:B:20:HIS:CD2	1:B:22:LYS:H	2.29	0.51
1:B:368:GLN:NE2	1:C:368:GLN:HE21	2.09	0.50
1:B:108:ASN:ND2	1:B:295:GLY:HA3	2.26	0.50
1:A:205:ASP:OD1	1:A:230:LYS:HE2	2.12	0.50
1:C:237:ASN:ND2	1:C:239:SER:H	2.08	0.50
1:B:169:LEU:O	1:B:172:SER:HB2	2.11	0.50
1:A:24:LEU:N	1:A:24:LEU:CD2	2.74	0.50
1:A:141:LYS:NZ	3:B:412:AKG:H31	2.26	0.50
1:D:341:MSE:HE2	1:D:342:HIS:CA	2.42	0.49
1:C:209:LEU:HD11	1:C:221:MSE:HG3	1.94	0.49
1:C:342:HIS:CD2	1:C:344:HIS:CD2	2.97	0.49
1:D:342:HIS:HD2	1:D:344:HIS:CD2	2.30	0.49
1:A:310:GLY:O	1:A:314:LYS:HG3	2.13	0.49
1:B:131:ASN:O	1:B:135:HIS:HD2	1.96	0.49
1:B:5:SER:HA	1:B:8:LYS:HB2	1.94	0.48
1:C:147:PHE:HB3	1:C:152:LYS:HE2	1.95	0.48
1:C:71:ASN:ND2	1:C:97:ARG:HH21	2.12	0.47
1:B:246:ILE:HB	1:B:247:PRO:HD3	1.97	0.46
1:A:22:LYS:CE	1:A:302:GLU:OE2	2.62	0.46
1:B:123:LEU:HD23	1:B:128:PRO:HG2	1.98	0.46
1:D:352:THR:O	1:D:356:LYS:HB2	2.16	0.46
1:B:120:LEU:C	1:B:120:LEU:HD12	2.36	0.46
1:C:292:HIS:HB3	1:D:141:LYS:HE2	1.98	0.46
1:B:229:MSE:HE2	1:B:233:SER:OG	2.16	0.46
1:D:209:LEU:HD11	1:D:221:MSE:HG3	1.98	0.45
1:A:342:HIS:HB2	1:A:397:MSE:HE3	1.98	0.45
1:C:245:ASP:OD1	1:C:247:PRO:HD2	2.16	0.45
1:D:330:VAL:HG13	1:D:369:TYR:CG	2.52	0.45
1:B:368:GLN:HE21	1:C:368:GLN:HE21	1.64	0.45
1:D:246:ILE:HB	1:D:247:PRO:HD3	1.97	0.45
1:B:407:ARG:HG3	6:B:702:HOH:O	2.17	0.45
1:C:342:HIS:ND1	1:C:397:MSE:HE3	2.32	0.45
1:A:354:LEU:HD13	1:A:400:ILE:CD1	2.47	0.45
1:C:164:THR:HG23	1:C:188:LEU:HG	1.99	0.45
1:A:407:ARG:CD	6:A:707:HOH:O	2.65	0.44
1:D:342:HIS:HE1	1:D:397:MSE:O	2.00	0.44
1:D:318:ASN:ND2	1:D:318:ASN:C	2.70	0.44
1:A:338:ARG:HB2	1:A:383:ILE:HG13	2.00	0.44
1:C:282:CYS:O	1:D:135:HIS:HD2	2.01	0.43
1:C:24:LEU:O	1:C:28:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LYS:HB3	1:C:138:VAL:HB	2.00	0.43
1:B:358:PHE:CZ	1:B:397:MSE:HE2	2.53	0.43
1:B:185:LYS:NZ	6:B:696:HOH:O	2.51	0.43
1:D:340:LEU:HD22	1:D:397:MSE:SE	2.68	0.43
1:C:55:HIS:HD2	6:C:606:HOH:O	2.00	0.43
1:D:214:ASN:HB2	1:D:215:PRO:CD	2.48	0.43
1:C:374:ALA:CB	1:C:375[B]:GLN:NE2	2.82	0.43
1:C:346:ASN:HD21	1:C:377:GLY:HA3	1.83	0.43
1:C:123:LEU:HD23	1:C:128:PRO:HG2	2.01	0.43
1:C:48:LYS:HE2	1:C:69:VAL:HG22	2.01	0.43
1:A:397:MSE:HE2	1:A:406:ALA:HB1	2.01	0.43
1:C:61:SER:OG	3:C:412:AKG:C5	2.67	0.42
1:D:160:GLY:O	1:D:164:THR:HB	2.19	0.42
1:A:97:ARG:HD3	6:A:557:HOH:O	2.20	0.42
1:A:246:ILE:HB	1:A:247:PRO:HD3	2.02	0.42
1:A:342:HIS:CD2	1:A:344:HIS:HD2	2.28	0.42
1:D:161:HIS:CG	6:D:656:HOH:O	2.73	0.42
1:A:344:HIS:HE1	6:A:435:HOH:O	2.02	0.42
1:D:240:ARG:HD3	6:D:768:HOH:O	2.19	0.42
1:D:318:ASN:HD21	1:D:320:SER:HB2	1.85	0.41
