



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:12 PM GMT

PDB ID : 1NVM  
Title : Crystal structure of a bifunctional aldolase-dehydrogenase : sequestering a reactive and volatile intermediate  
Authors : Manjasetty, A.B.; Powlowski, J.; Vrielink, A.  
Deposited on : 2003-02-04  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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

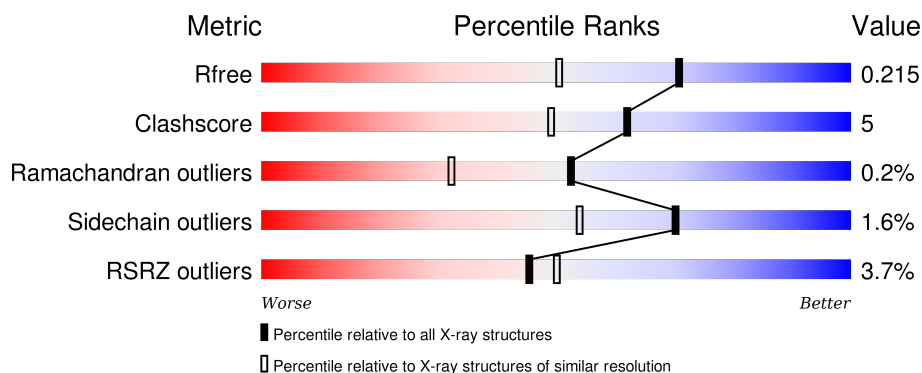
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	345	 2% 88% 10% •
1	C	345	 2% 88% 9% ••
1	E	345	 3% 88% 8% ••
1	G	345	 3% 85% 12% ••
2	B	312	 3% 87% 11% •

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	D	312	
2	F	312	
2	H	312	

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
4	OXL	A	3508	-	-	-	X
4	OXL	C	3509	-	-	-	X
4	OXL	E	3510	-	-	-	X
4	OXL	G	3511	-	-	-	X
5	SO4	A	3512	-	-	-	X
5	SO4	C	3514	-	-	-	X
5	SO4	E	3517	-	-	-	X
5	SO4	E	3518	-	-	-	X
5	SO4	F	3523	-	-	-	X
7	MPD	A	3525	-	-	-	X
7	MPD	B	3528	-	-	X	X
7	MPD	C	3524	-	-	-	X
7	MPD	C	3529	-	-	-	X
7	MPD	E	3527	-	-	-	X
7	MPD	G	3526	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22561 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 4-hydroxy-2-oxovalerate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	13	5	0
			2599	1619	470	491	19			
1	C	337	Total	C	N	O	S	5	4	0
			2568	1598	462	489	19			
1	E	338	Total	C	N	O	S	8	6	0
			2579	1606	461	492	20			
1	G	339	Total	C	N	O	S	12	5	0
			2588	1613	467	489	19			

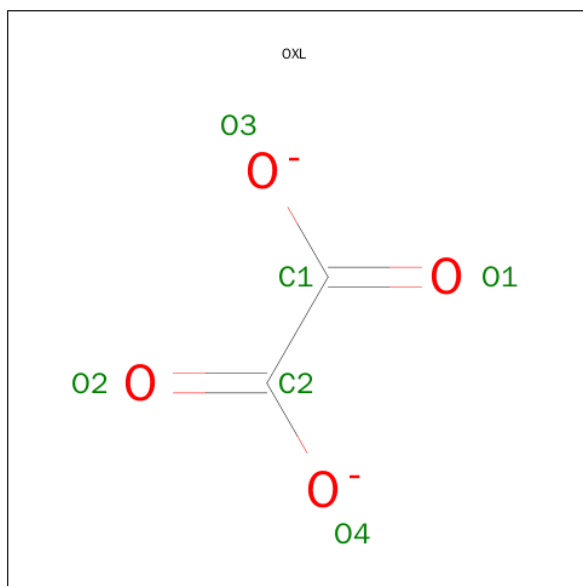
- Molecule 2 is a protein called acetaldehyde dehydrogenase (acylating).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	312	Total	C	N	O	S	19	13	0
			2316	1463	392	442	19			
2	D	308	Total	C	N	O	S	15	10	0
			2280	1441	389	433	17			
2	F	309	Total	C	N	O	S	10	13	0
			2289	1450	387	434	18			
2	H	307	Total	C	N	O	S	20	7	0
			2263	1433	384	430	16			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

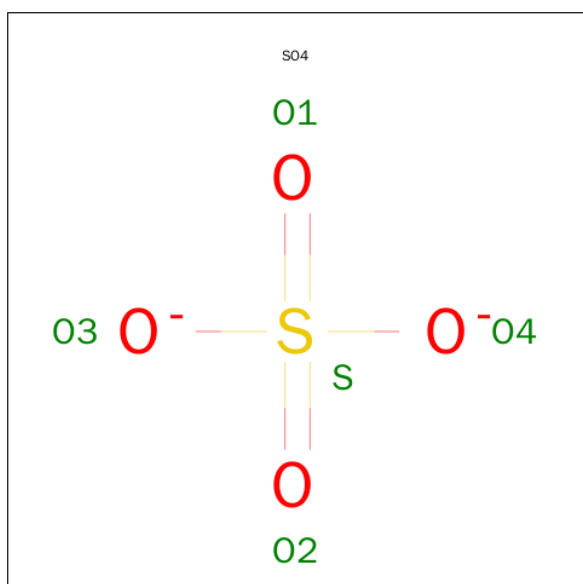
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		

- Molecule 4 is OXALATE ION (three-letter code: OXL) (formula:  $C_2O_4$ ).



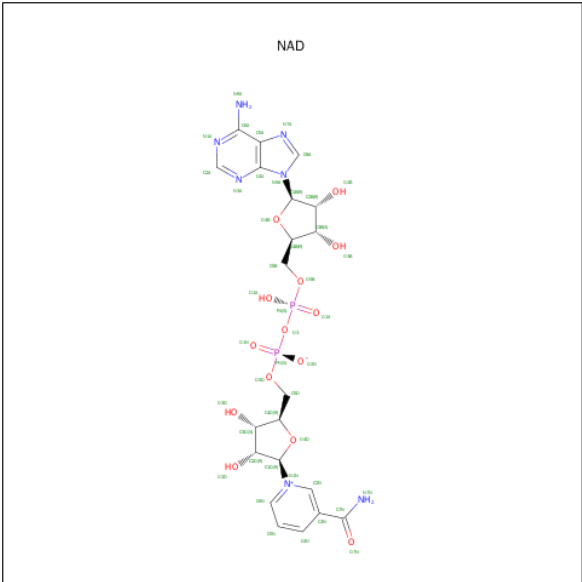
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	2	4		
4	C	1	Total	C	O	0	0
			6	2	4		
4	E	1	Total	C	O	0	0
			6	2	4		
4	G	1	Total	C	O	0	0
			6	2	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



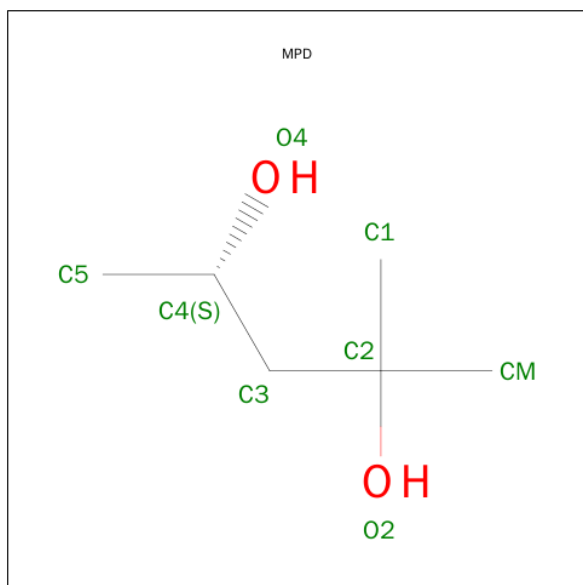
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	2	0
			8	6	2		
7	G	1	Total	C	O	0	0
			8	6	2		
7	E	1	Total	C	O	4	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		
7	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is water.

