Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:28 PM GMT

PDB ID	:	1XAJ
Title	:	CRYSTAL STRUCTURE OF STAPHLYOCOCCUS AUREUS 3-DEHYDROQUINATE SYNTHASE (DHQS) IN COMPLEX WITH ZN2+, NAD+ AND CARBAPHOSPHONATE
Authors	:	Nichols, C.E.; Ren, J.; Leslie, K.; Dhaliwal, B.; Lockyer, M.; Charles, I.; Hawkins, A.R.; Stammers, D.K.
Deposited on	:	2004-08-25
Resolution	:	2.35 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

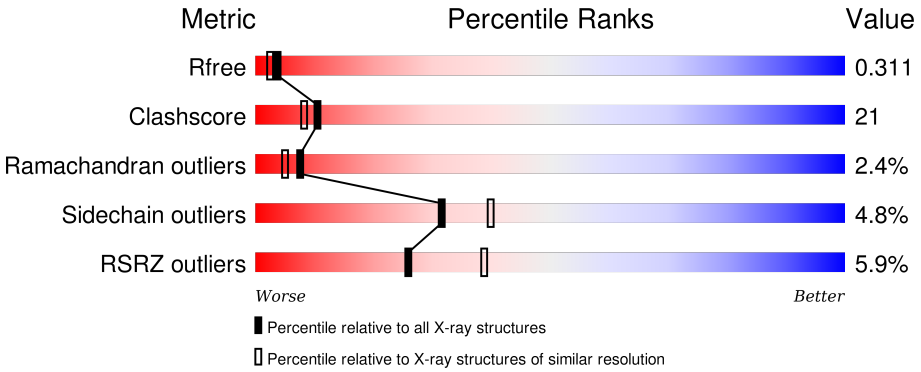
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 <=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	354	5%, 53%, 38%, 5%
1	B	354	6%, 51%, 40%, 5%

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	ZN	A	600	-	-	-	X
2	ZN	B	601	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5760 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 3-dehydroquinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2701	1746	450	497	8			
1	B	337	Total	C	N	O	S	0	0	0
			2701	1746	450	497	8			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	LYS	ASP	see remark 999	UNP Q6GGU4
A	23	TYR	HIS	see remark 999	UNP Q6GGU4
A	25	GLY	SER	see remark 999	UNP Q6GGU4
A	28	LEU	ILE	see remark 999	UNP Q6GGU4
A	29	ASN	ASP	see remark 999	UNP Q6GGU4
A	36	LEU	ILE	see remark 999	UNP Q6GGU4
A	41	TYR	HIS	see remark 999	UNP Q6GGU4
A	48	ASN	ASP	see remark 999	UNP Q6GGU4
A	109	VAL	ILE	see remark 999	UNP Q6GGU4
A	170	LYS	GLU	see remark 999	UNP Q6GGU4
A	226	VAL	ILE	see remark 999	UNP Q6GGU4
A	282	SER	ASN	see remark 999	UNP Q6GGU4
A	326	MET	ILE	see remark 999	UNP Q6GGU4
B	22	LYS	ASP	see remark 999	UNP Q6GGU4
B	23	TYR	HIS	see remark 999	UNP Q6GGU4
B	25	GLY	SER	see remark 999	UNP Q6GGU4
B	28	LEU	ILE	see remark 999	UNP Q6GGU4
B	29	ASN	ASP	see remark 999	UNP Q6GGU4
B	36	LEU	ILE	see remark 999	UNP Q6GGU4
B	41	TYR	HIS	see remark 999	UNP Q6GGU4
B	48	ASN	ASP	see remark 999	UNP Q6GGU4
B	109	VAL	ILE	see remark 999	UNP Q6GGU4
B	170	LYS	GLU	see remark 999	UNP Q6GGU4
B	226	VAL	ILE	see remark 999	UNP Q6GGU4
B	282	SER	ASN	see remark 999	UNP Q6GGU4

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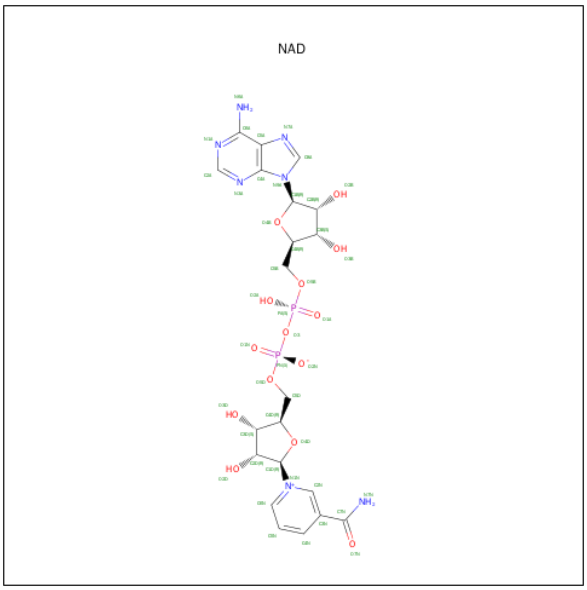
Chain	Residue	Modelled	Actual	Comment	Reference
B	326	MET	ILE	see remark 999	UNP Q6GGU4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

