



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:34 am GMT

PDB ID : 1ORR
Title : Crystal Structure of CDP-Tyvelose 2-Epimerase complexed with NAD and CDP
Authors : Koropatkin, N.M.; Liu, H.; Holden, H.M.
Deposited on : 2003-03-14
Resolution : 1.50 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	:	trunk28620
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)	:	recalc28949

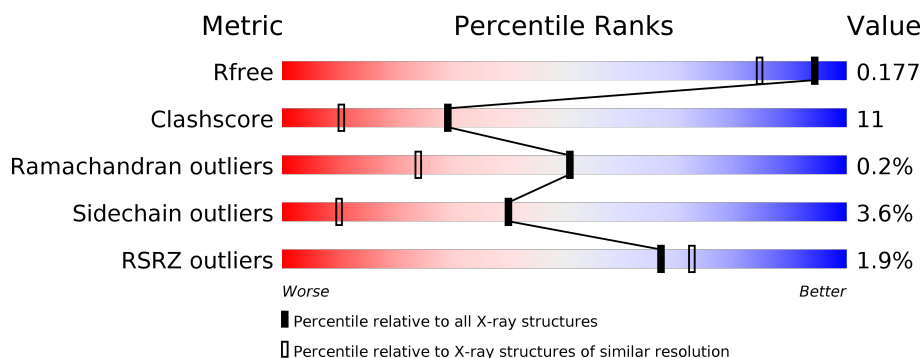
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (1.50-1.50)

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	347	<div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
1	B	347	<div> <div>%</div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
1	C	347	<div> <div>5%</div> <div>68%</div> <div>25%</div> <div>• •</div> </div>
1	D	347	<div> <div>2%</div> <div>67%</div> <div>25%</div> <div>• •</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12059 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 CDP-tyvelose-2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	11	0
			2706	1712	458	520	16			
1	B	338	Total	C	N	O	S	0	4	0
			2676	1695	451	514	16			
1	C	335	Total	C	N	O	S	0	6	0
			2661	1686	448	511	16			
1	D	336	Total	C	N	O	S	0	5	0
			2661	1685	450	510	16			

There are 40 discrepancies between the modelled and reference sequences:

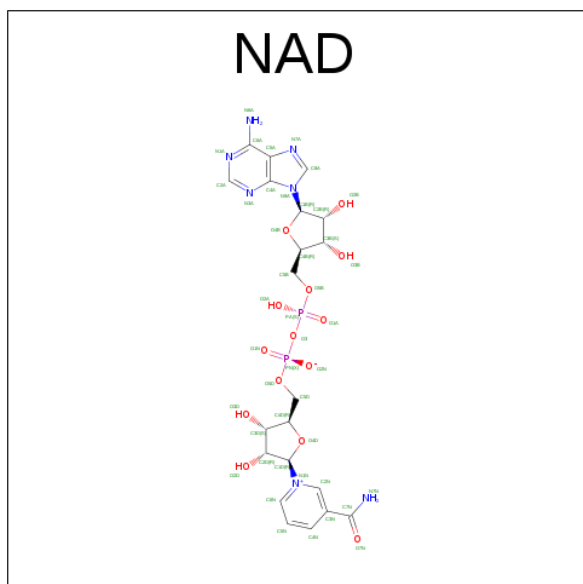
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP P14169
A	2	ALA	-	CLONING ARTIFACT	UNP P14169
A	340	LEU	-	EXPRESSION TAG	UNP P14169
A	341	GLU	-	EXPRESSION TAG	UNP P14169
A	342	HIS	-	EXPRESSION TAG	UNP P14169
A	343	HIS	-	EXPRESSION TAG	UNP P14169
A	344	HIS	-	EXPRESSION TAG	UNP P14169
A	345	HIS	-	EXPRESSION TAG	UNP P14169
A	346	HIS	-	EXPRESSION TAG	UNP P14169
A	347	HIS	-	EXPRESSION TAG	UNP P14169
B	1	MET	-	CLONING ARTIFACT	UNP P14169
B	2	ALA	-	CLONING ARTIFACT	UNP P14169
B	340	LEU	-	EXPRESSION TAG	UNP P14169
B	341	GLU	-	EXPRESSION TAG	UNP P14169
B	342	HIS	-	EXPRESSION TAG	UNP P14169
B	343	HIS	-	EXPRESSION TAG	UNP P14169
B	344	HIS	-	EXPRESSION TAG	UNP P14169
B	345	HIS	-	EXPRESSION TAG	UNP P14169
B	346	HIS	-	EXPRESSION TAG	UNP P14169
B	347	HIS	-	EXPRESSION TAG	UNP P14169
C	1	MET	-	CLONING ARTIFACT	UNP P14169

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	-	CLONING ARTIFACT	UNP P14169
C	340	LEU	-	EXPRESSION TAG	UNP P14169
C	341	GLU	-	EXPRESSION TAG	UNP P14169
C	342	HIS	-	EXPRESSION TAG	UNP P14169
C	343	HIS	-	EXPRESSION TAG	UNP P14169
C	344	HIS	-	EXPRESSION TAG	UNP P14169
C	345	HIS	-	EXPRESSION TAG	UNP P14169
C	346	HIS	-	EXPRESSION TAG	UNP P14169
C	347	HIS	-	EXPRESSION TAG	UNP P14169
D	1	MET	-	CLONING ARTIFACT	UNP P14169
D	2	ALA	-	CLONING ARTIFACT	UNP P14169
D	340	LEU	-	EXPRESSION TAG	UNP P14169
D	341	GLU	-	EXPRESSION TAG	UNP P14169
D	342	HIS	-	EXPRESSION TAG	UNP P14169
D	343	HIS	-	EXPRESSION TAG	UNP P14169
D	344	HIS	-	EXPRESSION TAG	UNP P14169
D	345	HIS	-	EXPRESSION TAG	UNP P14169
D	346	HIS	-	EXPRESSION TAG	UNP P14169
D	347	HIS	-	EXPRESSION TAG	UNP P14169

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



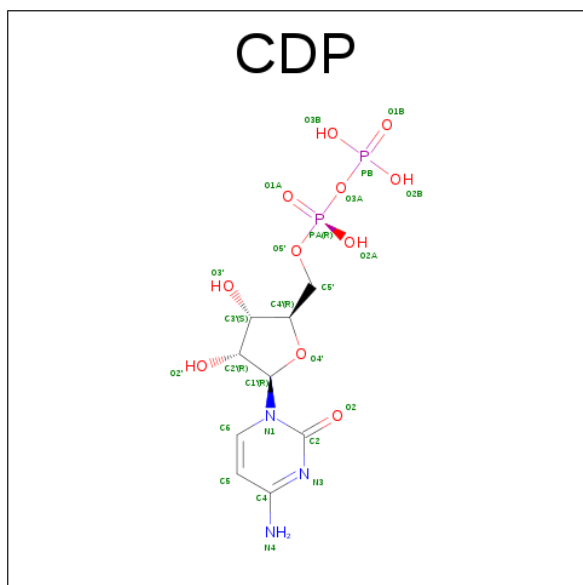
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			44	21	7	14	2	