1:C:211:VAL:HG11	1:C:220:MSE:HE1	2.02	0.41
1:C:195:GLN:NE2	6:C:595:HOH:O	2.52	0.41
1:C:142:LEU:C	1:C:142:LEU:HD22	2.40	0.41
1:D:120:LEU:HD12	1:D:120:LEU:C	2.41	0.41
1:C:344:HIS:HE1	6:C:537:HOH:O	2.04	0.41
1:D:168:ILE:HD11	1:D:188:LEU:HD23	2.02	0.41
1:C:209:LEU:HD22	1:C:220:MSE:CE	2.50	0.41
1:D:332:LEU:HD13	1:D:369:TYR:HB2	2.02	0.41
1:C:229:MSE:HE2	1:C:233:SER:OG	2.21	0.41
1:D:77:VAL:HG12	1:D:315:TYR:HE2	1.86	0.41
1:A:46:GLN:HA	1:A:46:GLN:NE2	2.36	0.41
1:D:392:LYS:HE2	6:D:661:HOH:O	2.21	0.41
1:A:179:PHE:CZ	1:A:193:GLN:HB2	2.56	0.41
1:A:354:LEU:HD13	1:A:400:ILE:HD13	2.03	0.41
1:B:60:ARG:HD3	6:B:423:HOH:O	2.20	0.40
1:A:220:MSE:HG2	1:A:243:VAL:HG13	2.04	0.40
1:D:318:ASN:ND2	1:D:320:SER:H	2.20	0.40
1:C:123:LEU:HD11	1:C:262:ALA:HB2	2.03	0.40
1:D:173:LEU:HD12	1:D:173:LEU:HA	1.91	0.40
1:C:374:ALA:HB3	1:C:375[B]:GLN:NE2	2.37	0.40
1:D:123:LEU:HD11	1:D:262:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLU:HB2	6:B:661:HOH:O	2.22	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	405/410 (99%)	386 (95%)	18 (4%)	1 (0%)	52	60
1	B	405/410 (99%)	389 (96%)	14 (4%)	2 (0%)	34	34
1	C	406/410 (99%)	393 (97%)	13 (3%)	0	100	100
1	D	406/410 (99%)	383 (94%)	21 (5%)	2 (0%)	34	34
All	All	1622/1640 (99%)	1551 (96%)	66 (4%)	5 (0%)	46	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	74	GLU
1	B	43	ASP
1	D	6	LEU
1	A	386	ASP
1	B	215	PRO

5.3.2 Protein sidechains [i](#)

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	329/323 (102%)	307 (93%)	22 (7%)	20	18
1	B	329/323 (102%)	305 (93%)	24 (7%)	17	14
1	C	330/323 (102%)	313 (95%)	17 (5%)	29	29
1	D	330/323 (102%)	307 (93%)	23 (7%)	19	16
All	All	1318/1292 (102%)	1232 (94%)	86 (6%)	21	19

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	24	LEU
1	A	39	LYS
1	A	42	LEU
1	A	45	GLU
1	A	52	ARG
1	A	68	ASP
1	A	74	GLU
1	A	75	LYS
1	A	108	ASN
1	A	136	ARG
1	A	142	LEU
1	A	173	LEU
1	A	195	GLN
1	A	274	SER
1	A	286	ASN
1	A	341	MSE
1	A	354	LEU
1	A	356	LYS
1	A	369	TYR
1	A	388	ASP
1	A	407	ARG
1	B	5	SER
1	B	6	LEU
1	B	59	LEU
1	B	109	THR
1	B	142	LEU
1	B	192	THR
1	B	256	LYS
1	B	274	SER
1	B	307	GLU
1	B	312	LEU
1	B	325	VAL

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Mol	Chain	Res	Type
1	B	327	PHE
1	B	338	ARG
1	B	341	MSE
1	B	346	ASN
1	B	347	ARG
1	B	369	TYR
1	B	373	SER
1	B	375	GLN
1	B	376	MSE
1	B	381	ILE
1	B	387	GLU
1	B	388	ASP
1	B	392	LYS
1	C	24	LEU
1	C	34	ASN
1	C	42	LEU
1	C	45	GLU
1	C	59	LEU
1	C	92	ASP
1	C	97	ARG
1	C	125	ARG
1	C	142	LEU
1	C	188	LEU
1	C	195	GLN
1	C	286	ASN
1	C	323	SER