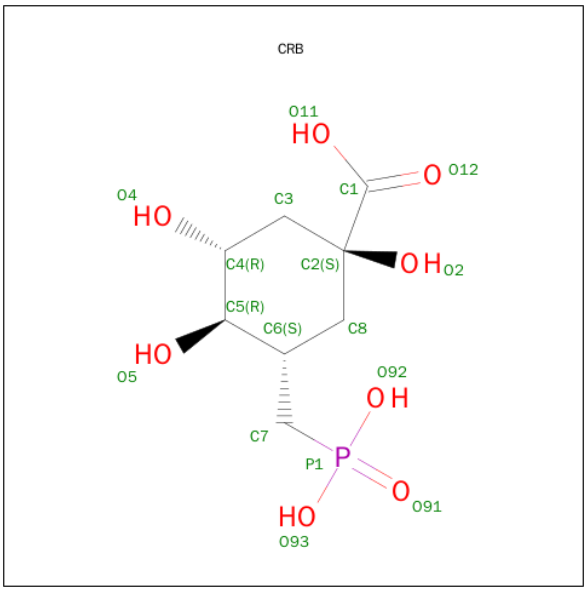
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is [1R-(1ALPHA,3BETA,4ALPHA,5BETA)]-5-(PHOSPHONOMETHYL)-1 ,3,4-TRIHYDROXYCYCLOHEXANE-1-CARBOXYLIC ACID (three-letter code: CRB) (formula: $C_8H_{15}O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 17 8 8 1	0	0
4	B	1	Total C O P 17 8 8 1	0	0

- Molecule 5 is water.

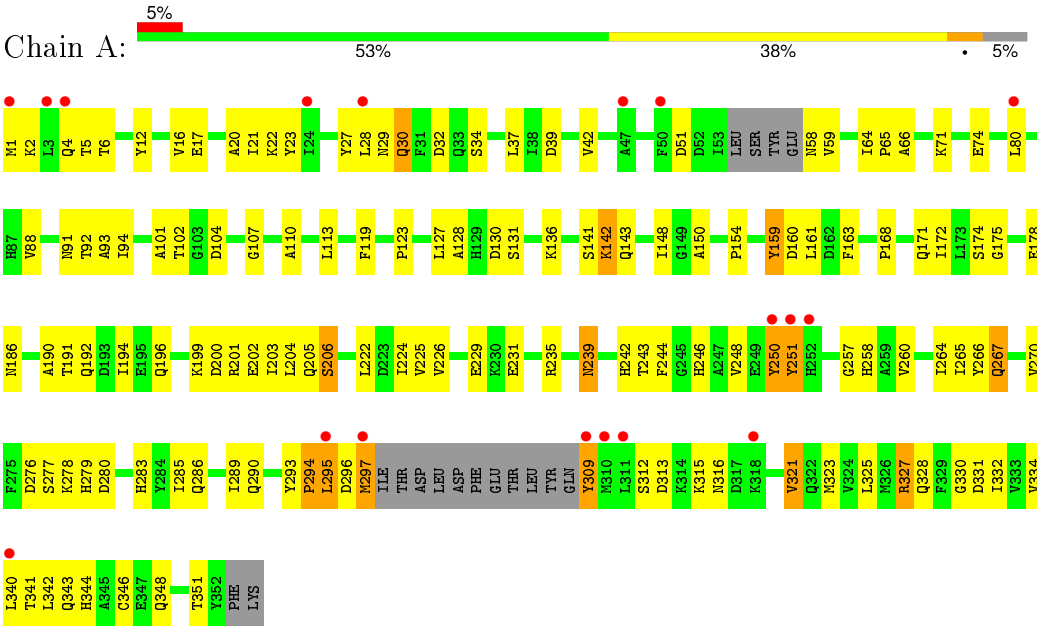
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	131	Total O 131 131	0	0
5	B	103	Total O 103 103	0	0

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.