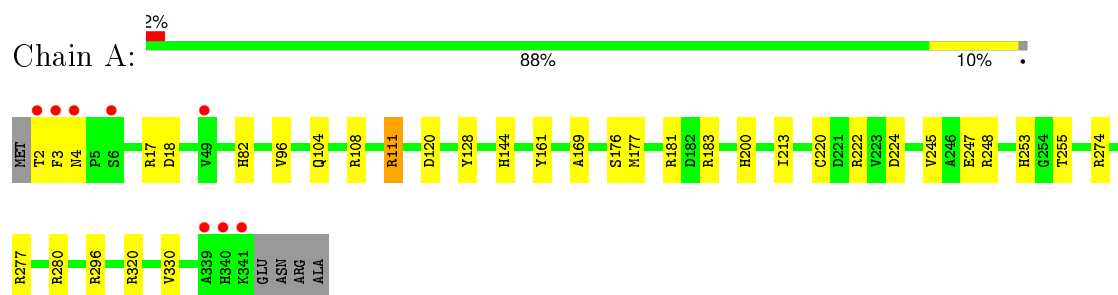
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	414	Total 414	O 414	0	0
8	B	378	Total 378	O 378	0	0
8	C	412	Total 412	O 412	0	0
8	D	293	Total 293	O 293	0	0
8	E	363	Total 363	O 363	0	0
8	F	338	Total 338	O 338	0	0
8	G	340	Total 340	O 340	0	0
8	H	273	Total 273	O 273	0	0



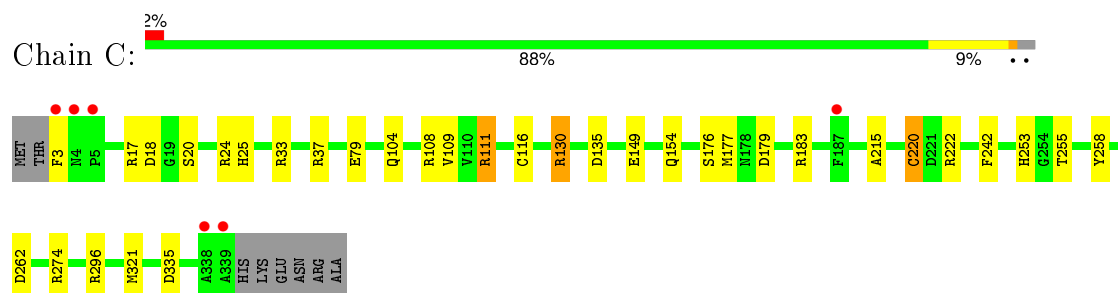
### 3 Residue-property plots [i](#)

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.

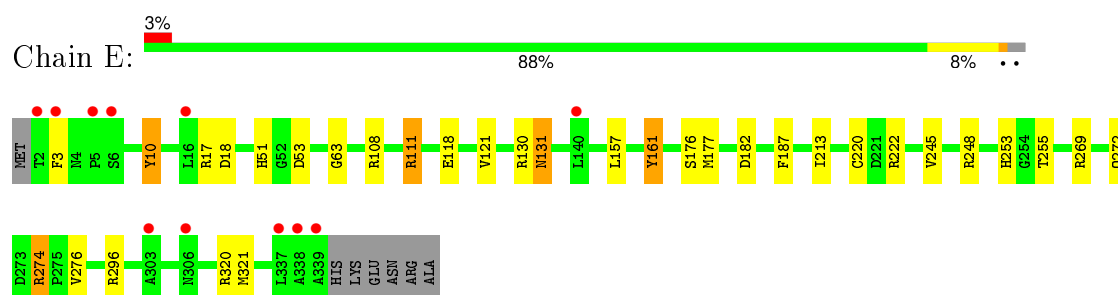
- Molecule 1: 4-hydroxy-2-oxovalerate aldolase



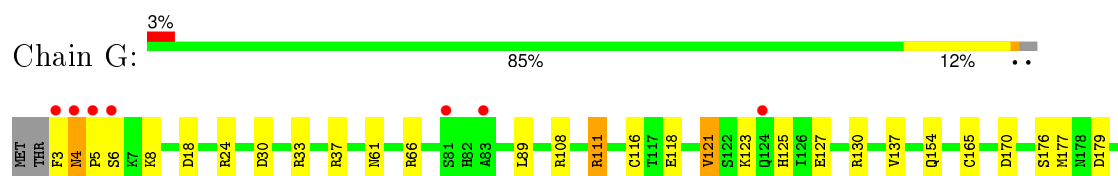
- Molecule 1: 4-hydroxy-2-oxovalerate aldolase



- Molecule 1: 4-hydroxy-2-oxovalerate aldolase

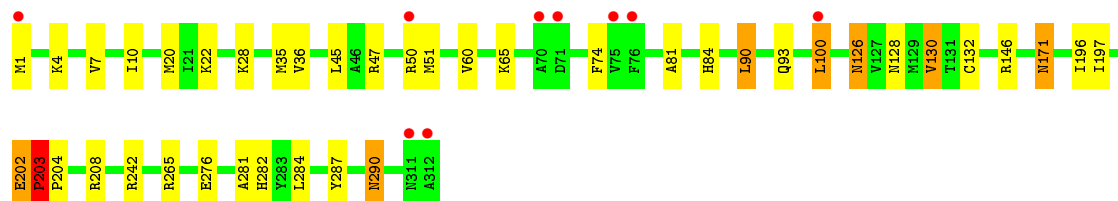
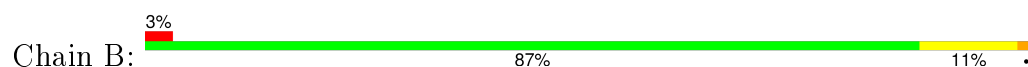


- Molecule 1: 4-hydroxy-2-oxovalerate aldolase

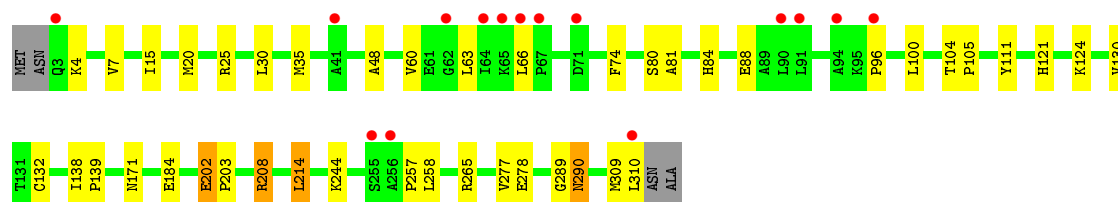
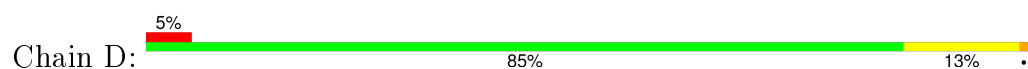




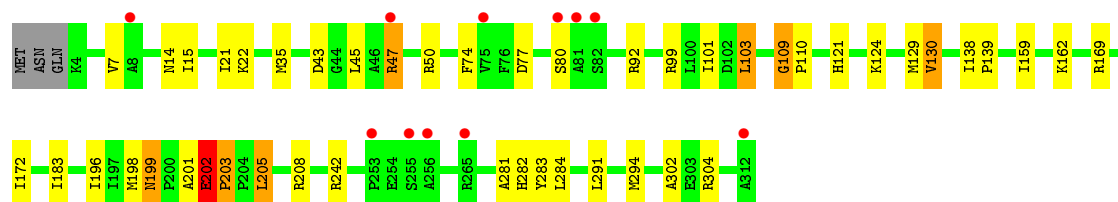
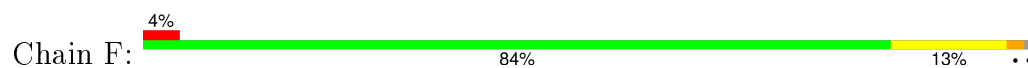
- Molecule 2: acetaldehyde dehydrogenase (acylating)