1	C	325	VAL
1	C	338	ARG
1	C	341	MSE
1	C	369	TYR
1	D	33	THR
1	D	34	ASN
1	D	42	LEU
1	D	87	ASN
1	D	100	PRO
1	D	106	PHE
1	D	142	LEU
1	D	173	LEU
1	D	217	THR
1	D	268	THR
1	D	274	SER
1	D	318	ASN

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Mol	Chain	Res	Type
1	D	327	PHE
1	D	331	SER
1	D	338	ARG
1	D	341	MSE
1	D	347	ARG
1	D	352	THR
1	D	369	TYR
1	D	376	MSE
1	D	386	ASP
1	D	387	GLU
1	D	392	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	87	ASN
1	A	108	ASN
1	A	273	ASN
1	A	286	ASN
1	A	303	ASN
1	A	342	HIS
1	A	344	HIS
1	A	346	ASN
1	A	368	GLN
1	B	20	HIS
1	B	46	GLN
1	B	55	HIS
1	B	71	ASN
1	B	161	HIS
1	B	184	ASN
1	B	190	ASN
1	B	193	GLN
1	B	257	HIS
1	B	273	ASN
1	B	303	ASN
1	B	346	ASN
1	B	355	ASN
1	B	368	GLN
1	B	395	GLN
1	C	20	HIS
1	C	34	ASN

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Mol	Chain	Res	Type
1	C	46	GLN
1	C	71	ASN
1	C	108	ASN
1	C	140	ASN
1	C	190	ASN
1	C	195	GLN
1	C	237	ASN
1	C	273	ASN
1	C	286	ASN
1	C	303	ASN
1	C	342	HIS
1	C	344	HIS
1	C	346	ASN
1	C	364	ASN
1	D	34	ASN
1	D	140	ASN
1	D	161	HIS
1	D	210	HIS
1	D	257	HIS
1	D	273	ASN
1	D	303	ASN
1	D	318	ASN
1	D	342	HIS
1	D	346	ASN
1	D	355	ASN
1	D	368	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 20 ligands modelled in this entry, 7 are unknown - leaving 13 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$
2	PO4	A	411	-	4,4,4	1.08	0	6,6,6	0.27	0
2	PO4	A	412	-	4,4,4	0.26	0	6,6,6	0.27	0
3	AKG	A	413	-	3,9,9	0.25	0	4,11,11	1.77	1 (25%)
5	NAD	A	416	-	38,48,48	1.85	3 (7%)	47,73,73	1.85	4 (8%)
2	PO4	B	411	-	4,4,4	0.57	0	6,6,6	0.43	0
3	AKG	B	412	-	3,9,9	1.41	1 (33%)	4,11,11	1.44	1 (25%)
5	NAD	B	414	-	38,48,48	1.66	4 (10%)	47,73,73	2.11	7 (14%)
2	PO4	C	411	-	4,4,4	0.64	0	6,6,6	0.28	0
3	AKG	C	412	-	3,9,9	1.61	1 (33%)	4,11,11	2.16	2 (50%)
5	NAD	C	415	-	38,48,48	1.75	2 (5%)	47,73,73	2.26	8 (17%)
2	PO4	D	411	-	4,4,4	0.81	0	6,6,6	0.41	0
3	AKG	D	412	-	3,9,9	1.71	1 (33%)	4,11,11	1.28	1 (25%)
5	NAD	D	415	-	38,48,48	1.62	3 (7%)	47,73,73	2.31	9 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	411	-	-	0/0/0/0	0/0/0/0
2	PO4	A	412	-	-	0/0/0/0	0/0/0/0
3	AKG	A	413	-	-	0/3/9/9	0/0/0/0
5	NAD	A	416	-	-	0/22/62/62	0/5/5/5
2	PO4	B	411	-	-	0/0/0/0	0/0/0/0
3	AKG	B	412	-	-	0/3/9/9	0/0/0/0
5	NAD	B	414	-	-	0/22/62/62	0/5/5/5
2	PO4	C	411	-	-	0/0/0/0	0/0/0/0
3	AKG	C	412	-	-	0/3/9/9	0/0/0/0
5	NAD	C	415	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	D	411	-	-	0/0/0/0	0/0/0/0
3	AKG	D	412	-	-	0/3/9/9	0/0/0/0
5	NAD	D	415	-	-	0/22/62/62	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	415	NAD	O4B-C4B	-2.02	1.40	1.45