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

- Molecule 3 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	3	11	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	310	Total O 310 310	0	0
4	B	277	Total O 277 277	0	0

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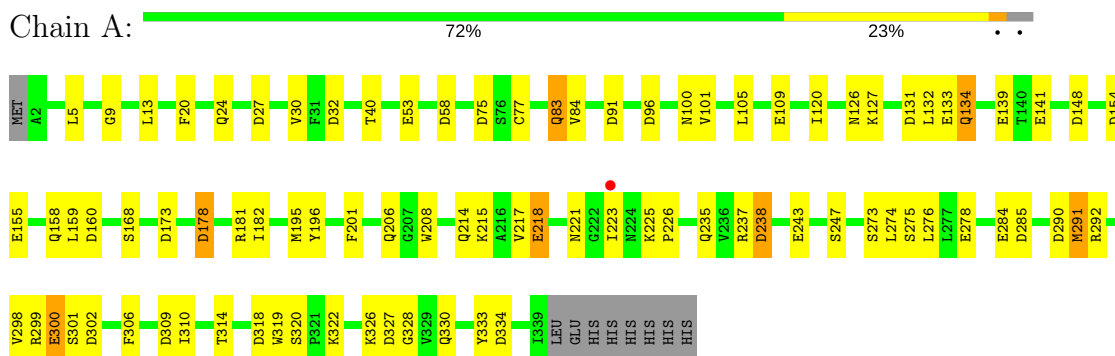
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	259	Total 259	O 259	0	0
4	D	233	Total 233	O 233	0	0

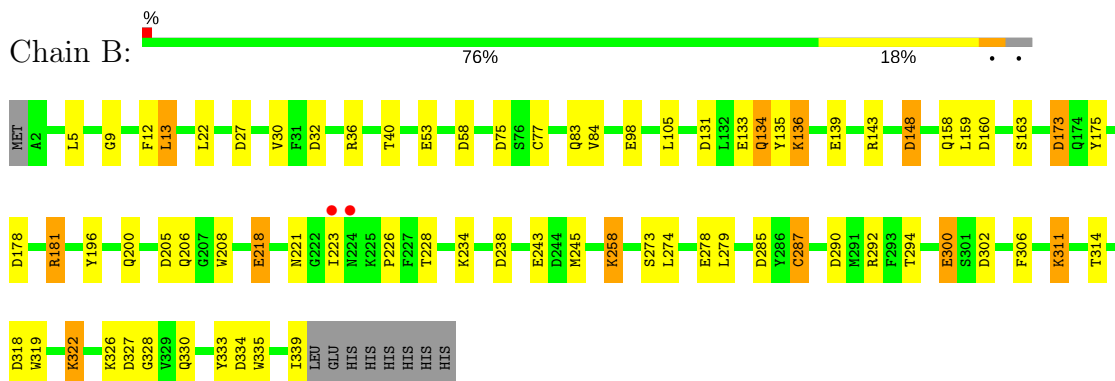
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