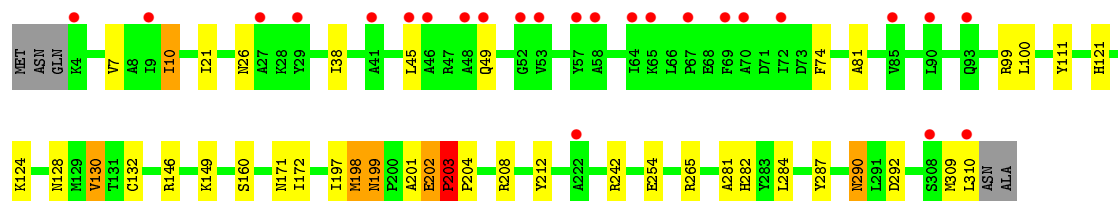
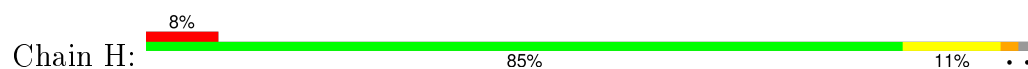
- Molecule 2: acetaldehyde dehydrogenase (acylating)



- Molecule 2: acetaldehyde dehydrogenase (acylating)



- Molecule 2: acetaldehyde dehydrogenase (acylating)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.20 Å   140.00 Å   191.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.96 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-1.70) 99.4 (19.96-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.70 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.189   ,   0.230 0.179   ,   0.215	Depositor DCC
$R_{free}$ test set	15061 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 59.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 298400 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	22561	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OXL, MPD, MN, SO4, 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	0.61	0/2671	1.30	19/3607 (0.5%)
1	C	0.63	0/2634	1.37	23/3558 (0.6%)
1	E	0.58	0/2653	1.30	22/3585 (0.6%)
1	G	0.58	0/2660	1.27	21/3593 (0.6%)
2	B	0.58	0/2412	1.24	15/3273 (0.5%)
2	D	0.58	1/2366 (0.0%)	1.17	9/3211 (0.3%)
2	F	0.57	0/2395	1.33	26/3251 (0.8%)
2	H	0.54	0/2332	1.21	18/3167 (0.6%)
All	All	0.59	1/20123 (0.0%)	1.28	153/27245 (0.6%)

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	A	0	1
1	C	0	1
2	B	0	2
2	D	0	2
2	F	0	5
2	H	0	3
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	278	GLU	CD-OE2	-6.01	1.19	1.25

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	47	ARG	NE-CZ-NH2	-19.91	110.34	120.30
1	C	296	ARG	NE-CZ-NH1	15.73	128.16	120.30
1	C	111	ARG	NE-CZ-NH1	14.31	127.45	120.30
1	E	274	ARG	NE-CZ-NH1	14.06	127.33	120.30
1	C	274	ARG	NE-CZ-NH1	13.90	127.25	120.30
1	E	18	ASP	CB-CG-OD2	13.52	130.47	118.30
1	C	17	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	A	108	ARG	NE-CZ-NH1	12.34	126.47	120.30
2	F	47	ARG	NE-CZ-NH1	12.15	126.38	120.30
1	C	18	ASP	CB-CG-OD1	12.11	129.20	118.30
2	B	208	ARG	NE-CZ-NH2	-11.51	114.54	120.30
1	A	18	ASP	CB-CG-OD2	11.07	128.27	118.30
1	C	108	ARG	NE-CZ-NH1	11.02	125.81	120.30
2	B	50	ARG	NE-CZ-NH1	-10.75	114.93	120.30
1	C	18	ASP	CB-CG-OD2	-10.69	108.68	118.30
1	C	33	ARG	NE-CZ-NH2	-10.69	114.95	120.30
1	A	222	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	E	18	ASP	CB-CG-OD1	-10.54	108.82	118.30
1	E	108	ARG	NE-CZ-NH1	10.41	125.50	120.30
2	H	99	ARG	NE-CZ-NH2	-10.35	115.12	120.30
2	F	109	GLY	CA-C-O	-9.80	102.96	120.60
1	A	181	ARG	CD-NE-CZ	9.61	137.05	123.60
2	F	242	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	A	296	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	C	296	ARG	CD-NE-CZ	9.42	136.78	123.60
1	G	170	ASP	CB-CG-OD1	9.39	126.75	118.30
1	G	33	ARG	NE-CZ-NH1	-9.27	115.67	120.30
2	F	99	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	A	18	ASP	CB-CG-OD1	-9.06	110.14	118.30
2	H	111	TYR	CB-CG-CD1	-9.03	115.58	121.00
1	C	108	ARG	NE-CZ-NH2	-8.88	115.86	120.30
2	B	50	ARG	NE-CZ-NH2	8.68	124.64	120.30
2	H	242	ARG	NE-CZ-NH2	-8.53	116.04	120.30
2	F	110	PRO	CA-N-CD	-8.50	99.60	111.50
2	F	202	GLU	CA-C-O	-8.50	102.25	120.10
1	E	296	ARG	NE-CZ-NH1	8.38	124.49	120.30
2	H	10	ILE	CB-CG1-CD1	8.28	137.08	113.90
1	A	280	ARG	NE-CZ-NH2	-8.18	116.21	120.30
2	F	208	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	C	222	ARG	NE-CZ-NH2	-8.04	116.28	120.30
2	F	110	PRO	N-CA-CB	8.03	112.94	103.30
1	E	296	ARG	CD-NE-CZ	7.98	134.77	123.60
2	B	242	ARG	NE-CZ-NH2	-7.97	116.31	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	10	TYR	CB-CG-CD2	-7.97	116.22	121.00
2	H	203	PRO	CA-N-CD	-7.97	100.34	111.50
1	G	37	ARG	NE-CZ-NH2	-7.94	116.33	120.30
2	H	146	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	G	111	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	E	17	ARG	NE-CZ-NH1	7.71	124.16	120.30
2	D	184	GLU	OE1-CD-OE2	-7.67	114.10	123.30
2	H	146	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	A	277	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	E	111	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	274	ARG	NE-CZ-NH2	-7.58	116.51	120.30
2	F	99	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	D	202	GLU	CA-C-O	-7.56	104.23	120.10
1	A	224	ASP	CB-CG-OD2	-7.54	111.51	118.30
2	F	242	ARG	CD-NE-CZ	7.46	134.05	123.60
1	G	296	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	108	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	111	ARG	NE-CZ-NH1	7.42	124.01	120.30
2	F	169	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	E	274	ARG	NE-CZ-NH2	-7.32	116.64	120.30
2	H	203	PRO	N-CA-CB	7.17	111.91	103.30
1	G	18	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	E	10	TYR	CB-CG-CD1	7.06	125.23	121.00
2	B	208	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	C	296	ARG	NE-CZ-NH2	-7.02	116.79	120.30
2	F	77	ASP	CB-CG-OD2	7.00	124.60	118.30
2	H	111	TYR	CB-CG-CD2	6.83	125.10	121.00
1	G	66	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	E	111	ARG	NE-CZ-NH2	-6.79	116.91	120.30
2	H	202	GLU	CA-C-O	-6.73	105.97	120.10
2	D	203	PRO	CA-N-CD	-6.71	102.11	111.50
2	D	111	TYR	CB-CG-CD1	6.65	124.99	121.00
2	F	203	PRO	CA-N-CD	-6.63	102.21	111.50
1	E	248	ARG	NE-CZ-NH1	6.61	123.60	120.30
2	D	203	PRO	N-CA-CB	6.59	111.21	103.30
2	H	208	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	C	262	ASP	CB-CG-OD1	6.53	124.17	118.30
1	A	296	ARG	CG-CD-NE	6.45	125.33	111.80
2	D	208	ARG	NE-CZ-NH2	-6.43	117.08	120.30
2	F	50	ARG	NE-CZ-NH2	-6.39	117.10	120.30
2	D	25	ARG	NE-CZ-NH2	-6.39	117.11	120.30
2	B	276	GLU	N-CA-CB	6.37	122.07	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	G	296	ARG	CD-NE-CZ	6.34	132.48	123.60
1	A	17	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	F	304	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	D	111	TYR	CB-CG-CD2	-6.30	117.22	121.00
2	B	202	GLU	CA-C-O	-6.28	106.92	120.10
1	G	262	ASP	CB-CG-OD2	-6.25	112.68	118.30
2	B	265	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	G	320	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	G	222	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	G	24	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	G	296	ARG	CG-CD-NE	6.06	124.53	111.80
1	E	182	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	120	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	161	TYR	CB-CG-CD1	5.99	124.59	121.00
2	F	43	ASP	CB-CG-OD2	5.99	123.69	118.30
2	B	203	PRO	CA-N-CD	-5.99	103.12	111.50
1	C	296	ARG	CG-CD-NE	5.98	124.36	111.80
1	G	108	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	E	269	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	G	111	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	G	130	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	183	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	277	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	H	198[A]	MET	CA-CB-CG	5.83	123.20	113.30
2	H	198[B]	MET	CA-CB-CG	5.83	123.20	113.30
2	B	50	ARG	CD-NE-CZ	5.83	131.76	123.60
2	H	212	TYR	CB-CG-CD2	-5.83	117.50	121.00
2	H	242	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	G	262	ASP	CB-CG-OD1	5.73	123.46	118.30
1	E	269	ARG	CG-CD-NE	-5.72	99.78	111.80
2	F	92	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	B	203	PRO	N-CA-CB	5.60	110.02	103.30
1	G	30	ASP	CB-CG-OD1	5.58	123.32	118.30
1	E	3	PHE	CB-CG-CD1	-5.57	116.90	120.80
2	H	265	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	E	248	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	130	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	B	287	TYR	CB-CG-CD2	5.46	124.27	121.00
2	B	287	TYR	CB-CG-CD1	-5.45	117.73	121.00
2	F	242	ARG	NE-CZ-NH2	-5.39	117.60	120.30
2	F	203	PRO	N-CA-CB	5.38	109.76	103.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	G	108	ARG	CD-NE-CZ	5.32	131.04	123.60
2	H	242	ARG	CD-NE-CZ	5.32	131.04	123.60
2	D	25	ARG	CB-CA-C	-5.31	99.78	110.40
1	E	130	ARG	NE-CZ-NH1	-5.30	117.65	120.30
2	F	92	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	183	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	E	320	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	E	187	PHE	CB-CG-CD2	-5.27	117.11	120.80
2	B	100	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	E	161	TYR	CB-CG-CD1	5.26	124.15	121.00
1	C	24	ARG	NE-CZ-NH2	-5.21	117.70	120.30
2	F	129[A]	MET	O-C-N	-5.19	114.39	122.70
2	F	129[B]	MET	O-C-N	-5.19	114.39	122.70
1	C	335	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	B	146	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	C	242	PHE	CB-CG-CD2	-5.15	117.19	120.80
1	C	321	MET	CG-SD-CE	5.12	108.38	100.20
1	G	66	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	G	18	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	183	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	111	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	F	203	PRO	N-CD-CG	5.03	110.75	103.20
2	H	254	GLU	OE1-CD-OE2	-5.03	117.26	123.30
2	F	129[A]	MET	N-CA-C	-5.01	97.47	111.00
2	F	129[B]	MET	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	GLN	Sidechain
2	B	202	GLU	Mainchain,Peptide
1	C	258	TYR	Sidechain
2	D	202	GLU	Mainchain,Peptide
2	F	109	GLY	Mainchain,Peptide
2	F	130[B]	VAL	Mainchain
2	F	202	GLU	Mainchain,Peptide
2	H	202	GLU	Mainchain,Peptide
2	H	26	ASN	Sidechain