3	B	412	AKG	O5-C2	2.15	1.26	1.22
3	D	412	AKG	C3-C2	2.20	1.54	1.51
5	D	415	NAD	C2A-N3A	2.24	1.36	1.32
3	C	412	AKG	C3-C2	2.33	1.54	1.51
5	A	416	NAD	C2A-N1A	2.57	1.38	1.33
5	B	414	NAD	O4D-C1D	2.81	1.44	1.41
5	B	414	NAD	C2A-N1A	2.95	1.39	1.33
5	C	415	NAD	C2A-N3A	4.00	1.39	1.32
5	B	414	NAD	C2A-N3A	4.16	1.39	1.32
5	A	416	NAD	C2A-N3A	4.85	1.40	1.32
5	B	414	NAD	O7N-C7N	7.28	1.39	1.24
5	C	415	NAD	O7N-C7N	8.14	1.41	1.24
5	D	415	NAD	O7N-C7N	8.31	1.41	1.24
5	A	416	NAD	O7N-C7N	8.64	1.42	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	415	NAD	N3A-C2A-N1A	-11.27	120.26	128.89
5	C	415	NAD	N3A-C2A-N1A	-9.75	121.43	128.89
5	B	414	NAD	N3A-C2A-N1A	-9.56	121.57	128.89
5	A	416	NAD	N3A-C2A-N1A	-7.20	123.38	128.89
5	A	416	NAD	C4A-C5A-N7A	-5.49	104.43	109.48
5	C	415	NAD	O7N-C7N-C3N	-5.04	114.09	119.59
5	D	415	NAD	C4A-C5A-N7A	-3.46	106.29	109.48
5	D	415	NAD	PN-O3-PA	-3.25	123.61	132.73
5	B	414	NAD	C1B-N9A-C4A	-3.16	122.18	126.94
5	D	415	NAD	C1B-N9A-C4A	-3.14	122.20	126.94
5	B	414	NAD	O7N-C7N-N7N	-2.98	118.41	122.59
3	A	413	AKG	C3-C4-C5	-2.85	107.53	112.75
3	C	412	AKG	C3-C4-C5	-2.79	107.64	112.75
3	B	412	AKG	C3-C2-C1	-2.76	114.90	121.51
5	B	414	NAD	O3-PN-O5D	-2.64	95.92	102.94
5	B	414	NAD	O4B-C1B-N9A	-2.57	102.72	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	416	NAD	PN-O3-PA	-2.52	125.65	132.73
5	C	415	NAD	PN-O3-PA	-2.26	126.39	132.73
5	D	415	NAD	O4B-C4B-C5B	-2.24	101.32	109.32
3	D	412	AKG	C3-C4-C5	-2.23	108.67	112.75
5	C	415	NAD	C1B-N9A-C4A	-2.10	123.77	126.94
5	C	415	NAD	C4A-C5A-N7A	-2.09	107.55	109.48
5	D	415	NAD	C2B-C1B-N9A	2.05	117.42	114.29
5	C	415	NAD	C2N-C3N-C4N	2.27	120.82	118.29
5	D	415	NAD	C2N-C3N-C4N	2.28	120.82	118.29
3	C	412	AKG	O5-C2-C3	2.45	124.90	120.28
5	B	414	NAD	C3N-C7N-N7N	2.80	120.88	117.82
5	D	415	NAD	O3-PA-O5B	3.87	113.21	102.94
5	C	415	NAD	C3N-C7N-N7N	4.53	122.78	117.82
5	D	415	NAD	O4D-C1D-N1N	4.70	113.29	108.13
5	A	416	NAD	O4D-C1D-N1N	6.12	114.85	108.13
5	B	414	NAD	O4D-C1D-N1N	6.44	115.20	108.13
5	C	415	NAD	O4D-C1D-N1N	6.96	115.78	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	412	AKG	4	0
5	B	414	NAD	1	0
3	C	412	AKG	2	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 ⓘ

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	398/410 (97%)	0.63	27 (6%)	20 21	36, 43, 50, 55	0
1	B	398/410 (97%)	0.51	8 (2%)	68 70	35, 43, 51, 69	0
1	C	398/410 (97%)	0.50	14 (3%)	48 50	35, 43, 51, 56	0
1	D	398/410 (97%)	0.65	31 (7%)	16 17	34, 43, 50, 65	0