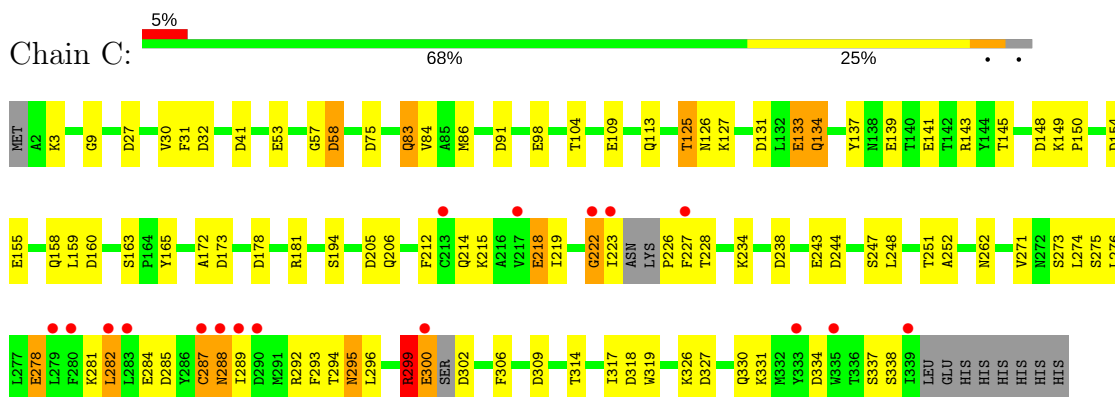
• Molecule 1: CDP-tyvelose-2-epimerase



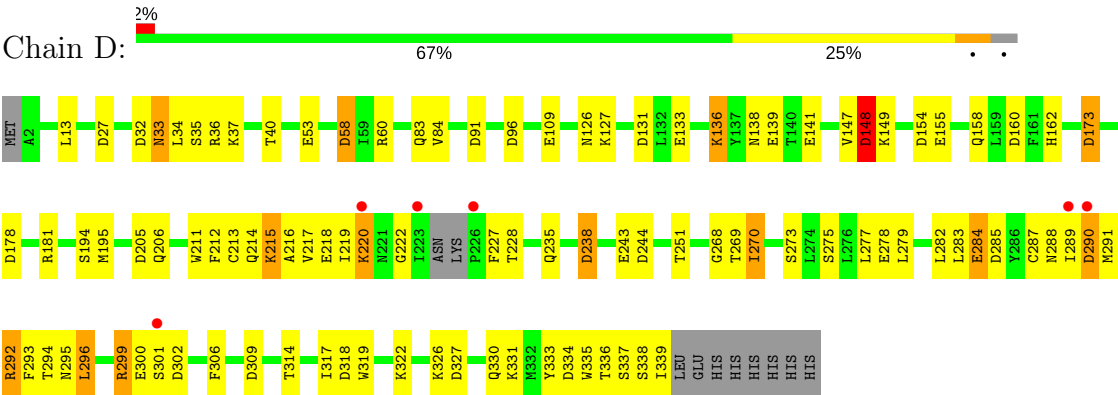
• Molecule 1: CDP-tyvelose-2-epimerase



• Molecule 1: CDP-tyvelose-2-epimerase



● Molecule 1: CDP-tyvelose-2-epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.00Å 168.10Å 89.60Å 90.00° 105.40° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 47.01 – 1.46	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-1.50) 95.4 (47.01-1.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 1.46Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.178 , 0.229 0.175 , 0.177	Depositor DCC
R_{free} test set	20900 reflections (11.10%)	DCC
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 80.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12059	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDP, 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	0.87	10/2828 (0.4%)	1.31	43/3830 (1.1%)
1	B	0.88	8/2761 (0.3%)	1.30	32/3738 (0.9%)
1	C	0.87	12/2757 (0.4%)	1.32	42/3729 (1.1%)
1	D	0.90	10/2740 (0.4%)	1.32	42/3704 (1.1%)
All	All	0.88	40/11086 (0.4%)	1.31	159/15001 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	1	0
All	All	2	0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	GLU	CD-OE2	7.30	1.33	1.25
1	D	278	GLU	CD-OE2	7.02	1.33	1.25
1	C	155	GLU	CD-OE2	6.87	1.33	1.25
1	C	284	GLU	CD-OE2	6.69	1.33	1.25
1	D	133	GLU	CD-OE2	6.65	1.32	1.25
1	D	300	GLU	CD-OE2	6.61	1.32	1.25
1	C	141	GLU	CD-OE2	6.50	1.32	1.25
1	A	155	GLU	CD-OE2	6.49	1.32	1.25
1	D	155	GLU	CD-OE2	6.49	1.32	1.25
1	D	284	GLU	CD-OE2	6.47	1.32	1.25
1	C	53	GLU	CD-OE2	6.23	1.32	1.25
1	B	243	GLU	CD-OE2	6.19	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	243	GLU	CD-OE2	6.14	1.32	1.25
1	C	109	GLU	CD-OE2	6.09	1.32	1.25
1	B	278	GLU	CD-OE2	6.06	1.32	1.25
1	A	300	GLU	CD-OE2	5.98	1.32	1.25
1	C	300	GLU	CD-OE2	5.95	1.32	1.25
1	A	218	GLU	CD-OE2	5.70	1.31	1.25
1	A	243	GLU	CD-OE2	5.68	1.31	1.25
1	D	141	GLU	CD-OE2	5.64	1.31	1.25
1	C	243	GLU	CD-OE2	5.59	1.31	1.25
1	A	133	GLU	CD-OE2	5.56	1.31	1.25
1	A	109	GLU	CD-OE2	5.54	1.31	1.25
1	B	53	GLU	CD-OE2	5.52	1.31	1.25
1	D	53	GLU	CD-OE2	5.49	1.31	1.25
1	A	141	GLU	CD-OE2	5.48	1.31	1.25
1	B	300	GLU	CD-OE2	5.46	1.31	1.25
1	B	139	GLU	CD-OE2	5.44	1.31	1.25
1	A	278	GLU	CD-OE2	5.39	1.31	1.25
1	C	139	GLU	CD-OE2	5.37	1.31	1.25
1	B	133	GLU	CD-OE2	5.37	1.31	1.25
1	D	109	GLU	CD-OE2	5.34	1.31	1.25
1	C	278	GLU	CD-OE2	5.32	1.31	1.25
1	C	218	GLU	CD-OE2	5.31	1.31	1.25
1	D	139	GLU	CD-OE2	5.29	1.31	1.25
1	B	98	GLU	CD-OE2	5.21	1.31	1.25
1	A	53	GLU	CD-OE2	5.18	1.31	1.25
1	C	133	GLU	CD-OE2	5.16	1.31	1.25
1	C	98	GLU	CD-OE2	5.16	1.31	1.25
1	A	139	GLU	CD-OE2	5.11	1.31	1.25

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	A	292	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	C	178	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	A	302	ASP	CB-CG-OD1	8.37	125.83	118.30
1	A	96	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	B	58	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	D	32	ASP	CB-CG-OD1	7.97	125.48	118.30
1	D	290	ASP	CB-CG-OD1	7.97	125.47	118.30
1	B	306	PHE	N-CA-CB	7.89	124.81	110.60
1	B	148	ASP	CB-CG-OD2	-7.86	111.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ASP	CB-CG-OD1	7.74	125.27	118.30
1	C	178	ASP	CB-CG-OD1	7.74	125.26	118.30
1	C	205	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	C	148	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	B	131	ASP	CB-CG-OD1	7.48	125.03	118.30
1	D	178	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	C	91	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	C	306	PHE	N-CA-CB	7.42	123.96	110.60
1	D	131	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	A	154	ASP	CB-CG-OD1	7.24	124.82	118.30
1	B	32	ASP	CB-CG-OD1	7.22	124.80	118.30
1	B	287	CYS	CB-CA-C	-7.22	95.96	110.40
1	D	154	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	58	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	C	58	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	285	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	D	306	PHE	N-CA-CB	7.11	123.40	110.60
1	A	173	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	D	290	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	D	285	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	B	178	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	306	PHE	N-CA-CB	7.03	123.26	110.60
1	A	160	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	237	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	D	148	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	A	75	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	D	244	ASP	CB-CG-OD1	6.90	124.51	118.30
1	C	334	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	A	302	ASP	CB-CG-OD2	-6.87	112.11	118.30
1	C	32	ASP	CB-CG-OD1	6.87	124.48	118.30
1	B	334	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	D	302	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	B	131	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	C	244	ASP	CB-CG-OD1	6.83	124.44	118.30
1	A	238	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	309	ASP	CB-CG-OD1	6.75	124.38	118.30
1	C	27	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	B	292	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	131	ASP	CB-CG-OD1	6.73	124.36	118.30
1	B	334	ASP	CB-CG-OD1	6.71	124.34	118.30
1	C	125[A]	THR	CA-CB-CG2	-6.70	103.02	112.40
1	C	125[B]	THR	CA-CB-CG2	-6.70	103.02	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125[C]	THR	CA-CB-CG2	-6.70	103.02	112.40
1	D	309	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	178	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	D	91	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	B	205	ASP	CB-CG-OD2	-6.63	112.34	118.30
1	A	238	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	B	32	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	B	173	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	163	SER	N-CA-CB	6.48	120.22	110.50
1	C	91	ASP	CB-CG-OD1	6.47	124.13	118.30
1	C	173	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	318	ASP	CB-CG-OD1	6.44	124.10	118.30
1	C	299	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	309	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	D	154	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	D	160	ASP	CB-CG-OD1	6.37	124.03	118.30
1	D	244	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	131	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	C	75	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	148	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	178	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	D	318	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	D	318	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	181	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	285	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	C	285	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	A	91	ASP	CB-CG-OD1	6.22	123.89	118.30
1	D	299	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	300	GLU	N-CA-CB	6.20	121.75	110.60
1	A	96	ASP	CB-CG-OD1	6.18	123.86	118.30
1	C	327	ASP	CB-CG-OD2	-6.13	112.79	118.30
1	C	244	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	173	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	274	LEU	CB-CA-C	-6.12	98.58	110.20
1	D	178	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	309	ASP	CB-CG-OD1	6.08	123.77	118.30
1	D	60	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	32	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	D	327	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	C	302	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	A	58	ASP	CB-CG-OD1	6.04	123.74	118.30
1	C	334	ASP	CB-CG-OD1	6.04	123.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	27	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	A	91	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	C	154	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	178	ASP	CB-CG-OD1	5.96	123.67	118.30
1	D	285	ASP	CB-CG-OD1	5.96	123.67	118.30
1	D	299	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	D	58	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	327	ASP	CB-CG-OD1	5.90	123.61	118.30
1	D	27	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	A	27	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	131	ASP	CB-CG-OD1	5.77	123.49	118.30
1	D	91	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	32	ASP	CB-CG-OD1	5.76	123.48	118.30
1	D	333	TYR	CA-CB-CG	-5.74	102.49	113.40
1	B	75	ASP	CB-CG-OD1	5.74	123.46	118.30
1	D	238	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	C	302	ASP	CB-CG-OD1	5.67	123.40	118.30
1	D	96	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	D	60	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	334	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	238	ASP	CB-CG-OD1	5.61	123.34	118.30
1	D	302	ASP	CB-CG-OD1	5.60	123.34	118.30
1	C	131	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	27	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	C	299	ARG	CB-CA-C	5.54	121.47	110.40
1	C	41	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	C	131	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	C	309	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	226	PRO	N-CA-CB	5.51	109.92	103.30
1	A	274	LEU	CB-CA-C	-5.50	99.74	110.20
1	D	27	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	334	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	290	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	C	205	ASP	CB-CG-OD1	5.42	123.18	118.30
1	D	160	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	327	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	181	ARG	CB-CA-C	-5.34	99.72	110.40
1	D	334	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	C	160	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	154	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	75	ASP	CB-CG-OD1	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	318	ASP	CB-CG-OD1	5.27	123.05	118.30
1	A	160	ASP	CB-CG-OD1	5.26	123.03	118.30
1	D	205	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	B	302	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	148	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	D	148	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	309	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	154	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	318	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	285	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	274	LEU	CB-CA-C	-5.17	100.38	110.20
1	C	181	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	83	GLN	N-CA-C	-5.13	97.14	111.00
1	C	318	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	327	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	160	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	292	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	58	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	318	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	C	83	GLN	N-CA-C	-5.06	97.34	111.00
1	B	290	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	D	292	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	C	262	ASN	CB-CA-C	-5.04	100.31	110.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	300	GLU	CA
1	C	299	ARG	CA