## 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	2599	0	2570	17	0
1	C	2568	0	2533	14	0
1	E	2579	0	2547	14	0
1	G	2588	0	2555	32	0
2	B	2316	0	2385	39	0
2	D	2280	0	2346	35	0
2	F	2289	0	2348	30	0
2	H	2263	0	2335	27	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	6	0	0	0	0
4	C	6	0	0	0	0
4	E	6	0	0	0	0
4	G	6	0	0	0	0
5	A	10	0	0	0	0
5	C	15	0	0	0	0
5	E	15	0	0	0	0
5	F	10	0	0	0	0
5	G	10	0	0	0	0
6	B	44	0	26	1	0
6	D	44	0	26	4	0
6	H	44	0	26	5	0
7	A	8	0	14	1	0
7	B	8	0	14	14	0
7	C	16	0	28	6	0
7	E	8	0	14	1	0
7	G	8	0	14	5	0
8	A	414	0	0	5	0
8	B	378	0	0	6	0
8	C	412	0	0	3	0
8	D	293	0	0	1	0
8	E	363	0	0	1	0
8	F	338	0	0	3	0
8	G	340	0	0	0	0
8	H	273	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22561	0	19781	212	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 5.

All (212) 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:E:177[B]:MET:SD	1:G:177[B]:MET:SD	2.60	0.97
1:A:177[B]:MET:SD	1:C:177[B]:MET:SD	2.63	0.97
7:B:3528:MPD:C5	7:B:3528:MPD:HM2	1.96	0.96
1:G:3:PHE:CE1	1:G:4:ASN:O	2.20	0.95
1:G:4:ASN:HD22	1:G:5:PRO:HD2	1.29	0.95
2:B:81:ALA:H	2:B:171[B]:ASN:HD21	1.15	0.93
1:G:3:PHE:CD1	1:G:4:ASN:N	2.39	0.91
2:B:20[B]:MET:HE2	2:B:35[B]:MET:SD	2.15	0.86
7:B:3528:MPD:H52	7:B:3528:MPD:HM2	1.55	0.86
2:H:81:ALA:H	2:H:171:ASN:HD22	1.22	0.86
2:B:81:ALA:H	2:B:171[B]:ASN:ND2	1.75	0.84
1:G:322:VAL:H	1:G:325:GLN:HE21	1.24	0.84
2:H:290:ASN:HD22	6:H:3503:NAD:H72N	1.26	0.84
7:G:3526:MPD:HM2	7:G:3526:MPD:H52	1.61	0.81
1:E:51:HIS:HD2	1:E:53:ASP:H	1.24	0.81
2:B:90:LEU:HD12	7:B:3528:MPD:H11	1.66	0.77
1:E:176:SER:OG	7:E:3527:MPD:H51	1.88	0.74
1:E:253:HIS:HD2	1:E:255:THR:H	1.37	0.72
1:G:176:SER:OG	7:G:3526:MPD:H51	1.88	0.72
2:B:60:VAL:HG13	2:B:90:LEU:HD23	1.69	0.71
2:D:81:ALA:H	2:D:171[A]:ASN:HD22	1.36	0.71
1:G:4:ASN:HD22	1:G:5:PRO:CD	2.04	0.69
2:B:81:ALA:N	2:B:171[B]:ASN:HD21	1.87	0.69
2:B:84:HIS:CE1	2:B:100:LEU:HD21	2.26	0.69
2:F:138[B]:ILE:CD1	2:F:183:ILE:HA	2.23	0.69
1:A:2:THR:HG22	1:A:4:ASN:OD1	1.93	0.69
1:E:253:HIS:CD2	1:E:255:THR:H	2.11	0.69
2:F:138[B]:ILE:HD11	2:F:183:ILE:HG13	1.76	0.68
2:B:51:MET:HE1	8:B:3870:HOH:O	1.93	0.67
1:A:96:VAL:HG13	1:A:128:TYR:CD2	2.30	0.67
1:E:51:HIS:CD2	1:E:53:ASP:H	2.11	0.66
7:B:3528:MPD:H53	7:B:3528:MPD:HM2	1.77	0.66
2:B:90:LEU:HD11	7:B:3528:MPD:H4	1.77	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:NH2	7:C:3524:MPD:O2	2.29	0.66
1:A:253:HIS:CD2	1:A:255:THR:H	2.14	0.65
7:G:3526:MPD:CM	7:G:3526:MPD:H52	2.26	0.65
2:F:138[B]:ILE:HD12	2:F:183:ILE:HA	1.78	0.65
2:B:290:ASN:H	2:B:290:ASN:HD22	1.45	0.64
1:G:121[B]:VAL:HG11	2:H:198[B]:MET:CE	2.28	0.64
2:B:90:LEU:HD12	7:B:3528:MPD:C1	2.27	0.64
1:C:176:SER:OG	7:C:3524:MPD:H51	1.99	0.63
1:G:213[A]:ILE:HD11	1:G:245:VAL:HG11	1.79	0.63
2:B:128:ASN:ND2	2:B:130:VAL:H	1.97	0.62
2:D:20[A]:MET:CE	2:D:48:ALA:HB2	2.30	0.62
1:A:253:HIS:HD2	1:A:255:THR:H	1.47	0.61
2:F:199:ASN:HD22	2:F:201:ALA:H	1.46	0.61
2:F:138[B]:ILE:HD11	2:F:183:ILE:CG1	2.30	0.61
2:B:196[B]:ILE:HD13	2:B:197:ILE:N	2.15	0.61
2:B:60:VAL:HG12	8:B:3648:HOH:O	2.00	0.61
2:B:20[B]:MET:CE	2:B:35[B]:MET:SD	2.88	0.61
1:C:253:HIS:CD2	1:C:255:THR:H	2.19	0.61
1:G:121[A]:VAL:CG2	2:H:172:ILE:HG13	2.31	0.60
1:G:253:HIS:CD2	1:G:255:THR:H	2.20	0.59
1:C:130:ARG:O	7:C:3529:MPD:HM1	2.02	0.59
1:G:253:HIS:HD2	1:G:255:THR:H	1.50	0.59
2:D:88:GLU:OE2	2:D:100:LEU:HD22	2.03	0.59
2:D:290:ASN:ND2	2:D:290:ASN:H	2.01	0.58
2:F:162:LYS:HE3	2:F:202:GLU:OE2	2.03	0.58
1:C:253:HIS:HD2	1:C:255:THR:H	1.51	0.57
1:C:20:SER:OG	1:C:25:HIS:HD2	1.86	0.57
2:B:10[B]:ILE:HG22	2:B:36:VAL:HB	1.84	0.57
2:D:290:ASN:HD22	2:D:290:ASN:H	1.50	0.57
2:F:172[B]:ILE:HD11	2:F:196:ILE:HG21	1.85	0.57
2:F:205:LEU:HD21	8:F:3816:HOH:O	2.04	0.56
2:H:199:ASN:HD22	2:H:201:ALA:H	1.53	0.56
2:D:81:ALA:H	2:D:171[B]:ASN:ND2	2.03	0.56
1:G:121[B]:VAL:HG11	2:H:198[B]:MET:HE3	1.87	0.56
2:B:290:ASN:ND2	2:B:290:ASN:H	2.02	0.56
1:G:3:PHE:CE1	1:G:4:ASN:C	2.78	0.56
2:F:22[A]:LYS:NZ	2:F:282:HIS:HD2	2.04	0.56
2:F:101:ILE:CD1	2:F:302:ALA:HB2	2.36	0.56
2:H:45:LEU:O	2:H:49:GLN:HG3	2.06	0.55
2:D:4:LYS:HE3	2:D:30:LEU:O	2.06	0.55
2:F:121:HIS:HA	2:F:124:LYS:HG3	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:ALA:H	2:D:171[B]:ASN:HD21	1.53	0.55
2:D:20[A]:MET:HE1	2:D:48:ALA:CB	2.36	0.55
2:F:21:ILE:HD12	2:F:283:TYR:HB2	1.88	0.55
2:D:121:HIS:HD2	2:D:124:LYS:NZ	2.04	0.55
2:B:1:MET:O	2:B:4:LYS:HE3	2.07	0.55
7:B:3528:MPD:C5	7:B:3528:MPD:CM	2.72	0.55
2:H:128:ASN:ND2	2:H:130:VAL:H	2.05	0.55
2:D:214:LEU:HD22	2:D:258:LEU:HD12	1.89	0.54
2:B:84:HIS:CE1	2:B:100:LEU:CD2	2.90	0.54
2:D:309:MET:O	2:D:310:LEU:HB2	2.07	0.54
1:G:3:PHE:HD1	1:G:4:ASN:H	1.49	0.53
2:D:20[A]:MET:HE1	2:D:48:ALA:HB2	1.90	0.53
2:D:132[A]:CYS:HB3	6:D:3502:NAD:H4N	1.91	0.53
2:B:20[B]:MET:HE2	2:B:35[B]:MET:CE	2.39	0.52
2:D:20[A]:MET:HE2	2:D:35:MET:HE2	1.91	0.52
2:H:160[A]:SER:HG	2:H:287:TYR:HE1	1.56	0.52
2:F:159[A]:ILE:HD11	2:F:198[A]:MET:SD	2.49	0.52
2:H:309:MET:O	2:H:310:LEU:HB2	2.09	0.52
2:B:10[B]:ILE:HG22	2:B:36:VAL:CB	2.40	0.52
1:G:121[B]:VAL:HG11	2:H:198[B]:MET:HE1	1.92	0.52
2:H:281:ALA:HA	2:H:284:LEU:O	2.10	0.52
2:D:257:PRO:HG2	2:D:265:ARG:HD2	1.91	0.52
1:A:176:SER:OG	7:A:3525:MPD:H51	2.09	0.52
1:A:144:HIS:HD2	8:A:3534:HOH:O	1.92	0.51
2:H:121:HIS:HD2	2:H:124:LYS:NZ	2.09	0.51
7:B:3528:MPD:H11	7:B:3528:MPD:H52	1.91	0.51
7:B:3528:MPD:H51	8:B:3848:HOH:O	2.11	0.51
7:C:3524:MPD:H13	8:C:3676:HOH:O	2.10	0.51
2:H:149:LYS:HD2	8:H:3697:HOH:O	2.09	0.51
2:F:199:ASN:ND2	2:F:201:ALA:H	2.09	0.50
2:B:93:GLN:OE1	7:B:3528:MPD:HM3	2.11	0.50
2:D:63:LEU:O	2:D:66:LEU:HB2	2.12	0.50