All	All	1592/1640 (97%)	0.57	80 (5%)	32 34	34, 43, 51, 69	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	5	SER	6.7
1	D	6	LEU	6.6
1	D	64	HIS	5.8
1	A	52	ARG	5.2
1	A	48	LYS	4.9
1	A	6	LEU	4.8
1	C	52	ARG	4.8
1	A	49	GLU	4.7
1	B	5	SER	4.3
1	A	74	GLU	4.2
1	D	45	GLU	4.2
1	B	6	LEU	4.1
1	D	69	VAL	4.1
1	D	73	ALA	4.0
1	D	52	ARG	4.0
1	C	46	GLN	3.9
1	C	362	GLY	3.9
1	D	43	ASP	3.7
1	A	42	LEU	3.6
1	A	73	ALA	3.6
1	D	42	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	45	GLU	3.5
1	B	64	HIS	3.4
1	D	46	GLN	3.3
1	D	65	LEU	3.3
1	D	49	GLU	3.2
1	C	73	ALA	3.1
1	D	93	ALA	3.0
1	D	68	ASP	3.0
1	A	43	ASP	3.0
1	A	5	SER	2.9
1	D	70	ILE	2.9
1	A	37	PHE	2.9
1	A	70	ILE	2.8
1	A	72	ALA	2.8
1	C	48	LYS	2.8
1	A	50	SER	2.7
1	D	375	GLN	2.7
1	B	271	ALA	2.7
1	C	71	ASN	2.7
1	D	66	THR	2.7
1	D	71	ASN	2.6
1	A	16	VAL	2.6
1	C	6	LEU	2.6
1	A	127	VAL	2.5
1	D	44	ASP	2.4
1	A	68	ASP	2.4
1	B	45[A]	GLU	2.4
1	C	41	ALA	2.3
1	A	46	GLN	2.3
1	A	35	ILE	2.3
1	D	363	VAL	2.3
1	A	45	GLU	2.3
1	A	71	ASN	2.3
1	D	41	ALA	2.3
1	A	9	ASP	2.3
1	D	75	LYS	2.3
1	D	74	GLU	2.3
1	B	199	ASP	2.3
1	D	122	LEU	2.2
1	A	57	ILE	2.2
1	D	118	GLY	2.2
1	D	127	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	122	LEU	2.2
1	D	51	ILE	2.2
1	A	124	LEU	2.2
1	A	10	LYS	2.1
1	B	113	ALA	2.1
1	A	288	LEU	2.1
1	C	5	SER	2.1
1	C	10	LYS	2.1
1	C	289	LEU	2.1
1	C	360	GLU	2.1
1	D	48	LYS	2.1
1	A	282	CYS	2.0
1	A	128	PRO	2.0
1	D	62	ARG	2.0
1	D	126	GLY	2.0
1	D	50	SER	2.0
1	B	200	LEU	2.0

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(Å ²)	Q<0.9
2	PO4	A	412	5/5	0.82	0.30	6.30	100,101,101,102	0
3	AKG	D	412	10/10	0.81	0.22	3.32	45,60,66,69	0
4	UNL	C	414	10/-	0.87	0.32	3.04	62,69,77,79	0
4	UNL	D	413	10/-	0.93	0.18	2.00	25,51,62,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	AKG	C	412	10/10	0.85	0.17	1.14	54,67,73,74	0
4	UNL	D	414	10/-	0.87	0.32	0.82	67,79,80,82	0
4	UNL	B	413	10/-	0.89	0.23	0.81	80,83,86,86	0
4	UNL	A	415	10/-	0.81	0.27	0.48	68,71,74,76	0
3	AKG	A	413	10/10	0.86	0.14	-0.18	63,64,69,71	0
2	PO4	B	411	5/5	0.97	0.14	-0.70	33,36,42,42	0
3	AKG	B	412	10/10	0.87	0.14	-0.75	55,58,61,63	0
5	NAD	B	414	44/44	0.95	0.12	-1.43	34,42,47,48	0
5	NAD	A	416	44/44	0.97	0.11	-1.46	28,31,36,38	0
5	NAD	C	415	44/44	0.96	0.11	-1.69	27,35,38,40	0
5	NAD	D	415	44/44	0.97	0.09	-1.74	33,39,41,42	0
2	PO4	C	411	5/5	0.99	0.09	-2.45	32,33,34,34	0
4	UNL	A	414	10/-	0.88	0.27	-	57,61,71,74	0
4	UNL	C	413	10/-	0.92	0.29	-	52,63,76,77	0
2	PO4	D	411	5/5	0.99	0.09	-	27,31,35,39	0
2	PO4	A	411	5/5	0.99	0.07	-	27,28,29,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.