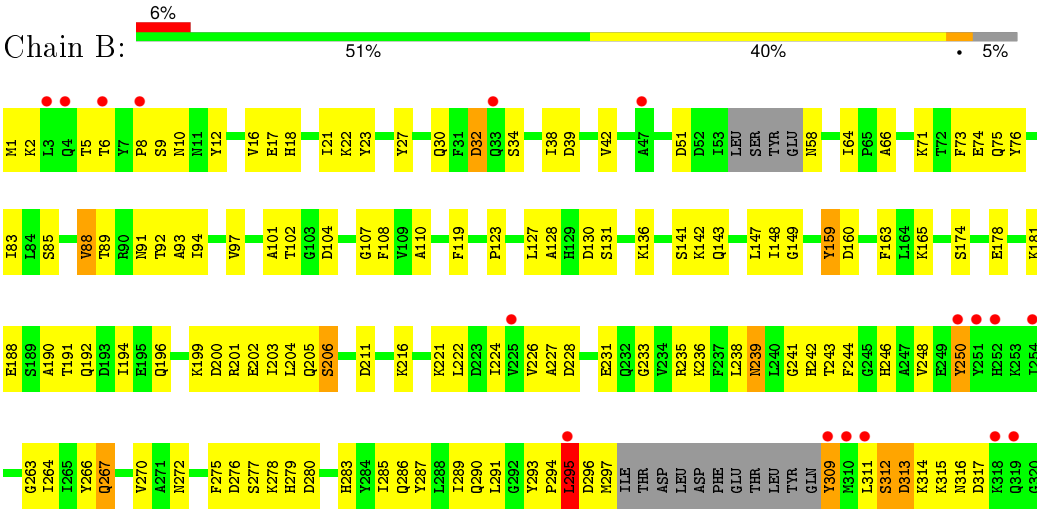
- Molecule 1: 3-dehydroquinate synthase

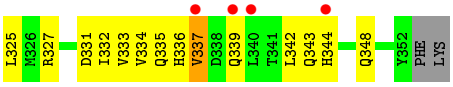
Chain A:



- Molecule 1: 3-dehydroquinate synthase

Chain B:




L325
M326
R327
D331
I332
V333
V334
Q335
H336
V337
D338
Q339
L340
T341
L342
Q343
H344
Q348
Y352
PHE
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	54.74Å 54.74Å 231.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.55 – 2.35 25.55 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.4 (25.55-2.35) 97.5 (25.55-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.58 (at 2.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.311 0.219 , 0.311	Depositor DCC
R_{free} test set	2739 reflections (9.99%)	DCC
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.0	EDS
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 27413 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5760	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CRB, ZN, 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	0.35	0/2762	0.61	0/3735
1	B	0.34	0/2762	0.60	0/3735
All	All	0.35	0/5524	0.61	0/7470

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	2701	0	2677	117	0
1	B	2701	0	2677	119	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	44	0	26	3	0
3	B	44	0	26	2	0
4	A	17	0	12	0	0
4	B	17	0	12	1	0
5	A	131	0	0	5	0
5	B	103	0	0	8	0
All	All	5760	0	5430	234	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 21.