2:D:7:VAL:HG12	2:D:74:PHE:HB2	1.92	0.50
2:D:20[A]:MET:HE3	2:D:48:ALA:HB2	1.93	0.50
2:D:132[A]:CYS:HB3	6:D:3502:NAD:C4N	2.42	0.50
1:G:118:GLU:O	1:G:121[B]:VAL:HG22	2.12	0.49
1:E:213:ILE:HD11	1:E:245:VAL:HG11	1.94	0.49
1:G:213[A]:ILE:CD1	1:G:245:VAL:HG11	2.42	0.49
2:D:132[B]:CYS:SG	6:D:3502:NAD:C4N	3.02	0.48
2:D:4:LYS:HG2	8:D:3756:HOH:O	2.13	0.48
2:B:90:LEU:CD1	7:B:3528:MPD:H4	2.41	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:HE3	8:B:3887:HOH:O	2.14	0.48
7:B:3528:MPD:H12	8:B:3626:HOH:O	2.13	0.47
2:D:84:HIS:HE1	2:D:100:LEU:HD23	1.78	0.47
2:H:81:ALA:N	2:H:171:ASN:HD22	2.03	0.47
2:B:100:LEU:HD23	2:B:126:ASN:OD1	2.13	0.47
2:H:199:ASN:ND2	2:H:201:ALA:H	2.13	0.47
1:G:116:CYS:O	1:G:154:GLN:HG3	2.14	0.47
1:A:330:VAL:HG23	8:A:3882:HOH:O	2.14	0.47
2:H:199:ASN:C	2:H:199:ASN:HD22	2.18	0.47
1:A:213:ILE:HD11	1:A:245:VAL:HG11	1.96	0.47
2:F:47:ARG:NE	8:F:3775:HOH:O	2.46	0.47
2:F:103:LEU:HD13	2:F:294[B]:MET:HG3	1.96	0.47
1:G:209:VAL:HG23	1:G:238:PRO:HD2	1.96	0.47
2:F:199:ASN:HD22	2:F:199:ASN:C	2.18	0.47
2:H:7:VAL:HG12	2:H:74:PHE:HB2	1.96	0.47
1:A:82:HIS:HE1	8:A:3675:HOH:O	1.98	0.46
2:B:93:GLN:OE1	7:B:3528:MPD:H13	2.16	0.46
2:F:281:ALA:HA	2:F:284:LEU:O	2.14	0.46
2:B:1:MET:N	2:B:28:LYS:O	2.48	0.46
2:F:15:ILE:HD11	2:F:291:LEU:HD22	1.98	0.46
2:F:205:LEU:HD23	8:F:3656:HOH:O	2.15	0.46
2:D:277:VAL:O	2:D:289:GLY:HA3	2.16	0.46
1:G:4:ASN:ND2	1:G:6:SER:H	2.14	0.46
2:F:14:ASN:HB3	2:F:284:LEU:HD21	1.99	0.45
1:A:169:ALA:HA	1:A:200:HIS:HB3	1.98	0.45
1:G:3:PHE:HE1	1:G:4:ASN:O	1.87	0.45
2:B:35[B]:MET:HG2	2:B:45:LEU:HD23	1.99	0.45
1:C:179:ASP:OD2	7:C:3524:MPD:H52	2.17	0.45
1:A:247:GLU:OE1	1:A:253:HIS:HE1	2.00	0.45
2:D:81:ALA:H	2:D:171[B]:ASN:CG	2.20	0.45
7:C:3524:MPD:HM2	7:C:3524:MPD:H52	1.98	0.45
1:G:121[A]:VAL:HG22	2:H:172:ILE:HG13	1.96	0.45
2:D:208:ARG:NH2	2:D:244:LYS:HG2	2.30	0.45
1:E:118:GLU:O	1:E:121:VAL:HG22	2.17	0.45
2:B:126:ASN:C	2:B:126:ASN:HD22	2.20	0.45
2:D:80:SER:HA	2:D:171[B]:ASN:HD21	1.82	0.44
1:G:325:GLN:HG2	2:H:197[A]:ILE:HD13	1.98	0.44
2:B:281:ALA:HA	2:B:284:LEU:O	2.17	0.44
2:B:93:GLN:HB2	7:B:3528:MPD:H13	2.00	0.44
1:C:215:ALA:O	1:C:220[A]:CYS:HB3	2.18	0.44
2:H:132[A]:CYS:HB3	6:H:3503:NAD:C4N	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ASN:HB3	8:E:3702:HOH:O	2.17	0.44
2:F:138[B]:ILE:HD11	2:F:183:ILE:HA	1.95	0.44
2:F:7:VAL:HG12	2:F:74:PHE:HB2	1.99	0.44
2:D:15:ILE:HD11	6:D:3502:NAD:C4N	2.48	0.44
1:G:229:GLY:O	1:G:230:MET:C	2.56	0.43
1:E:272:GLN:NE2	1:E:276:VAL:H	2.16	0.43
2:D:257:PRO:HG2	2:D:265:ARG:CD	2.47	0.43
2:B:7:VAL:HG12	2:B:74:PHE:HB2	2.00	0.43
1:G:4:ASN:HA	1:G:5:PRO:HD3	1.25	0.43
1:A:96:VAL:HG13	1:A:128:TYR:CE2	2.53	0.43
1:A:320:ARG:HD3	8:A:3917:HOH:O	2.17	0.43
2:D:138:ILE:N	2:D:139:PRO:CD	2.82	0.43
1:C:116:CYS:O	1:C:154:GLN:HG3	2.17	0.43
2:B:132[B]:CYS:SG	6:B:3501:NAD:C4N	3.07	0.43
2:H:132[B]:CYS:SG	6:H:3503:NAD:C4N	3.07	0.43
2:D:60:VAL:O	2:D:63:LEU:HB3	2.19	0.43
1:A:144:HIS:HE1	8:A:3628:HOH:O	2.02	0.42
1:G:3:PHE:CG	1:G:4:ASN:N	2.85	0.42
2:F:203:PRO:O	2:F:205:LEU:HD22	2.19	0.42
2:B:203:PRO:HA	2:B:204:PRO:HD3	1.90	0.42
1:G:137:VAL:HG22	1:G:165:CYS:HB3	2.02	0.42
2:H:21:ILE:HD13	2:H:282:HIS:O	2.18	0.42
2:H:132[A]:CYS:HB3	6:H:3503:NAD:H4N	2.00	0.42
1:E:51:HIS:HE1	1:E:63:GLY:O	2.02	0.42
2:B:47:ARG:O	2:B:51:MET:HG3	2.19	0.42
2:F:22[A]:LYS:HZ2	2:F:282:HIS:CD2	2.37	0.42
7:G:3526:MPD:CM	7:G:3526:MPD:C5	2.96	0.42
2:F:35[B]:MET:HG2	2:F:45:LEU:HD23	2.01	0.42
2:D:81:ALA:N	2:D:171[B]:ASN:HD21	2.16	0.42
1:G:321:MET:CE	1:G:321:MET:HA	2.49	0.42
2:F:205:LEU:N	2:F:205:LEU:HD22	2.35	0.41
2:D:257:PRO:HB2	2:D:265:ARG:HG2	2.02	0.41
2:B:22:LYS:NZ	2:B:282:HIS:HD2	2.18	0.41
2:B:84:HIS:HE1	2:B:100:LEU:CD2	2.33	0.41
1:G:89:LEU:HD21	1:G:125:HIS:HD2	1.86	0.41
1:G:123:LYS:HE2	1:G:127:GLU:OE2	2.20	0.41
2:B:65:LYS:HD2	8:B:3713:HOH:O	2.19	0.41
1:E:157[B]:LEU:HG	1:E:161:TYR:CZ	2.55	0.41
2:H:203:PRO:HA	2:H:204:PRO:HD3	1.88	0.41
1:C:3:PHE:HA	8:C:3892:HOH:O	2.20	0.41
2:D:104:THR:HB	2:D:105:PRO:HD2	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:ASP:OD2	7:G:3526:MPD:H52	2.20	0.41
1:A:96:VAL:HG13	1:A:128:TYR:CG	2.55	0.41
1:E:321:MET:HA	1:E:321:MET:CE	2.50	0.41
2:D:20[A]:MET:HE3	2:D:35:MET:HE3	2.03	0.41
1:E:10:TYR:HB3	1:E:222:ARG:HG2	2.02	0.41
1:C:149:GLU:H	1:C:149:GLU:CD	2.24	0.41
2:H:121:HIS:HD2	2:H:124:LYS:HZ3	1.69	0.40
2:H:38:ILE:HG23	6:H:3503:NAD:C2A	2.51	0.40
1:C:104:GLN:NE2	8:C:3795:HOH:O	2.54	0.40
1:C:109:VAL:HG22	1:C:135:ASP:HB3	2.04	0.40
1:C:37:ARG:NH1	1:C:79:GLU:OE1	2.48	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	343/345 (99%)	331 (96%)	12 (4%)	0	100	100
1	C	339/345 (98%)	330 (97%)	9 (3%)	0	100	100
1	E	342/345 (99%)	335 (98%)	7 (2%)	0	100	100
1	G	342/345 (99%)	334 (98%)	8 (2%)	0	100	100
2	B	323/312 (104%)	315 (98%)	6 (2%)	2 (1%)	30	12
2	D	316/312 (101%)	306 (97%)	9 (3%)	1 (0%)	46	26
2	F	320/312 (103%)	310 (97%)	8 (2%)	2 (1%)	30	12
2	H	312/312 (100%)	302 (97%)	8 (3%)	2 (1%)	30	12
All	All	2637/2628 (100%)	2563 (97%)	67 (2%)	7 (0%)	52	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	130[A]	VAL
2	F	130[B]	VAL
2	B	203	PRO
2	H	203	PRO
2	B	130	VAL
2	D	130	VAL
2	H	130	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	271/270 (100%)	267 (98%)	4 (2%)	72	56
1	C	267/270 (99%)	264 (99%)	3 (1%)	80	69
1	E	270/270 (100%)	265 (98%)	5 (2%)	65	46
1	G	270/270 (100%)	262 (97%)	8 (3%)	48	26
2	B	250/237 (106%)	245 (98%)	5 (2%)	63	44
2	D	244/237 (103%)	241 (99%)	3 (1%)	78	65
2	F	247/237 (104%)	243 (98%)	4 (2%)	70	54
2	H	240/237 (101%)	235 (98%)	5 (2%)	61	42
All	All	2059/2028 (102%)	2022 (98%)	37 (2%)	70	49