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	2706	0	2639	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2676	0	2612	49	0
1	C	2661	0	2592	68	0
1	D	2661	0	2584	60	0
2	A	44	0	26	4	0
2	B	44	0	26	0	0
2	C	44	0	26	3	0
2	D	44	0	26	1	0
3	A	25	0	12	0	0
3	B	25	0	12	0	0
3	C	25	0	12	1	0
3	D	25	0	12	1	0
4	A	310	0	0	12	0
4	B	277	0	0	5	0
4	C	259	0	0	4	0
4	D	233	0	0	6	0
All	All	12059	0	10579	233	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 11.

All (233) 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:C:125[C]:THR:HG22	1:C:127:LYS:H	1.00	1.11
1:C:218:GLU:HA	1:C:223:ILE:HD12	1.34	1.05
1:C:218:GLU:HB3	1:C:223:ILE:HB	1.42	0.99
1:B:134:GLN:H	1:B:134:GLN:HE21	1.14	0.94
1:C:125[C]:THR:HG22	1:C:127:LYS:N	1.85	0.90
1:C:134:GLN:H	1:C:134:GLN:HE21	1.13	0.90
1:B:13:LEU:HD22	1:B:245:MET:HE2	1.54	0.90
1:A:134:GLN:HE21	1:A:134:GLN:H	1.18	0.89
1:C:218:GLU:CA	1:C:223:ILE:HD12	2.04	0.88
1:B:335:TRP:CZ2	1:B:339:ILE:HD11	2.09	0.86
1:C:295:ASN:HD22	1:C:295:ASN:N	1.77	0.83
1:D:314[A]:THR:HG22	1:D:319:TRP:O	1.82	0.80
1:D:326:LYS:O	1:D:330:GLN:HG3	1.82	0.79
1:C:125[C]:THR:CG2	1:C:127:LYS:H	1.92	0.78
1:A:310:ILE:O	1:A:314[C]:THR:HG22	1.83	0.78
1:C:314[B]:THR:HG21	4:C:1644:HOH:O	1.84	0.78
1:C:314[B]:THR:HG22	1:C:319:TRP:O	1.85	0.76
1:C:125[A]:THR:HG21	1:C:165:TYR:OH	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:GLN:O	1:C:218:GLU:HG3	1.87	0.75
1:D:314[A]:THR:HG21	4:D:1697:HOH:O	1.85	0.75
1:A:314[B]:THR:HG22	1:A:319:TRP:O	1.85	0.75
1:A:84[B]:VAL:HG13	4:A:1343:HOH:O	1.85	0.75
1:C:326:LYS:O	1:C:330:GLN:HG3	1.88	0.73
1:C:282:LEU:HD21	1:C:326:LYS:HA	1.70	0.73
1:C:134:GLN:N	1:C:134:GLN:HE21	1.86	0.72
1:A:238:ASP:HA	1:A:273:SER:HA	1.73	0.71
1:C:295:ASN:ND2	1:C:295:ASN:N	2.38	0.71
1:C:3[B]:LYS:HE3	4:C:1415:HOH:O	1.90	0.70
1:B:13:LEU:HD22	1:B:245:MET:CE	2.20	0.70
1:A:158[B]:GLN:HE21	1:A:159:LEU:H	1.40	0.70
1:A:314[C]:THR:HG23	4:A:1442:HOH:O	1.89	0.70
1:B:13:LEU:HB3	1:B:245:MET:HE1	1.73	0.70
1:B:326:LYS:O	1:B:330:GLN:HG3	1.91	0.70
1:A:221:ASN:HB2	1:A:223:ILE:CD1	2.22	0.69
1:D:136:LYS:HD2	1:D:148:ASP:OD1	1.92	0.69
1:A:158[B]:GLN:HE22	1:C:159:LEU:H	1.40	0.69
1:A:218:GLU:HA	1:A:223:ILE:HD13	1.76	0.68
1:B:22:LEU:HD23	4:B:1391:HOH:O	1.94	0.68
1:C:134:GLN:NE2	1:C:134:GLN:H	1.90	0.67
1:C:226:PRO:HA	1:C:292:ARG:O	1.93	0.67
1:B:13:LEU:CB	1:B:245:MET:HE1	2.24	0.67
1:A:223:ILE:HG22	1:A:225:LYS:HG3	1.77	0.67
1:A:215:LYS:HA	1:A:215:LYS:HE2	1.77	0.66
1:B:314:THR:HG22	1:B:319:TRP:O	1.95	0.66
1:B:322:LYS:HD2	4:B:1572:HOH:O	1.95	0.66
1:A:226:PRO:HB3	4:A:1458:HOH:O	1.94	0.66
1:D:284:GLU:O	1:D:288:ASN:N	2.29	0.66
1:D:279:LEU:O	1:D:283:LEU:HD23	1.95	0.66
1:A:84[B]:VAL:HG22	2:A:1200:NAD:C2D	2.27	0.65
1:C:299:ARG:NH2	3:C:1401:CDP:O2A	2.29	0.65
1:C:251[A]:THR:HG23	1:C:317:ILE:HD12	1.77	0.65
1:D:289:ILE:HG22	1:D:290:ASP:N	2.12	0.65
1:B:36:ARG:NH2	1:B:206:GLN:HG3	2.11	0.64
1:A:320:SER:OG	1:A:322:LYS:NZ	2.30	0.64
1:C:143:ARG:HA	1:C:234:LYS:HB3	1.79	0.64
1:C:212:PHE:CE1	1:C:276[B]:LEU:HD21	2.33	0.64
1:B:12:PHE:CD1	1:B:200:GLN:HB2	2.33	0.64
1:B:221:ASN:HB2	1:B:223:ILE:CD1	2.28	0.64
1:C:125[A]:THR:HG22	2:C:1400:NAD:H5N	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314[B]:THR:HG21	4:A:1446:HOH:O	1.98	0.63
1:A:182[B]:ILE:CD1	1:C:163:SER:HA	2.29	0.62
1:D:219:ILE:O	1:D:222:GLY:N	2.32	0.62
1:A:182[B]:ILE:HD13	1:C:163:SER:HA	1.80	0.62
1:D:211:TRP:O	1:D:214:GLN:HB3	1.98	0.62
1:D:289:ILE:HG22	1:D:290:ASP:H	1.66	0.61
1:D:238:ASP:HA	1:D:273:SER:HA	1.82	0.61
1:D:214:GLN:HG2	4:D:1716:HOH:O	2.01	0.61
1:B:135:TYR:HB3	1:B:148:ASP:OD1	2.01	0.60
1:D:299:ARG:HD2	3:D:1501:CDP:O2'	2.01	0.60
1:D:213:CYS:O	1:D:216:ALA:HB3	2.01	0.60
1:D:36:ARG:HD3	2:D:1500:NAD:O1A	2.02	0.60