All (234) 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:272:ASN:HD21	1:A:279:HIS:HB2	1.13	1.08
1:B:272:ASN:HD21	1:B:279:HIS:HB2	1.21	0.99
1:B:250:TYR:HD2	1:B:309:TYR:HH	0.99	0.97
1:A:294:PRO:O	1:A:296:ASP:N	2.00	0.94
1:A:94:ILE:HG13	1:A:110:ALA:HB2	1.52	0.92
1:B:289:ILE:HG12	1:B:295:LEU:HD11	1.53	0.91
1:B:294:PRO:O	1:B:296:ASP:N	2.06	0.88
1:A:327:ARG:NH1	1:A:331:ASP:OD1	2.11	0.82
1:A:244:PHE:O	1:A:248:VAL:HG23	1.83	0.79
1:B:244:PHE:O	1:B:248:VAL:HG23	1.83	0.79
1:A:250:TYR:HD2	1:A:309:TYR:HH	1.33	0.77
1:B:94:ILE:HG13	1:B:110:ALA:HB2	1.67	0.77
1:A:272:ASN:ND2	1:A:279:HIS:HB2	1.97	0.75
1:A:289:ILE:HG12	1:A:295:LEU:HD11	1.70	0.74
1:A:321:VAL:O	1:A:336:HIS:HA	1.88	0.73
1:B:272:ASN:ND2	1:B:279:HIS:HB2	2.03	0.72
1:B:323:MET:O	1:B:334:VAL:HA	1.89	0.71
1:A:39:ASP:HB3	1:A:42:VAL:HG23	1.73	0.70
1:A:270:VAL:HG12	1:A:325:LEU:HD11	1.71	0.70
1:A:174:SER:O	1:A:257:GLY:HA3	1.91	0.70
1:B:32:ASP:OD2	1:B:91:ASN:HB3	1.93	0.69
1:A:313:ASP:HB3	1:A:316:ASN:OD1	1.94	0.68
1:A:94:ILE:CG1	1:A:110:ALA:HB2	2.21	0.68
1:A:32:ASP:OD2	1:A:91:ASN:HB3	1.95	0.67
1:B:141:SER:C	1:B:143:GLN:H	1.97	0.67
1:B:64:ILE:HD11	1:B:102:THR:HG23	1.77	0.66
1:B:289:ILE:HG12	1:B:295:LEU:CD1	2.25	0.66
1:A:141:SER:C	1:A:143:GLN:H	1.98	0.66
1:A:6:THR:OG1	1:A:226:VAL:HG11	1.95	0.66
1:B:39:ASP:HB3	1:B:42:VAL:HG23	1.77	0.66
1:B:6:THR:OG1	1:B:226:VAL:HG11	1.97	0.65
1:A:330:GLY:HA2	5:A:645:HOH:O	1.95	0.65
1:A:128:ALA:HA	1:A:131:SER:OG	1.97	0.64
1:B:275:PHE:CB	1:B:327:ARG:HG3	2.28	0.64
1:B:94:ILE:CG1	1:B:110:ALA:HB2	2.28	0.64
1:A:92:THR:HG22	1:A:93:ALA:N	2.12	0.64
1:B:192:GLN:O	1:B:196:GLN:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASP:HB3	1:A:42:VAL:CG2	2.29	0.63
1:A:323:MET:O	1:A:334:VAL:HA	1.99	0.63
1:B:92:THR:HG22	1:B:93:ALA:N	2.13	0.62
1:A:266:TYR:OH	1:A:342:LEU:HD22	1.98	0.62
1:A:267:GLN:HG2	1:A:325:LEU:HD23	1.82	0.62
1:A:243:THR:HG21	1:A:323:MET:HA	1.82	0.62
1:A:191:THR:O	1:A:194:ILE:HG22	1.99	0.62
1:B:191:THR:O	1:B:194:ILE:HG22	2.00	0.62
1:A:250:TYR:O	1:A:251:TYR:HB2	1.99	0.61
1:A:276:ASP:OD2	1:A:278:LYS:HE2	2.00	0.60
1:B:39:ASP:HB3	1:B:42:VAL:CG2	2.32	0.60
1:A:192:GLN:O	1:A:196:GLN:HG3	2.03	0.59
1:B:8:PRO:O	1:B:9:SER:HB3	2.04	0.58
1:B:216:LYS:HD3	5:B:1051:HOH:O	2.03	0.58
1:B:275:PHE:HB3	1:B:327:ARG:HG3	1.85	0.58
1:B:128:ALA:HA	1:B:131:SER:OG	2.02	0.58
1:A:199:LYS:HG3	1:A:203:ILE:HD12	1.85	0.58
1:B:174:SER:O	1:B:257:GLY:HA3	2.03	0.58
1:B:246:HIS:HE1	5:B:1018:HOH:O	1.86	0.58
1:B:260:VAL:O	1:B:264:ILE:HG13	2.03	0.58
1:B:243:THR:HG21	1:B:323:MET:HA	1.85	0.57
1:A:37:LEU:HD13	1:A:94:ILE:HG23	1.85	0.56
1:A:94:ILE:HG13	1:A:110:ALA:CB	2.32	0.56
1:A:286:GLN:O	1:A:290:GLN:HG3	2.04	0.56
1:B:239:ASN:CB	1:B:315:LYS:HD3	2.35	0.56
1:A:21:ILE:HG12	1:A:21:ILE:O	2.05	0.55
1:B:141:SER:HB3	1:B:148:ILE:CD1	2.36	0.55
1:B:201:ARG:HE	1:B:205:GLN:NE2	2.05	0.55
1:A:225:VAL:HG12	1:A:235:ARG:CZ	2.37	0.55
1:B:313:ASP:HB3	1:B:316:ASN:OD1	2.07	0.54
1:A:250:TYR:HD2	1:A:309:TYR:OH	1.89	0.54
1:A:344:HIS:O	1:A:348:GLN:HB2	2.08	0.54
1:B:199:LYS:HD3	5:B:1098:HOH:O	2.05	0.54
1:B:92:THR:HG22	1:B:93:ALA:H	1.73	0.54
1:B:267:GLN:HG2	1:B:325:LEU:HD23	1.87	0.54
1:A:92:THR:HG22	1:A:93:ALA:H	1.73	0.54
1:B:83:ILE:HG22	1:B:88:VAL:HG11	1.89	0.54
1:B:201:ARG:HE	1:B:205:GLN:HE22	1.56	0.53
1:A:27:TYR:HA	1:A:30:GLN:NE2	2.24	0.53
1:B:286:GLN:O	1:B:290:GLN:HG3	2.08	0.53
1:B:1:MET:HG2	1:B:2:LYS:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASP:HB3	1:A:163:PHE:CE2	2.44	0.53
1:B:276:ASP:OD2	1:B:278:LYS:HE2	2.09	0.52