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	A	220[A]	CYS
1	A	220[B]	CYS
1	A	274	ARG
2	B	90	LEU
2	B	126	ASN
2	B	171[A]	ASN
2	B	171[B]	ASN
2	B	290	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	111	ARG
1	C	220[A]	CYS
1	C	220[B]	CYS
2	D	96	PRO
2	D	214	LEU
2	D	290	ASN
1	E	111	ARG
1	E	131	ASN
1	E	220[A]	CYS
1	E	220[B]	CYS
1	E	274	ARG
2	F	80	SER
2	F	103	LEU
2	F	199	ASN
2	F	205	LEU
1	G	4	ASN
1	G	8	LYS
1	G	61	ASN
1	G	111	ARG
1	G	121[A]	VAL
1	G	121[B]	VAL
1	G	220[A]	CYS
1	G	220[B]	CYS
2	H	10	ILE
2	H	100	LEU
2	H	199	ASN
2	H	290	ASN
2	H	292	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	144	HIS
1	A	253	HIS
1	A	318	HIS
2	B	26	ASN
2	B	49	GLN
2	B	126	ASN
2	B	128	ASN
2	B	282	HIS
1	C	25	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	104	GLN
1	C	131	ASN
1	C	253	HIS
2	D	49	GLN
2	D	121	HIS
2	D	246	GLN
2	D	248	GLN
1	E	51	HIS
1	E	82	HIS
1	E	253	HIS
1	E	272	GLN
2	F	86	GLN
2	F	199	ASN
2	F	235	GLN
2	F	282	HIS
1	G	4	ASN
1	G	61	ASN
1	G	82	HIS
1	G	97	HIS
1	G	253	HIS
1	G	325	GLN
2	H	121	HIS
2	H	128	ASN
2	H	151	HIS
2	H	171	ASN
2	H	199	ASN
2	H	235	GLN
2	H	246	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 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 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	$\# Z  > 2$
4	OXL	A	3508	3	0,5,5	0.00	-	0,6,6	0.00	-
5	SO4	A	3512	-	4,4,4	0.89	0	6,6,6	0.09	0
5	SO4	A	3513	-	4,4,4	0.89	0	6,6,6	0.07	0
7	MPD	A	3525	-	6,7,7	1.15	1 (16%)	7,10,10	0.69	0
6	NAD	B	3501	-	38,48,48	1.18	3 (7%)	47,73,73	2.04	11 (23%)
7	MPD	B	3528	-	6,7,7	0.59	0	7,10,10	1.49	1 (14%)
4	OXL	C	3509	3	0,5,5	0.00	-	0,6,6	0.00	-
5	SO4	C	3514	-	4,4,4	0.90	0	6,6,6	0.48	0
5	SO4	C	3515	-	4,4,4	0.90	0	6,6,6	0.16	0
5	SO4	C	3516	-	4,4,4	0.89	0	6,6,6	0.11	0
7	MPD	C	3524	-	6,7,7	0.48	0	7,10,10	0.60	0
7	MPD	C	3529	-	6,7,7	0.53	0	7,10,10	0.80	0
6	NAD	D	3502	-	38,48,48	1.26	4 (10%)	47,73,73	1.92	11 (23%)
4	OXL	E	3510	3	0,5,5	0.00	-	0,6,6	0.00	-
5	SO4	E	3517	-	4,4,4	0.98	0	6,6,6	0.29	0
5	SO4	E	3518	-	4,4,4	0.92	0	6,6,6	0.13	0
5	SO4	E	3522	-	4,4,4	0.89	0	6,6,6	0.25	0
7	MPD	E	3527	-	6,7,7	0.48	0	7,10,10	1.68	2 (28%)
5	SO4	F	3519	-	4,4,4	0.96	0	6,6,6	0.34	0
5	SO4	F	3523	-	4,4,4	1.17	0	6,6,6	0.44	0
4	OXL	G	3511	3	0,5,5	0.00	-	0,6,6	0.00	-
5	SO4	G	3520	-	4,4,4	0.88	0	6,6,6	0.31	0
5	SO4	G	3521	-	4,4,4	0.90	0	6,6,6	0.13	0
7	MPD	G	3526	-	6,7,7	0.53	0	7,10,10	0.59	0
6	NAD	H	3503	-	38,48,48	1.19	4 (10%)	47,73,73	1.90	10 (21%)

