



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:57 PM GMT

PDB ID : 2V7G
Title : Crystal Structure of an Engineered Urocanase Tetramer
Authors : Treiber, N.; Schulz, G.E.
Deposited on : 2007-07-30
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

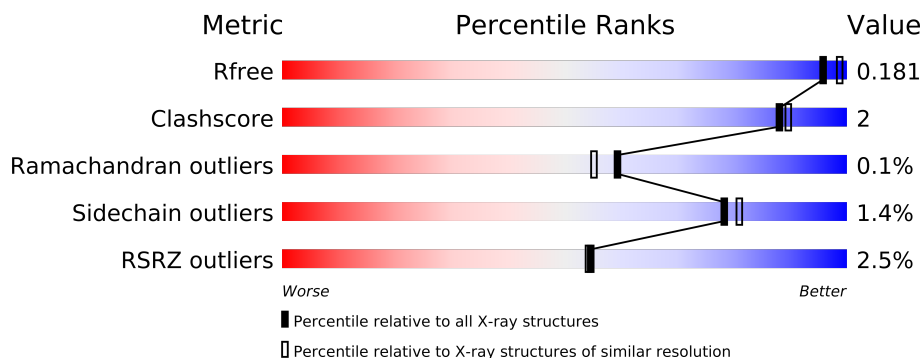
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	557	
1	B	557	
1	C	557	
1	D	557	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ACT	A	1559	-	X
3	GOL	A	1560	-	X
3	GOL	A	1561	-	X
3	GOL	B	1561	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	B	1563	-	X
3	GOL	D	1559	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18528 atoms, of which 0 are hydrogen and 0 are deuterium.

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 UROCANATE HYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4240	2664	757	797	22			
1	B	553	Total	C	N	O	S	0	0	0
			4240	2664	757	797	22			
1	C	553	Total	C	N	O	S	0	0	0
			4240	2664	757	797	22			
1	D	553	Total	C	N	O	S	0	0	0
			4240	2664	757	797	22			

There are 28 discrepancies between the modelled and reference sequences:

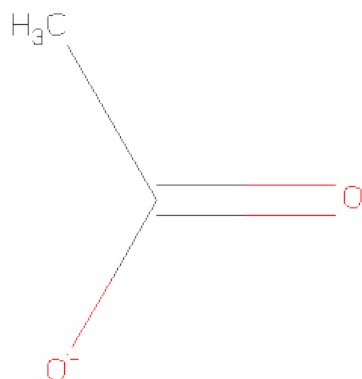
Chain	Residue	Modelled	Actual	Comment	Reference
A	198	SER	CYS	ENGINEERED MUTATION	UNP P25080
A	277	ILE	ALA	ENGINEERED MUTATION	UNP P25080
A	291	ILE	GLU	ENGINEERED MUTATION	UNP P25080
A	301	ALA	GLN	ENGINEERED MUTATION	UNP P25080
A	164	SER	THR	CONFLICT	UNP P25080
A	165	LEU	VAL	CONFLICT	UNP P25080
A	167	GLY	ALA	CONFLICT	UNP P25080
B	198	SER	CYS	ENGINEERED MUTATION	UNP P25080
B	277	ILE	ALA	ENGINEERED MUTATION	UNP P25080
B	291	ILE	GLU	ENGINEERED MUTATION	UNP P25080
B	301	ALA	GLN	ENGINEERED MUTATION	UNP P25080
B	164	SER	THR	CONFLICT	UNP P25080
B	165	LEU	VAL	CONFLICT	UNP P25080
B	167	GLY	ALA	CONFLICT	UNP P25080
C	198	SER	CYS	ENGINEERED MUTATION	UNP P25080
C	277	ILE	ALA	ENGINEERED MUTATION	UNP P25080
C	291	ILE	GLU	ENGINEERED MUTATION	UNP P25080
C	301	ALA	GLN	ENGINEERED MUTATION	UNP P25080
C	164	SER	THR	CONFLICT	UNP P25080
C	165	LEU	VAL	CONFLICT	UNP P25080
C	167	GLY	ALA	CONFLICT	UNP P25080

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Chain	Residue	Modelled	Actual	Comment	Reference
D	198	SER	CYS	ENGINEERED MUTATION	UNP P25080
D	277	ILE	ALA	ENGINEERED MUTATION	UNP P25080
D	291	ILE	GLU	ENGINEERED MUTATION	UNP P25080
D	301	ALA	GLN	ENGINEERED MUTATION	UNP P25080
D	164	SER	THR	CONFLICT	UNP P25080
D	165	LEU	VAL	CONFLICT	UNP P25080
D	167	GLY	ALA	CONFLICT	UNP P25080