1:B:141:SER:C	1:B:143:GLN:N	2.61	0.52
1:B:178:GLU:HA	1:B:178:GLU:OE2	2.10	0.52
1:A:141:SER:C	1:A:143:GLN:N	2.63	0.52
1:A:178:GLU:OE2	1:A:178:GLU:HA	2.10	0.52
1:B:74:GLU:HG2	5:B:1089:HOH:O	2.10	0.52
1:B:287:TYR:O	1:B:291:LEU:HG	2.11	0.51
1:A:340:LEU:HD11	1:A:344:HIS:CE1	2.45	0.51
1:B:270:VAL:HG12	1:B:325:LEU:HD11	1.92	0.51
1:A:239:ASN:CB	1:A:315:LYS:HD3	2.41	0.51
1:A:39:ASP:OD1	1:A:66:ALA:HA	2.10	0.51
1:B:71:LYS:HD2	1:B:101:ALA:HA	1.93	0.50
1:B:74:GLU:HA	5:B:1049:HOH:O	2.11	0.50
1:B:221:LYS:HG3	1:B:238:LEU:HD11	1.94	0.50
1:B:79:THR:O	1:B:83:ILE:HG13	2.11	0.50
1:A:127:LEU:HB2	1:A:175:GLY:HA2	1.94	0.50
1:A:71:LYS:HD2	1:A:101:ALA:HA	1.92	0.50
1:B:321:VAL:O	1:B:336:HIS:HA	2.12	0.50
1:B:200:ASP:OD1	1:B:203:ILE:HG13	2.13	0.49
1:B:337:VAL:HG12	1:B:342:LEU:HG	1.94	0.49
1:B:199:LYS:HD2	5:B:1040:HOH:O	2.11	0.49
1:A:351:THR:HG21	5:A:621:HOH:O	2.12	0.49
1:A:16:VAL:O	1:A:17:GLU:HB3	2.12	0.49
1:A:199:LYS:HE2	1:A:200:ASP:OD2	2.12	0.49
1:B:242:HIS:HB3	1:B:246:HIS:CD2	2.48	0.49
1:A:17:GLU:O	1:A:160:ASP:HA	2.13	0.49
1:B:202:GLU:O	1:B:206:SER:HB3	2.13	0.49
1:B:127:LEU:HD23	1:B:127:LEU:O	2.13	0.48
1:B:16:VAL:O	1:B:17:GLU:HB3	2.13	0.48
1:A:5:THR:HG21	1:A:12:TYR:CE1	2.47	0.48
1:B:334:VAL:O	1:B:335:GLN:HB3	2.12	0.48
1:B:222:LEU:O	1:B:226:VAL:HG23	2.14	0.48
1:B:327:ARG:NH1	1:B:331:ASP:OD1	2.46	0.48
1:A:127:LEU:O	1:A:127:LEU:HD23	2.13	0.48
1:A:171:GLN:NE2	1:A:171:GLN:HA	2.28	0.48
1:A:201:ARG:HE	1:A:205:GLN:HE22	1.61	0.48
1:A:142:LYS:HE2	1:B:81:GLU:OE2	2.13	0.48
1:A:104:ASP:OD1	3:A:400:NAD:H2N	2.13	0.48
1:A:136:LYS:HB2	3:A:400:NAD:H72N	1.78	0.48
1:B:104:ASP:OD1	3:B:401:NAD:H2N	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:TYR:HA	1:B:30:GLN:OE1	2.13	0.48
1:A:224:ILE:N	1:A:224:ILE:HD13	2.28	0.48
1:A:258:HIS:HB3	1:A:297:MET:CE	2.44	0.48
1:A:142:LYS:HG3	1:B:81:GLU:OE2	2.14	0.48
1:B:5:THR:HG21	1:B:12:TYR:CE1	2.49	0.48
1:A:260:VAL:O	1:A:264:ILE:HG13	2.13	0.48
1:A:34:SER:N	1:A:58:ASN:O	2.47	0.47
1:B:1:MET:CG	1:B:2:LYS:N	2.77	0.47
1:B:141:SER:O	1:B:143:GLN:N	2.48	0.47
1:B:39:ASP:OD1	1:B:66:ALA:HA	2.14	0.47
1:A:141:SER:HB3	1:A:148:ILE:CD1	2.44	0.47
1:A:231:GLU:HA	1:A:235:ARG:HB3	1.95	0.47
1:B:231:GLU:HA	1:B:235:ARG:HB3	1.96	0.47
1:B:186:ASN:HB2	1:B:190:ALA:HB3	1.95	0.47
1:B:332:ILE:HD12	1:B:332:ILE:N	2.30	0.47
1:B:107:GLY:HA2	1:B:119:PHE:CZ	2.50	0.47
1:B:17:GLU:O	1:B:160:ASP:HA	2.15	0.47
1:B:241:GLY:O	1:B:263:GLY:HA3	2.15	0.47
1:A:4:GLN:HG3	1:A:12:TYR:O	2.16	0.46
1:B:314:LYS:HD2	5:B:1007:HOH:O	2.15	0.46
1:A:64:ILE:HD11	1:A:102:THR:HG23	1.97	0.46
1:A:92:THR:CG2	1:A:93:ALA:N	2.78	0.46
1:B:141:SER:OG	1:B:147:LEU:HD23	2.16	0.46
1:B:199:LYS:HG3	1:B:203:ILE:HD12	1.97	0.46
1:B:76:TYR:CZ	1:B:80:LEU:HD11	2.51	0.46
1:B:266:TYR:OH	1:B:342:LEU:HD22	2.16	0.46
1:B:123:PRO:HG2	1:B:159:TYR:CD2	2.50	0.46
1:A:327:ARG:HH12	1:A:331:ASP:CG	2.20	0.46
1:B:181:LYS:CD	1:B:242:HIS:HE1	2.29	0.46
1:A:80:LEU:HD23	1:A:113:LEU:HD13	1.97	0.45
1:A:130:ASP:OD2	3:A:400:NAD:H5N	2.16	0.45
1:B:236:LYS:O	1:B:324:VAL:HG21	2.16	0.45
1:A:123:PRO:HG2	1:A:159:TYR:CD2	2.50	0.45
1:A:34:SER:O	1:A:59:VAL:HA	2.17	0.45
1:B:327:ARG:NH2	1:B:333:VAL:HG11	2.31	0.45
1:B:181:LYS:HD3	1:B:242:HIS:HE1	1.82	0.45
1:A:168:PRO:O	1:A:172:ILE:HG13	2.16	0.45
1:A:270:VAL:O	1:A:274:LEU:HG	2.17	0.45
1:A:328:GLN:HG3	5:A:638:HOH:O	2.17	0.44
1:B:280:ASP:HB3	1:B:283:HIS:HB3	1.99	0.44
1:A:280:ASP:HB3	1:A:283:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:HG13	1:B:97:VAL:O	2.18	0.44