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
4	OXL	A	3508	3	-	0/0/4/4	0/0/0/0
5	SO4	A	3512	-	-	0/0/0/0	0/0/0/0
5	SO4	A	3513	-	-	0/0/0/0	0/0/0/0
7	MPD	A	3525	-	-	0/5/5/5	0/0/0/0
6	NAD	B	3501	-	-	0/22/62/62	0/5/5/5
7	MPD	B	3528	-	-	0/5/5/5	0/0/0/0
4	OXL	C	3509	3	-	0/0/4/4	0/0/0/0
5	SO4	C	3514	-	-	0/0/0/0	0/0/0/0
5	SO4	C	3515	-	-	0/0/0/0	0/0/0/0
5	SO4	C	3516	-	-	0/0/0/0	0/0/0/0
7	MPD	C	3524	-	-	0/5/5/5	0/0/0/0
7	MPD	C	3529	-	-	0/5/5/5	0/0/0/0
6	NAD	D	3502	-	-	0/22/62/62	0/5/5/5
4	OXL	E	3510	3	-	0/0/4/4	0/0/0/0
5	SO4	E	3517	-	-	0/0/0/0	0/0/0/0
5	SO4	E	3518	-	-	0/0/0/0	0/0/0/0
5	SO4	E	3522	-	-	0/0/0/0	0/0/0/0
7	MPD	E	3527	-	-	0/5/5/5	0/0/0/0
5	SO4	F	3519	-	-	0/0/0/0	0/0/0/0
5	SO4	F	3523	-	-	0/0/0/0	0/0/0/0
4	OXL	G	3511	3	-	0/0/4/4	0/0/0/0
5	SO4	G	3520	-	-	0/0/0/0	0/0/0/0
5	SO4	G	3521	-	-	0/0/0/0	0/0/0/0
7	MPD	G	3526	-	-	0/5/5/5	0/0/0/0
6	NAD	H	3503	-	-	0/22/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3502	NAD	PA-O2A	-2.36	1.44	1.54
7	A	3525	MPD	C1-C2	-2.35	1.44	1.52
6	H	3503	NAD	PA-O2A	-2.03	1.46	1.54
6	H	3503	NAD	O4B-C1B	2.20	1.44	1.41
6	H	3503	NAD	C6N-N1N	2.24	1.41	1.35
6	B	3501	NAD	C6N-N1N	2.38	1.41	1.35
6	D	3502	NAD	C6N-N1N	2.68	1.42	1.35
6	D	3502	NAD	O4B-C1B	3.25	1.45	1.41
6	B	3501	NAD	O4B-C1B	3.35	1.45	1.41
6	D	3502	NAD	C3N-C7N	3.68	1.56	1.50
6	H	3503	NAD	C3N-C7N	3.89	1.56	1.50
6	B	3501	NAD	C3N-C7N	3.96	1.56	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	3503	NAD	C5N-C4N-C3N	-6.42	112.26	120.33
6	B	3501	NAD	C5N-C4N-C3N	-6.33	112.37	120.33
6	D	3502	NAD	C5N-C4N-C3N	-5.16	113.84	120.33
6	B	3501	NAD	C5N-C6N-N1N	-3.92	113.69	120.47
6	D	3502	NAD	C5N-C6N-N1N	-3.91	113.70	120.47
6	H	3503	NAD	C4N-C3N-C7N	-3.85	110.91	121.09
6	B	3501	NAD	C4N-C3N-C7N	-3.84	110.95	121.09
7	E	3527	MPD	C2-C3-C4	-3.62	99.54	116.66
6	D	3502	NAD	O4D-C1D-N1N	-3.56	104.22	108.13
6	D	3502	NAD	C4N-C3N-C7N	-3.55	111.70	121.09
6	D	3502	NAD	O4B-C1B-N9A	-3.27	101.25	108.10
6	B	3501	NAD	C1B-N9A-C4A	-3.25	122.04	126.94
6	B	3501	NAD	C4B-O4B-C1B	-3.09	106.33	109.72
6	H	3503	NAD	PN-O3-PA	-2.90	124.60	132.73
6	D	3502	NAD	C1B-N9A-C4A	-2.85	122.64	126.94
6	H	3503	NAD	C5N-C6N-N1N	-2.78	115.66	120.47
6	B	3501	NAD	N3A-C2A-N1A	-2.45	127.02	128.89
6	H	3503	NAD	O4B-C1B-N9A	-2.33	103.22	108.10
6	D	3502	NAD	C4B-O4B-C1B	-2.03	107.48	109.72
6	B	3501	NAD	C4A-C5A-N7A	2.09	111.41	109.48
6	H	3503	NAD	C2N-C3N-C7N	2.09	125.39	119.31
6	H	3503	NAD	O2N-PN-O3	2.15	114.87	105.09
6	H	3503	NAD	O7N-C7N-N7N	2.20	125.70	122.59
7	E	3527	MPD	CM-C2-C3	2.22	122.76	109.90
6	D	3502	NAD	C4A-C5A-N7A	2.34	111.63	109.48
6	B	3501	NAD	C2N-C3N-C7N	2.37	126.19	119.31
6	D	3502	NAD	C2N-C3N-C7N	2.43	126.37	119.31
6	B	3501	NAD	C2B-C1B-N9A	3.17	119.14	114.29
6	D	3502	NAD	C2N-C3N-C4N	3.27	121.93	118.29
7	B	3528	MPD	CM-C2-C1	3.53	117.94	110.24
6	B	3501	NAD	C2N-C3N-C4N	3.90	122.63	118.29
6	H	3503	NAD	C6N-C5N-C4N	4.81	126.71	119.44
6	H	3503	NAD	C2N-C3N-C4N	4.85	123.69	118.29
6	D	3502	NAD	C6N-C5N-C4N	5.33	127.50	119.44
6	B	3501	NAD	C6N-C5N-C4N	5.97	128.47	119.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3525	MPD	1	0
6	B	3501	NAD	1	0
7	B	3528	MPD	14	0
7	C	3524	MPD	5	0
7	C	3529	MPD	1	0
6	D	3502	NAD	4	0
7	E	3527	MPD	1	0
7	G	3526	MPD	5	0
6	H	3503	NAD	5	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	340/345 (98%)	-0.08	8 (2%) 62 66	16, 21, 32, 52	21 (6%)
1	C	337/345 (97%)	-0.10	6 (1%) 71 76	17, 22, 30, 51	13 (3%)
1	E	338/345 (97%)	0.03	11 (3%) 50 54	18, 24, 35, 51	13 (3%)