1:B:134:GLN:H	1:B:134:GLN:NE2	1.94	0.60
1:B:13:LEU:CD2	1:B:245:MET:HE2	2.30	0.59
1:C:275:SER:OG	1:C:278:GLU:HG3	2.02	0.59
1:A:221:ASN:HB2	1:A:223:ILE:HD11	1.83	0.59
1:B:13:LEU:HD13	1:B:245:MET:CE	2.34	0.58
1:B:181:ARG:HD2	4:B:1521:HOH:O	2.03	0.58
1:B:238:ASP:HA	1:B:273:SER:HA	1.85	0.58
1:A:158[B]:GLN:NE2	1:C:158[B]:GLN:OE1	2.37	0.58
1:D:127:LYS:HE3	4:D:1663:HOH:O	2.04	0.58
1:D:287:CYS:O	1:D:289:ILE:HG13	2.04	0.58
1:D:162:HIS:HB2	4:D:1649:HOH:O	2.03	0.58
1:A:84[A]:VAL:HG22	4:A:1319:HOH:O	2.04	0.57
1:D:214:GLN:O	1:D:218:GLU:HG3	2.04	0.57
1:B:258:LYS:O	1:B:258:LYS:HG2	2.03	0.57
1:A:314[C]:THR:HG21	4:A:1446:HOH:O	2.03	0.57
1:C:228:THR:HG22	1:C:294:THR:OG1	2.04	0.56
1:C:84:VAL:HG23	1:C:206:GLN:HG3	1.88	0.56
1:B:134:GLN:N	1:B:134:GLN:HE21	1.96	0.56
1:C:125[A]:THR:HG22	2:C:1400:NAD:C5N	2.35	0.56
1:C:218:GLU:HB3	1:C:223:ILE:CB	2.27	0.56
1:C:113:GLN:NE2	4:C:1529:HOH:O	2.39	0.55
1:D:335:TRP:CH2	1:D:339:ILE:HD11	2.41	0.55
1:A:158[B]:GLN:HE21	1:A:159:LEU:N	2.05	0.54
1:C:247:SER:O	1:C:251[A]:THR:HG22	2.08	0.54
1:A:223:ILE:HG21	1:A:225:LYS:HD2	1.89	0.54
1:B:221:ASN:HB2	1:B:223:ILE:HD11	1.90	0.54
1:D:228:THR:HG22	1:D:294:THR:OG1	2.08	0.54
1:A:223:ILE:CG2	1:A:225:LYS:HD2	2.37	0.54
1:C:228:THR:HB	1:C:296:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:TYR:C	1:B:136:LYS:HE3	2.27	0.53
1:A:9:GLY:HA3	1:A:30:VAL:HG13	1.90	0.53
1:D:212:PHE:O	1:D:215:LYS:HB2	2.09	0.53
1:A:84[C]:VAL:HG13	4:A:1319:HOH:O	2.07	0.53
1:A:84[B]:VAL:HG22	2:A:1200:NAD:H2D	1.90	0.53
1:D:13:LEU:HD11	1:D:195:MET:HE3	1.90	0.53
1:D:335:TRP:CZ2	1:D:339:ILE:HD11	2.44	0.53
1:D:219:ILE:HG22	1:D:220:LYS:N	2.24	0.53
1:A:182[A]:ILE:HG23	1:C:300:GLU:OE1	2.09	0.52
1:C:125[C]:THR:CG2	1:C:127:LYS:HG2	2.39	0.52
1:A:126[C]:ASN:HD21	1:A:127:LYS:NZ	2.07	0.52
1:B:12:PHE:CD2	1:B:13:LEU:HD23	2.44	0.52
1:A:214:GLN:HG2	4:A:1462:HOH:O	2.08	0.52
1:C:227:PHE:CE1	1:C:293:PHE:HB3	2.45	0.51
1:D:214:GLN:HA	1:D:214:GLN:OE1	2.09	0.51
1:B:218:GLU:O	1:B:223:ILE:HD12	2.10	0.51
1:D:37:LYS:HE3	4:D:1623:HOH:O	2.10	0.51
1:A:84[C]:VAL:HG23	4:A:1343:HOH:O	2.10	0.51
1:C:9:GLY:HA3	1:C:30:VAL:HG13	1.93	0.51
1:D:283:LEU:O	1:D:287:CYS:N	2.42	0.51
1:C:126:ASN:HD22	1:C:126:ASN:H	1.58	0.51
1:B:136:LYS:N	1:B:136:LYS:HE3	2.25	0.51
1:B:158:GLN:HA	1:D:158[A]:GLN:OE1	2.11	0.51
1:B:36:ARG:HH22	1:B:206:GLN:HG3	1.75	0.50
1:A:300:GLU:HG2	4:C:1609:HOH:O	2.11	0.50
1:A:134:GLN:NE2	1:A:134:GLN:H	1.97	0.50
1:A:298:VAL:HG22	1:A:299:ARG:N	2.27	0.50
1:D:220:LYS:C	1:D:222:GLY:H	2.14	0.50
1:B:158:GLN:OE1	1:D:158[B]:GLN:OE1	2.29	0.50
1:C:86:MET:HG2	1:C:86:MET:O	2.09	0.49
1:A:100:ASN:HB2	1:A:168:SER:HB2	1.93	0.49
1:A:206:GLN:NE2	4:A:1318:HOH:O	2.45	0.49
1:D:217:VAL:HG21	1:D:336:THR:HG22	1.93	0.49
1:C:125[A]:THR:HG23	2:C:1400:NAD:H6N	1.95	0.49
1:A:134:GLN:N	1:A:134:GLN:HE21	1.98	0.49
1:A:215:LYS:CA	1:A:215:LYS:HE2	2.43	0.49
1:A:235:GLN:O	1:A:275:SER:HA	2.13	0.49
1:B:13:LEU:HD13	1:B:245:MET:HE2	1.93	0.49
1:B:143:ARG:HA	1:B:234:LYS:HB3	1.96	0.48
1:C:248:LEU:O	1:C:251[A]:THR:HG22	2.14	0.48
1:B:228:THR:HG22	1:B:294[C]:THR:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ILE:CG2	1:D:290:ASP:H	2.27	0.48
1:A:20:PHE:CE2	1:A:24:GLN:HG3	2.49	0.48
1:C:287:CYS:O	1:C:288:ASN:C	2.51	0.48
1:D:289:ILE:CG2	1:D:290:ASP:N	2.77	0.48
1:C:58:ASP:OD2	1:D:58:ASP:OD2	2.32	0.47
1:C:251[A]:THR:HG23	1:C:252:ALA:N	2.30	0.47
1:A:84[B]:VAL:CG2	2:A:1200:NAD:H2D	2.44	0.47
1:A:20:PHE:CZ	1:A:24:GLN:HG3	2.49	0.47
1:D:138:ASN:ND2	1:D:147:VAL:HG22	2.29	0.47
1:A:178:ASP:OD2	1:A:182[B]:ILE:HD13	2.15	0.47
1:A:218:GLU:O	1:A:223:ILE:HD12	2.15	0.47
1:D:251:THR:HG22	1:D:317:ILE:HD12	1.96	0.46
1:B:105:LEU:HD21	1:B:175:TYR:CD1	2.51	0.46
1:B:221:ASN:CB	1:B:223:ILE:HD11	2.45	0.46
1:B:84:VAL:HG12	1:B:84:VAL:O	2.14	0.46