1:B:92:THR:CG2	1:B:93:ALA:N	2.79	0.44
1:B:339:GLN:O	1:B:343:GLN:HB2	2.17	0.44
1:A:289:ILE:CG1	1:A:295:LEU:HD21	2.47	0.44
1:A:17:GLU:HG2	1:A:20:ALA:HB2	1.99	0.44
1:A:339:GLN:O	1:A:343:GLN:HB2	2.18	0.44
1:A:293:TYR:HA	1:A:294:PRO:HD3	1.64	0.44
1:B:21:ILE:O	1:B:21:ILE:HG12	2.18	0.44
1:B:344:HIS:O	1:B:348:GLN:HB2	2.18	0.44
1:B:1:MET:CG	1:B:2:LYS:H	2.31	0.44
1:A:351:THR:HG22	1:A:351:THR:O	2.18	0.44
1:B:107:GLY:CA	1:B:119:PHE:CZ	3.00	0.44
1:A:199:LYS:CG	1:A:203:ILE:HD12	2.48	0.43
1:A:285:ILE:O	1:A:289:ILE:HG13	2.18	0.43
1:A:334:VAL:O	1:A:335:GLN:HB3	2.16	0.43
1:A:201:ARG:HE	1:A:205:GLN:NE2	2.15	0.43
1:A:74:GLU:HA	5:A:644:HOH:O	2.17	0.43
1:A:181:LYS:O	1:A:185:LEU:HD22	2.19	0.43
1:A:186:ASN:HB2	1:A:190:ALA:HB3	2.00	0.43
1:A:141:SER:O	1:A:143:GLN:N	2.52	0.43
1:A:229:GLU:O	1:A:229:GLU:HG2	2.18	0.43
1:B:130:ASP:OD2	3:B:401:NAD:H5N	2.18	0.43
1:B:224:ILE:HD13	1:B:224:ILE:N	2.34	0.43
1:A:332:ILE:HD12	1:A:332:ILE:N	2.34	0.43
1:A:22:LYS:HE3	1:A:23:TYR:CE1	2.53	0.43
1:B:285:ILE:O	1:B:289:ILE:HG13	2.19	0.43
1:B:186:ASN:CB	1:B:190:ALA:HB3	2.49	0.43
1:B:277:SER:HB3	1:B:327:ARG:O	2.19	0.42
1:B:228:ASP:O	1:B:235:ARG:HB2	2.19	0.42
1:A:242:HIS:O	1:A:246:HIS:HB2	2.19	0.42
1:A:1:MET:CG	1:A:2:LYS:N	2.83	0.42
1:A:107:GLY:CA	1:A:119:PHE:CZ	3.03	0.42
1:B:239:ASN:HB2	1:B:315:LYS:HD3	2.00	0.42
1:B:233:GLY:O	1:B:236:LYS:HB2	2.19	0.42
1:A:186:ASN:CB	1:A:190:ALA:HB3	2.49	0.42
1:A:328:GLN:O	1:A:331:ASP:HB3	2.20	0.42
1:B:315:LYS:HE3	1:B:324:VAL:HG23	2.02	0.42
1:B:275:PHE:O	1:B:276:ASP:C	2.58	0.42
1:A:28:LEU:C	1:A:30:GLN:H	2.23	0.42
1:B:108:PHE:CE1	1:B:149:GLY:HA2	2.55	0.41
1:B:293:TYR:HA	1:B:294:PRO:HD3	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HG21	1:A:285:ILE:HD11	2.03	0.41
1:A:277:SER:HB3	1:A:327:ARG:O	2.20	0.41
1:A:267:GLN:HG2	1:A:325:LEU:CD2	2.49	0.41
1:B:34:SER:N	1:B:58:ASN:O	2.53	0.41
1:B:94:ILE:HG13	1:B:110:ALA:CB	2.45	0.41
1:A:141:SER:OG	1:A:143:GLN:HB2	2.20	0.41
1:A:181:LYS:HD3	1:A:242:HIS:HE1	1.85	0.41
1:B:9:SER:O	1:B:10:ASN:HB2	2.21	0.41
1:A:346:CYS:SG	1:A:346:CYS:O	2.79	0.41
1:B:311:LEU:O	1:B:312:SER:HB3	2.20	0.41
1:B:136:LYS:NZ	4:B:501:CRB:H81	2.35	0.41
1:A:274:LEU:HD21	1:A:341:THR:HG21	2.03	0.41
1:B:243:THR:HG23	1:B:315:LYS:HZ1	1.85	0.41
1:B:313:ASP:OD2	1:B:315:LYS:NZ	2.50	0.41
1:A:199:LYS:HD2	5:A:633:HOH:O	2.20	0.41
1:B:75:GLN:NE2	1:B:79:THR:OG1	2.51	0.41
1:A:17:GLU:HA	1:A:161:LEU:HD12	2.03	0.41
1:B:160:ASP:HB3	1:B:163:PHE:CE2	2.56	0.41
1:A:119:PHE:HB3	1:A:154:PRO:HA	2.03	0.41
1:A:83:ILE:HG22	1:A:88:VAL:HG11	2.03	0.41
1:A:150:ALA:HB1	5:B:1006:HOH:O	2.21	0.41
1:B:73:PHE:O	1:B:76:TYR:HB3	2.20	0.41
1:B:22:LYS:HE3	1:B:23:TYR:CE1	2.56	0.41
1:A:222:LEU:O	1:A:226:VAL:HG23	2.21	0.40
1:B:18:HIS:NE2	1:B:211:ASP:OD1	2.44	0.40
1:B:32:ASP:OD2	1:B:89:THR:OG1	2.30	0.40
1:A:277:SER:HB2	1:A:279:HIS:CD2	2.56	0.40
1:A:327:ARG:NH1	1:A:331:ASP:CG	2.74	0.40
1:B:94:ILE:CB	1:B:110:ALA:HB2	2.51	0.40
1:A:92:THR:CG2	1:A:93:ALA:H	2.33	0.40
1:A:202:GLU:O	1:A:206:SER:HB3	2.22	0.40
1:B:27:TYR:O	1:B:30:GLN:HG2	2.21	0.40
1:A:84:LEU:C	1:A:86:HIS: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	331/354 (94%)	276 (83%)	48 (14%)	7 (2%)	9	6
1	B	331/354 (94%)	278 (84%)	44 (13%)	9 (3%)	6	3
All	All	662/708 (94%)	554 (84%)	92 (14%)	16 (2%)	7	5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	TYR
1	A	295	LEU
1	A	312	SER
1	B	295	LEU
1	B	312	SER
1	B	142	LYS
1	B	313	ASP
1	A	29	ASN
1	A	142	LYS
1	B	227	ALA
1	B	165	LYS
1	B	188	GLU
1	B	32	ASP
1	A	65	PRO
1	A	294	PRO
1	B	337	VAL