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



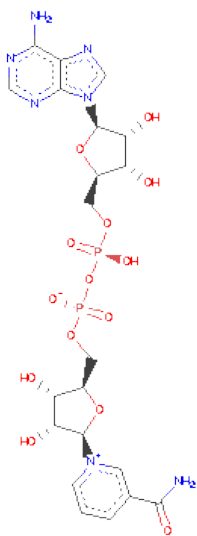
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

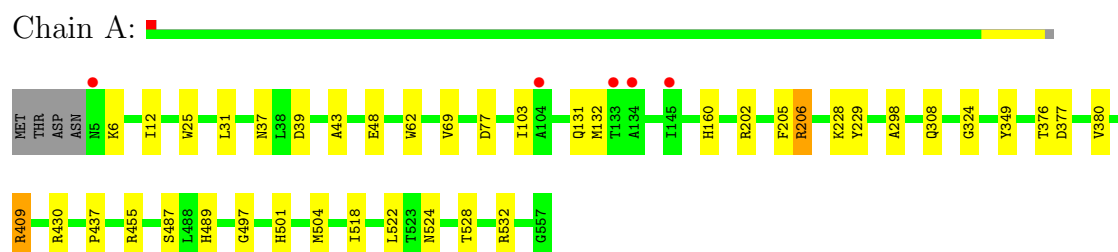
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	347	Total	O	0	0
			347	347		
5	B	341	Total	O	0	0
			341	341		
5	C	330	Total	O	0	0
			330	330		
5	D	292	Total	O	0	0
			292	292		