1:A:158[A]:GLN:HE22	1:C:159:LEU:H	1.62	0.46
1:D:215:LYS:HE2	1:D:215:LYS:CA	2.45	0.46
1:A:208:TRP:CZ3	1:A:276:LEU:CD2	2.99	0.46
1:D:84:VAL:HG23	1:D:206:GLN:HG3	1.97	0.46
1:A:84[A]:VAL:CG2	1:A:206:GLN:NE2	2.79	0.46
1:D:215:LYS:N	1:D:215:LYS:HE2	2.31	0.46
1:B:13:LEU:CA	1:B:245:MET:HE1	2.46	0.46
1:A:159:LEU:H	1:C:158[A]:GLN:HE22	1.63	0.45
1:B:287:CYS:SG	1:B:333:TYR:CE1	3.09	0.45
1:C:295:ASN:C	1:C:296:LEU:HD23	2.36	0.45
1:A:13:LEU:HD11	1:A:195:MET:HE3	1.99	0.45
1:C:149:LYS:HA	1:C:150:PRO:HD2	1.68	0.45
1:C:218:GLU:CB	1:C:223:ILE:HB	2.30	0.45
1:C:222:GLY:C	1:C:223:ILE:HG13	2.37	0.45
1:D:270:ILE:O	1:D:270:ILE:HG13	2.17	0.45
1:D:284:GLU:OE2	1:D:291:MET:N	2.34	0.45
1:B:12:PHE:CG	1:B:200:GLN:HB2	2.52	0.45
1:B:228:THR:HG22	1:B:294[C]:THR:HG22	1.99	0.45
1:C:133:GLU:HA	1:C:133:GLU:OE1	2.16	0.44
1:C:212:PHE:CE1	1:C:276[B]:LEU:CD2	2.99	0.44
1:A:40:THR:HG23	4:A:1222:HOH:O	2.17	0.44
1:A:126[C]:ASN:HD21	1:A:127:LYS:HZ2	1.64	0.44
1:C:125[C]:THR:HG21	1:C:165:TYR:HE2	1.82	0.44
1:D:126:ASN:ND2	1:D:126:ASN:H	2.16	0.44
1:D:126:ASN:HD22	1:D:126:ASN:H	1.65	0.44
1:D:228:THR:HB	1:D:296:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLY:HA3	1:B:30:VAL:HG13	2.00	0.44
1:D:227:PHE:CE1	1:D:293:PHE:HB3	2.53	0.44
1:C:31:PHE:CE1	1:C:57:GLY:HA3	2.53	0.43
1:A:217:VAL:CG2	1:A:333:TYR:CE1	3.01	0.43
1:A:84[B]:VAL:HG22	2:A:1200:NAD:O2D	2.18	0.43
1:D:138:ASN:ND2	1:D:147:VAL:CG2	2.81	0.43
1:D:283:LEU:N	1:D:283:LEU:HD22	2.33	0.43
1:D:235:GLN:O	1:D:275:SER:HA	2.18	0.43
1:D:33:ASN:ND2	1:D:35:SER:H	2.16	0.43
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.83	0.43
1:B:13:LEU:HA	1:B:245:MET:CE	2.48	0.43
1:B:40:THR:HG23	4:B:1317:HOH:O	2.19	0.42
1:A:201:PHE:HD1	4:A:1306:HOH:O	2.02	0.42
1:C:215:LYS:HA	1:C:215:LYS:HE2	2.02	0.42
1:C:215:LYS:N	1:C:215:LYS:HE2	2.34	0.42
1:A:225:LYS:N	1:A:226:PRO:HD3	2.35	0.42
1:C:215:LYS:HE2	1:C:215:LYS:CA	2.50	0.42
1:A:5:LEU:O	1:A:77:CYS:HA	2.20	0.42
1:B:221:ASN:CB	1:B:223:ILE:CD1	2.98	0.42
1:B:208:TRP:CZ3	1:B:279:LEU:HD22	2.54	0.42
1:D:288:ASN:C	1:D:289:ILE:HG13	2.40	0.42
1:A:326:LYS:O	1:A:330:GLN:HG3	2.19	0.42
1:C:137:TYR:HA	1:C:145:THR:O	2.20	0.42
1:D:295:ASN:N	1:D:295:ASN:OD1	2.53	0.41
1:A:217:VAL:HG22	1:A:333:TYR:CE1	2.56	0.41
1:D:335:TRP:CZ3	1:D:339:ILE:HD11	2.55	0.41
1:D:34:LEU:HD13	1:D:40:THR:HG22	2.02	0.41
1:D:148:ASP:C	1:D:149:LYS:HG2	2.40	0.41
1:A:284:GLU:HG3	1:A:291:MET:HG3	2.03	0.41
1:B:221:ASN:HB2	1:B:223:ILE:HD12	1.99	0.41
1:A:120:ILE:HD13	1:A:120:ILE:HG21	1.85	0.41
1:A:84[A]:VAL:HG21	1:A:206:GLN:CD	2.41	0.41
1:B:196:TYR:OH	1:B:328:GLY:HA3	2.20	0.41
1:A:101:VAL:O	1:A:105:LEU:HD23	2.21	0.41
1:C:219:ILE:HG21	1:C:289:ILE:HD12	2.03	0.41
1:D:277:LEU:HD23	1:D:277:LEU:HA	1.75	0.41
1:D:282:LEU:HA	1:D:282:LEU:HD12	1.86	0.41
1:C:104:THR:HG21	1:C:172:ALA:HB1	2.03	0.40
1:D:292:ARG:HA	4:D:1694:HOH:O	2.21	0.40
1:C:126:ASN:H	1:C:126:ASN:ND2	2.19	0.40
1:A:182[B]:ILE:HD11	1:C:163:SER:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:SER:O	1:C:251[C]:THR:HG23	2.21	0.40
1:D:268:GLY:O	1:D:269:THR:OG1	2.29	0.40
1:A:196:TYR:OH	1:A:328:GLY:HA3	2.21	0.40
1:C:238:ASP:HA	1:C:273:SER:HA	2.03	0.40
1:A:105:LEU:HA	1:A:105:LEU:HD13	1.88	0.40
1:B:311:LYS:NZ	4:B:1378:HOH:O	2.51	0.40
1:A:132:LEU:HA	1:A:134:GLN:NE2	2.36	0.40
1:B:5:LEU:O	1:B:77:CYS:HA	2.21	0.40
1:D:283:LEU:O	1:D:287:CYS:SG	2.80	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	350/347 (101%)	339 (97%)	11 (3%)	0	100	100
1	B	342/347 (99%)	332 (97%)	10 (3%)	0	100	100
1	C	337/347 (97%)	325 (96%)	11 (3%)	1 (0%)	44	19
1	D	337/347 (97%)	319 (95%)	17 (5%)	1 (0%)	44	19
All	All	1366/1388 (98%)	1315 (96%)	49 (4%)	2 (0%)	51	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	222	GLY
1	D	301	SER