1	G	339/345 (98%)	0.13	11 (3%) 51 55	19, 26, 35, 48	20 (5%)
2	B	312/312 (100%)	0.05	9 (2%) 55 59	17, 25, 38, 52	15 (4%)
2	D	308/312 (98%)	0.24	15 (4%) 33 36	18, 28, 43, 59	22 (7%)
2	F	309/312 (99%)	0.05	11 (3%) 46 51	20, 26, 36, 47	15 (4%)
2	H	307/312 (98%)	0.43	25 (8%) 15 16	21, 30, 45, 59	23 (7%)
All	All	2590/2628 (98%)	0.09	96 (3%) 45 50	16, 25, 39, 59	142 (5%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	3	PHE	8.2
1	E	3	PHE	7.9
1	E	2	THR	6.6
1	G	339	ALA	6.2
1	C	4	ASN	5.0
1	A	2	THR	4.9
2	F	80	SER	4.7
1	G	5	PRO	4.6
1	A	339	ALA	4.4
2	B	70	ALA	4.3
2	H	310	LEU	4.1
1	E	338	ALA	4.0
2	F	81	ALA	3.9
1	C	3	PHE	3.8
2	B	1	MET	3.7
1	A	3	PHE	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	4	ASN	3.7
2	D	90	LEU	3.7
2	D	67	PRO	3.7
1	C	339	ALA	3.7
2	H	72	ILE	3.6
1	C	338	ALA	3.6
1	E	306[A]	ASN	3.4
2	H	29	TYR	3.4
1	G	338	ALA	3.4
1	A	6	SER	3.3
1	C	5	PRO	3.3
2	D	96	PRO	3.3
2	H	9	ILE	3.3
2	D	94	ALA	3.3
2	B	71	ASP	3.3
2	H	52	GLY	3.2
1	E	339	ALA	3.2
2	H	67	PRO	3.2
2	F	312	ALA	3.1
1	E	5	PRO	3.0
2	D	3	GLN	3.0
2	F	265	ARG	3.0
2	H	69	PHE	3.0
2	D	255[A]	SER	2.9
2	F	255	SER	2.8
2	H	308	SER	2.8
1	E	303	ALA	2.8
2	H	93	GLN	2.8
2	B	311	ASN	2.8
1	G	81	SER	2.8
2	D	64	ILE	2.8
2	D	66	LEU	2.7
1	G	340	HIS	2.7
1	E	140	LEU	2.7
2	H	58	ALA	2.7
2	H	45	LEU	2.7
1	G	124	GLN	2.7
2	B	100	LEU	2.6
1	G	6	SER	2.6
2	F	253	PRO	2.6
2	H	41	ALA	2.6
2	H	48	ALA	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	64	ILE	2.6
2	B	76	PHE	2.5
2	F	75	VAL	2.5
1	A	4	ASN	2.5
2	H	49	GLN	2.5
2	H	57	TYR	2.4
1	A	340	HIS	2.4
2	B	312	ALA	2.4
2	F	8	ALA	2.4
2	F	256	ALA	2.4
2	B	75	VAL	2.4
2	H	90	LEU	2.4
1	C	187	PHE	2.4
2	F	82	SER	2.4
2	D	256	ALA	2.4
2	D	310	LEU	2.4
2	D	65	LYS	2.3
1	A	49	VAL	2.3
1	A	341	LYS	2.3
2	H	4	LYS	2.3
2	H	46	ALA	2.3
2	H	85	VAL	2.3
1	G	83	ALA	2.2
2	D	41	ALA	2.2
2	H	222	ALA	2.2
2	H	70	ALA	2.2
1	E	337	LEU	2.2
2	D	91	LEU	2.2
1	G	193	PRO	2.2
2	B	50	ARG	2.1
1	E	16	LEU	2.1
1	E	6	SER	2.1
2	H	53	VAL	2.1
2	D	62	GLY	2.1
2	H	27	ALA	2.1
2	D	71	ASP	2.0
2	H	65	LYS	2.0
2	F	47	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	OXL	E	3510	6/6	0.88	0.22	10.32	25,28,30,33	0
4	OXL	G	3511	6/6	0.90	0.22	9.50	26,29,31,34	0
7	MPD	G	3526	8/8	0.76	0.18	8.63	35,36,37,39	1
7	MPD	C	3524	8/8	0.69	0.27	8.53	26,27,27,27	7
5	SO4	A	3512	5/5	0.97	0.18	6.80	36,37,38,39	2
4	OXL	A	3508	6/6	0.86	0.18	6.47	22,24,28,29	0
7	MPD	B	3528	8/8	0.74	0.39	6.09	46,47,48,48	5
4	OXL	C	3509	6/6	0.88	0.18	5.91	21,24,26,31	0
5	SO4	E	3518	5/5	0.77	0.20	5.75	56,56,56,56	5
7	MPD	C	3529	8/8	0.68	0.21	4.52	47,48,49,49	0
5	SO4	C	3514	5/5	0.98	0.20	4.24	36,37,37,38	0
5	SO4	E	3517	5/5	0.97	0.21	3.94	44,44,45,46	0
5	SO4	F	3523	5/5	0.77	0.27	3.10	34,36,38,38	3
7	MPD	E	3527	8/8	0.86	0.13	2.37	28,29,41,41	4
7	MPD	A	3525	8/8	0.90	0.11	2.10	28,41,41,42	2
5	SO4	C	3516	5/5	0.91	0.13	1.19	52,52,52,52	5
5	SO4	G	3521	5/5	0.91	0.13	1.12	49,49,49,49	5
6	NAD	H	3503	44/44	0.94	0.13	0.79	28,33,37,38	0
5	SO4	F	3519	5/5	0.85	0.17	0.50	35,35,36,36	4
6	NAD	D	3502	44/44	0.95	0.11	0.46	26,28,33,36	0
6	NAD	B	3501	44/44	0.96	0.09	0.27	21,25,28,32	0
5	SO4	G	3520	5/5	0.94	0.12	0.13	28,30,30,30	5
3	MN	C	3505	1/1	0.99	0.03	-	20,20,20,20	0
3	MN	G	3507	1/1	0.99	0.03	-	24,24,24,24	0
5	SO4	A	3513	5/5	0.88	0.13	-	48,49,49,49	5
5	SO4	C	3515	5/5	0.93	0.14	-	51,51,51,52	5
3	MN	E	3506	1/1	1.00	0.01	-	22,22,22,22	0
3	MN	A	3504	1/1	1.00	0.02	-	19,19,19,19	0
5	SO4	E	3522	5/5	0.83	0.18	-	43,44,44,44	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.