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	289/306 (94%)	276 (96%)	13 (4%)	34	43
1	B	289/306 (94%)	274 (95%)	15 (5%)	29	35
All	All	578/612 (94%)	550 (95%)	28 (5%)	31	40

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	51	ASP
1	A	159	TYR
1	A	185	LEU
1	A	204	LEU
1	A	206	SER
1	A	239	ASN
1	A	250	TYR
1	A	267	GLN
1	A	297	MET
1	A	309	TYR
1	A	321	VAL
1	A	327	ARG
1	B	51	ASP
1	B	85	SER
1	B	88	VAL
1	B	159	TYR
1	B	185	LEU
1	B	204	LEU
1	B	206	SER
1	B	239	ASN
1	B	250	TYR
1	B	267	GLN
1	B	295	LEU
1	B	297	MET
1	B	309	TYR
1	B	317	ASP
1	B	321	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	30	GLN

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Mol	Chain	Res	Type
1	A	58	ASN
1	A	77	GLN
1	A	143	GLN
1	A	171	GLN
1	A	205	GLN
1	A	232	GLN
1	A	246	HIS
1	A	290	GLN
1	A	322	GLN
1	A	344	HIS
1	B	10	ASN
1	B	58	ASN
1	B	77	GLN
1	B	143	GLN
1	B	171	GLN
1	B	205	GLN
1	B	232	GLN
1	B	344	HIS