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	306/301 (102%)	300 (98%)	6 (2%)	60	28
1	B	298/301 (99%)	289 (97%)	9 (3%)	46	14
1	C	297/301 (99%)	284 (96%)	13 (4%)	33	6
1	D	294/301 (98%)	278 (95%)	16 (5%)	26	4
All	All	1195/1204 (99%)	1151 (96%)	44 (4%)	40	9

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	134	GLN
1	A	247[A]	SER
1	A	247[B]	SER
1	A	291	MET
1	A	301	SER
1	B	13	LEU
1	B	83	GLN
1	B	134	GLN
1	B	136	LYS
1	B	173	ASP
1	B	258	LYS
1	B	300	GLU
1	B	311	LYS
1	B	322	LYS
1	C	83	GLN
1	C	134	GLN
1	C	194	SER
1	C	271	VAL
1	C	281	LYS
1	C	282	LEU
1	C	287	CYS
1	C	288	ASN
1	C	295	ASN

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Mol	Chain	Res	Type
1	C	299	ARG
1	C	331	LYS
1	C	337	SER
1	C	338	SER
1	D	33	ASN
1	D	83	GLN
1	D	136	LYS
1	D	148	ASP
1	D	173	ASP
1	D	181	ARG
1	D	194	SER
1	D	215	LYS
1	D	220	LYS
1	D	270	ILE
1	D	296	LEU
1	D	322[A]	LYS
1	D	322[B]	LYS
1	D	331	LYS
1	D	337	SER
1	D	338	SER

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	113	GLN
1	A	134	GLN
1	A	200	GLN
1	A	206	GLN
1	A	303	GLN
1	B	113	GLN
1	B	134	GLN
1	B	200	GLN
1	B	206	GLN
1	B	330	GLN
1	C	44	HIS
1	C	113	GLN
1	C	126	ASN
1	C	134	GLN
1	C	200	GLN
1	C	295	ASN
1	D	33	ASN
1	D	113	GLN

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Mol	Chain	Res	Type
1	D	126	ASN
1	D	138	ASN

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 ⓘ

8 ligands 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
2	NAD	A	1200	-	41,48,48	1.81	6 (14%)	43,73,73	1.78	5 (11%)
3	CDP	A	1201	-	22,26,26	1.38	5 (22%)	23,40,40	1.35	2 (8%)
2	NAD	B	1300	-	41,48,48	1.86	6 (14%)	43,73,73	1.73	7 (16%)
3	CDP	B	1301	-	22,26,26	1.38	5 (22%)	23,40,40	1.26	2 (8%)
2	NAD	C	1400	-	41,48,48	2.06	8 (19%)	43,73,73	1.48	3 (6%)
3	CDP	C	1401	-	22,26,26	1.49	5 (22%)	23,40,40	1.43	3 (13%)
2	NAD	D	1500	-	41,48,48	1.88	5 (12%)	43,73,73	1.64	4 (9%)
3	CDP	D	1501	-	22,26,26	1.37	3 (13%)	23,40,40	1.41	4 (17%)

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	NAD	A	1200	-	-	0/22/62/62	0/5/5/5
3	CDP	A	1201	-	-	0/12/32/32	0/2/2/2
2	NAD	B	1300	-	-	0/22/62/62	0/5/5/5
3	CDP	B	1301	-	-	0/12/32/32	0/2/2/2
2	NAD	C	1400	-	-	0/22/62/62	0/5/5/5
3	CDP	C	1401	-	-	0/12/32/32	0/2/2/2
2	NAD	D	1500	-	-	0/22/62/62	0/5/5/5
3	CDP	D	1501	-	-	0/12/32/32	0/2/2/2

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1300	NAD	C3N-C7N	-4.11	1.44	1.50
2	A	1200	NAD	C3N-C7N	-3.15	1.45	1.50
2	A	1200	NAD	O4B-C1B	-2.98	1.37	1.41
3	C	1401	CDP	C6-C5	-2.91	1.31	1.38
2	D	1500	NAD	C6N-C5N	-2.90	1.32	1.38
3	B	1301	CDP	C6-C5	-2.84	1.31	1.38
3	D	1501	CDP	C6-C5	-2.75	1.32	1.38
2	C	1400	NAD	C6N-C5N	-2.67	1.32	1.38
2	B	1300	NAD	C6N-C5N	-2.61	1.32	1.38
3	A	1201	CDP	C6-C5	-2.56	1.32	1.38
2	A	1200	NAD	C6N-C5N	-2.49	1.33	1.38
2	C	1400	NAD	C3N-C7N	-2.06	1.47	1.50
2	C	1400	NAD	O4B-C1B	-2.00	1.38	1.41
3	B	1301	CDP	C4-N3	2.05	1.39	1.35
3	B	1301	CDP	C4-N4	2.12	1.42	1.35
3	D	1501	CDP	C4-N4	2.23	1.42	1.35
3	C	1401	CDP	C4-N4	2.26	1.42	1.35
3	C	1401	CDP	C6-N1	2.28	1.38	1.35
3	A	1201	CDP	C4-N4	2.28	1.42	1.35
2	B	1300	NAD	C6N-N1N	2.29	1.41	1.35
3	C	1401	CDP	C4-N3	2.33	1.39	1.35
3	A	1201	CDP	C4-N3	2.33	1.39	1.35
3	A	1201	CDP	C6-N1	2.35	1.39	1.35
2	C	1400	NAD	C2A-N1A	2.39	1.38	1.33
3	B	1301	CDP	C6-N1	2.49	1.39	1.35
2	D	1500	NAD	C6N-N1N	2.62	1.42	1.35
3	C	1401	CDP	PB-O1B	2.84	1.60	1.50
2	C	1400	NAD	C6N-N1N	2.86	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1301	CDP	PB-O1B	2.88	1.60	1.50
3	D	1501	CDP	PB-O1B	3.20	1.61	1.50
3	A	1201	CDP	PB-O1B	3.22	1.61	1.50
2	B	1300	NAD	C2N-C3N	5.11	1.46	1.39
2	D	1500	NAD	C2N-C3N	5.12	1.46	1.39
2	A	1200	NAD	C2N-C3N	5.22	1.46	1.39
2	A	1200	NAD	C5N-C4N	5.43	1.49	1.38
2	B	1300	NAD	C4N-C3N	5.47	1.48	1.39
2	A	1200	NAD	C4N-C3N	5.67	1.48	1.39
2	B	1300	NAD	C5N-C4N	5.86	1.50	1.38
2	C	1400	NAD	C5N-C4N	5.99	1.50	1.38
2	D	1500	NAD	C5N-C4N	6.10	1.50	1.38
2	C	1400	NAD	C2N-C3N	6.46	1.48	1.39
2	D	1500	NAD	C4N-C3N	6.96	1.50	1.39
2	C	1400	NAD	C4N-C3N	7.20	1.51	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1200	NAD	C5N-C4N-C3N	-8.79	110.01	120.35
2	B	1300	NAD	C5N-C4N-C3N	-6.95	112.18	120.35
2	C	1400	NAD	C5N-C4N-C3N	-6.71	112.45	120.35
2	D	1500	NAD	C5N-C4N-C3N	-4.98	114.50	120.35
2	D	1500	NAD	O7N-C7N-C3N	-4.35	114.54	119.62
2	B	1300	NAD	O7N-C7N-C3N	-4.20	114.72	119.62
3	A	1201	CDP	C5-C4-N3	-4.10	116.80	121.68
3	B	1301	CDP	C5-C4-N3	-3.88	117.05	121.68
3	C	1401	CDP	C5-C4-N3	-3.87	117.07	121.68
3	D	1501	CDP	C5-C4-N3	-3.71	117.26	121.68
3	C	1401	CDP	C4'-O4'-C1'	-3.23	106.33	109.77
3	B	1301	CDP	O3A-PB-O1B	-2.68	94.95	111.44
2	A	1200	NAD	O7N-C7N-C3N	-2.62	116.56	119.62
3	D	1501	CDP	C4'-O4'-C1'	-2.57	107.04	109.77
3	D	1501	CDP	C2'-C3'-C4'	-2.24	98.25	102.62
2	B	1300	NAD	C2D-C3D-C4D	-2.13	98.47	102.62
3	A	1201	CDP	O4'-C1'-N1	2.02	112.12	108.08
2	D	1500	NAD	C6N-C5N-C4N	2.19	122.75	119.44
2	C	1400	NAD	C6N-C5N-C4N	2.33	122.96	119.44
2	B	1300	NAD	C5A-C6A-N6A	2.43	125.42	120.47
2	B	1300	NAD	C3N-C2N-N1N	2.54	122.99	120.43
3	D	1501	CDP	N4-C4-N3	2.65	121.10	116.64
3	C	1401	CDP	N4-C4-N3	2.97	121.64	116.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1200	NAD	C3N-C2N-N1N	3.01	123.46	120.43
2	A	1200	NAD	C3N-C7N-N7N	3.21	121.44	117.77
2	A	1200	NAD	C6N-C5N-C4N	3.23	124.31	119.44
2	C	1400	NAD	C3N-C7N-N7N	3.53	121.81	117.77
2	B	1300	NAD	C6N-C5N-C4N	3.63	124.91	119.44
2	B	1300	NAD	C3N-C7N-N7N	4.21	122.58	117.77
2	D	1500	NAD	C3N-C7N-N7N	6.58	125.29	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1200	NAD	4	0
2	C	1400	NAD	3	0
3	C	1401	CDP	1	0
2	D	1500	NAD	1	0
3	D	1501	CDP	1	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	338/347 (97%)	-0.63	1 (0%) 93 94	11, 18, 48, 75	0
1	B	338/347 (97%)	-0.66	2 (0%) 89 91	11, 19, 50, 95	0
1	C	335/347 (96%)	-0.20	17 (5%) 29 32	11, 21, 57, 95	0
1	D	336/347 (96%)	-0.34	6 (1%) 69 74	11, 20, 58, 90	0
All	All	1347/1388 (97%)	-0.46	26 (1%) 67 72	11, 19, 55, 95	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	223	ILE	7.0
1	D	289	ILE	5.2
1	C	333	TYR	4.1
1	C	339	ILE	3.7
1	C	282	LEU	3.6
1	D	220	LYS	3.4
1	C	217	VAL	3.4
1	B	223	ILE	3.3
1	D	223	ILE	3.2
1	C	227	PHE	3.2
1	C	222	GLY	3.0
1	C	289	ILE	2.9
1	C	283	LEU	2.9
1	C	300	GLU	2.8
1	B	224	ASN	2.6
1	C	290	ASP	2.5
1	C	280	PHE	2.4
1	C	279	LEU	2.4
1	A	223	ILE	2.4
1	D	226	PRO	2.2
1	C	287	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	335	TRP	2.1
1	D	290	ASP	2.1
1	C	288	ASN	2.0
1	D	301	SER	2.0
1	C	213	CYS	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
3	CDP	A	1201	25/25	0.97	0.07	0.03	14,21,45,100	0
3	CDP	D	1501	25/25	0.96	0.07	-0.00	15,22,62,100	0
3	CDP	B	1301	25/25	0.97	0.06	-0.24	15,23,32,100	0
2	NAD	B	1300	44/44	0.99	0.05	-0.27	12,15,28,95	0
2	NAD	A	1200	44/44	0.99	0.05	-0.39	11,15,24,37	0
2	NAD	D	1500	44/44	0.99	0.05	-0.53	11,15,18,23	0
3	CDP	C	1401	25/25	0.95	0.08	-0.76	19,25,100,100	0
2	NAD	C	1400	44/44	0.99	0.05	-0.88	11,16,26,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.