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	400	-	38,48,48	1.73	8 (21%)	47,73,73	1.86	9 (19%)
4	CRB	A	500	2	13,17,17	2.21	5 (38%)	17,27,27	1.24	2 (11%)
3	NAD	B	401	-	38,48,48	1.91	8 (21%)	47,73,73	1.85	10 (21%)
4	CRB	B	501	2	13,17,17	2.21	5 (38%)	17,27,27	1.26	2 (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	400	-	-	0/22/62/62	0/5/5/5
4	CRB	A	500	2	-	0/5/29/29	0/1/1/1
3	NAD	B	401	-	-	0/22/62/62	0/5/5/5
4	CRB	B	501	2	-	0/5/29/29	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	CRB	C8-C6	-3.07	1.47	1.53
4	A	500	CRB	C8-C6	-2.79	1.47	1.53
3	B	401	NAD	C5N-C4N	2.22	1.43	1.38
3	B	401	NAD	C2A-N1A	2.25	1.38	1.33
3	A	400	NAD	C5N-C4N	2.25	1.43	1.38
3	A	400	NAD	C2A-N1A	2.48	1.38	1.33
4	B	501	CRB	C3-C2	2.96	1.56	1.53
4	B	501	CRB	C8-C2	2.97	1.56	1.53
4	A	500	CRB	C3-C2	2.98	1.56	1.53
4	A	500	CRB	P1-C7	3.16	1.82	1.79
4	B	501	CRB	P1-C7	3.29	1.82	1.79
3	A	400	NAD	O4B-C1B	3.40	1.45	1.41
4	A	500	CRB	C8-C2	3.44	1.56	1.53
3	A	400	NAD	C4N-C3N	3.46	1.45	1.39
3	A	400	NAD	C6N-N1N	3.50	1.44	1.35
3	A	400	NAD	C3N-C7N	3.54	1.56	1.50
3	B	401	NAD	C6N-N1N	3.61	1.45	1.35
3	A	400	NAD	C4A-N3A	3.62	1.41	1.35
4	A	500	CRB	C4-C5	3.80	1.57	1.52
3	B	401	NAD	C4N-C3N	3.81	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	CRB	C4-C5	4.00	1.58	1.52
3	B	401	NAD	C4A-N3A	4.06	1.41	1.35
3	B	401	NAD	C3N-C7N	4.08	1.57	1.50
3	B	401	NAD	O4B-C1B	4.42	1.46	1.41
3	A	400	NAD	O4D-C1D	4.42	1.46	1.41
3	B	401	NAD	O4D-C1D	5.12	1.47	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	NAD	C5N-C4N-C3N	-5.59	113.30	120.33
3	B	401	NAD	C5N-C4N-C3N	-5.56	113.34	120.33
3	A	400	NAD	O4B-C1B-N9A	-3.84	100.06	108.10
3	A	400	NAD	O4D-C1D-N1N	-3.82	103.93	108.13
3	B	401	NAD	O4B-C1B-N9A	-3.73	100.29	108.10
3	B	401	NAD	O4D-C1D-N1N	-3.46	104.33	108.13
3	B	401	NAD	C5N-C6N-N1N	-3.23	114.88	120.47
3	A	400	NAD	C5N-C6N-N1N	-3.02	115.24	120.47
3	B	401	NAD	C4N-C3N-C7N	-2.24	115.16	121.09
3	A	400	NAD	C4N-C3N-C7N	-2.22	115.22	121.09
4	A	500	CRB	O92-P1-C7	-2.22	101.41	106.84
4	B	501	CRB	O92-P1-C7	-2.09	101.72	106.84
4	B	501	CRB	O93-P1-O92	2.11	114.32	108.13
4	A	500	CRB	O93-P1-O92	2.12	114.34	108.13
3	B	401	NAD	C4B-O4B-C1B	2.32	112.27	109.72
3	A	400	NAD	O3-PA-O5B	2.38	109.24	102.94
3	B	401	NAD	O3-PA-O5B	2.61	109.85	102.94
3	B	401	NAD	C2N-C3N-C4N	3.68	122.39	118.29
3	A	400	NAD	C2N-C3N-C4N	3.77	122.49	118.29
3	A	400	NAD	C2B-C1B-N9A	4.26	120.80	114.29
3	B	401	NAD	C2B-C1B-N9A	4.29	120.84	114.29
3	B	401	NAD	C6N-C5N-C4N	4.49	126.23	119.44
3	A	400	NAD	C6N-C5N-C4N	4.75	126.61	119.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	NAD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	NAD	2	0
4	B	501	CRB	1	0

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, 95^{th} 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	337/354 (95%)	0.16	19 (5%)	28	42	23, 52, 102, 140	0
1	B	337/354 (95%)	0.18	21 (6%)	24	36	27, 52, 101, 138	0
All	All	674/708 (95%)	0.17	40 (5%)	26	39	23, 52, 102, 140	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	LYS	7.0
1	A	340	LEU	5.9
1	B	340	LEU	5.9
1	B	318	LYS	4.8
1	B	339	GLN	4.8
1	B	4	GLN	4.7
1	B	250	TYR	4.4
1	A	339	GLN	4.2
1	B	251	TYR	4.2
1	A	311	LEU	4.2
1	A	250	TYR	4.1
1	A	309	TYR	4.0
1	B	311	LEU	3.9
1	B	309	TYR	3.5
1	B	337	VAL	2.9
1	A	28	LEU	2.9
1	A	3	LEU	2.7
1	A	1	MET	2.6
1	A	47	ALA	2.6
1	B	3	LEU	2.6
1	B	6	THR	2.6
1	A	4	GLN	2.5
1	A	251	TYR	2.5
1	A	252	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	24	ILE	2.5
1	A	50	PHE	2.4
1	B	319	GLN	2.4
1	B	295	LEU	2.4
1	B	47	ALA	2.3
1	B	252	HIS	2.2
1	B	310	MET	2.2
1	B	225	VAL	2.2
1	A	310	MET	2.2
1	B	33	GLN	2.1
1	A	295	LEU	2.1
1	B	8	PRO	2.1
1	A	297	MET	2.1
1	B	344	HIS	2.0
1	B	254	ILE	2.0
1	A	80	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, 95^{th} 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	ZN	B	601	1/1	0.87	0.68	38.46	100,100,100,100	0
2	ZN	A	600	1/1	0.90	0.69	27.92	100,100,100,100	0
4	CRB	A	500	17/17	0.89	0.19	1.81	57,69,88,96	0
4	CRB	B	501	17/17	0.92	0.18	1.14	60,71,88,93	0
3	NAD	B	401	44/44	0.97	0.12	-0.33	19,38,52,70	0
3	NAD	A	400	44/44	0.97	0.10	-0.90	22,35,52,58	0

6.5 Other polymers (i)

There are no such residues in this entry.