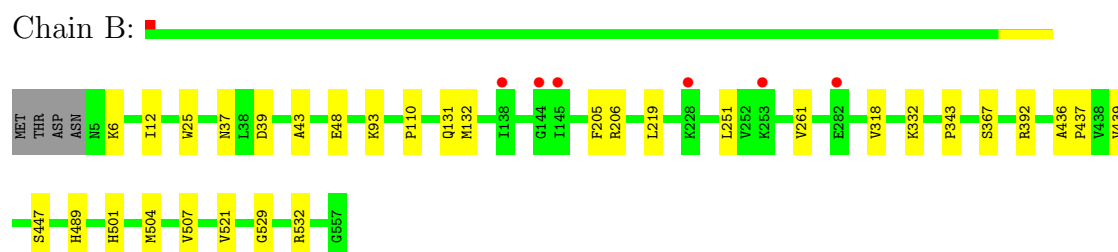
3 Residue-property plots

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

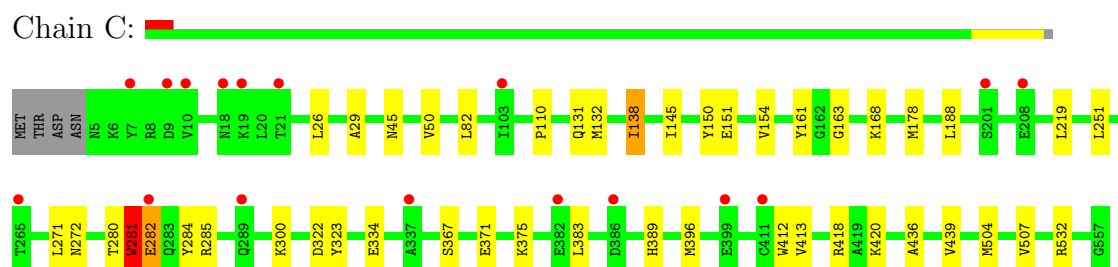
• Molecule 1: UROCANATE HYDRATASE



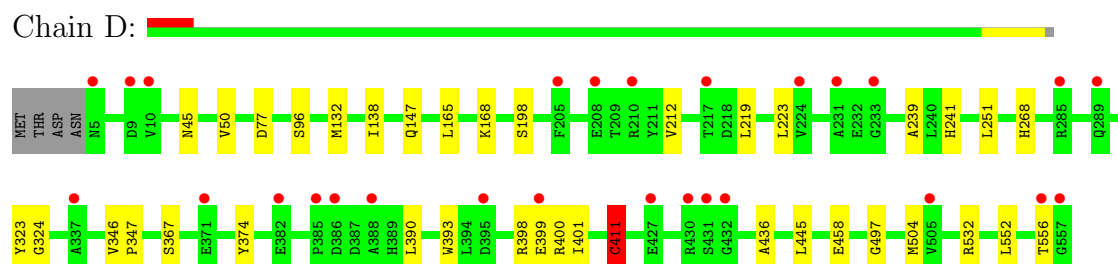
• Molecule 1: UROCANATE HYDRATASE



• Molecule 1: UROCANATE HYDRATASE



• Molecule 1: UROCANATE HYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.07Å 154.32Å 216.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.81 – 2.00 28.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.81-2.00) 97.0 (28.81-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.19 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.156 , 0.181 0.157 , 0.181	Depositor DCC
R_{free} test set	1498 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 149791 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18528	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 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.43	0/4333	0.57	0/5881
1	B	0.42	0/4333	0.55	0/5881
1	C	0.40	0/4333	0.55	1/5881 (0.0%)
1	D	0.40	1/4333 (0.0%)	0.53	0/5881
All	All	0.41	1/17332 (0.0%)	0.55	1/23524 (0.0%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	411	CYS	CB-SG	-5.74	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	TRP	N-CA-C	5.08	124.73	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	281	TRP	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4240	0	4160	22	0
1	B	4240	0	4160	18	0
1	C	4240	0	4160	27	0
1	D	4240	0	4160	20	0
2	A	8	0	6	0	0
2	B	12	0	9	0	0
2	C	8	0	6	0	0
3	A	12	0	16	1	0
3	B	18	0	24	1	0
3	D	24	0	32	0	0
4	A	44	0	26	0	0
4	B	44	0	26	0	0
4	C	44	0	26	0	0
4	D	44	0	26	2	0
5	A	347	0	0	0	0
5	B	341	0	0	0	0
5	C	330	0	0	0	0
5	D	292	0	0	1	0
All	All	18528	0	16837	83	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (83) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:377:ASP:OD1	1:A:409:ARG:HD2	1.97	0.64
1:C:413:VAL:HG23	1:C:418:ARG:HG2	1.82	0.60
1:C:281:TRP:N	1:C:282:GLU:HB2	2.17	0.60
1:C:300:LYS:HE3	1:C:334:GLU:OE2	2.03	0.58
1:C:280:THR:OG1	1:C:282:GLU:HB3	2.05	0.56
1:D:165:LEU:O	1:D:168:LYS:HB2	2.06	0.55
1:C:281:TRP:O	1:C:284:TYR:HB3	2.07	0.55
1:A:430:ARG:HH12	1:B:392:ARG:HD3	1.72	0.55
1:D:556:THR:HG23	5:D:2284:HOH:O	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:439:VAL:HG12	1:C:507:VAL:HG12	1.91	0.53
1:C:45:ASN:HB3	1:C:50:VAL:HB	1.89	0.53
1:B:6:LYS:O	1:B:48:GLU:HA	2.09	0.52
1:A:6:LYS:O	1:A:48:GLU:HA	2.08	0.52
1:A:31:LEU:HD11	1:A:69:VAL:HG13	1.92	0.52
1:D:147:GLN:HG2	1:D:393:TRP:CZ2	2.45	0.52
1:D:219:LEU:HD11	1:D:251:LEU:HD21	1.92	0.52
1:C:145:ILE:CD1	1:C:178:MET:HA	2.41	0.50
1:D:212:VAL:HG11	1:D:239:ALA:HB2	1.93	0.50
1:C:145:ILE:HD11	1:C:178:MET:HA	1.95	0.49
1:D:399:GLU:HG3	1:D:400:ARG:HG2	1.94	0.49
1:D:346:VAL:HB	1:D:347:PRO:HD3	1.93	0.49
1:B:219:LEU:HD11	1:B:251:LEU:HD21	1.95	0.49
1:D:324:GLY:HA3	4:D:3001:NAD:H71N	1.78	0.49
1:B:447:SER:OG	1:B:529:GLY:HA3	2.12	0.48
1:C:29:ALA:CB	1:C:507:VAL:HG11	2.43	0.48
1:C:271:LEU:O	1:C:285:ARG:NH2	2.42	0.48
1:D:390:LEU:HD11	1:D:411:CYS:SG	2.53	0.48
1:D:552:LEU:H	1:D:556:THR:CG2	2.27	0.48
1:B:489:HIS:HB2	1:B:501:HIS:CE1	2.49	0.48
1:A:298:ALA:HB1	3:A:1560:GOL:H31	1.95	0.48
1:A:160:HIS:HE1	1:A:349:TYR:OH	1.96	0.47
1:A:25:TRP:CD2	1:A:437:PRO:HG2	2.50	0.47
1:A:430:ARG:HH12	1:B:392:ARG:CD	2.28	0.46
1:B:504:MET:CE	1:B:521:VAL:CG1	2.93	0.46
1:A:37:ASN:O	1:A:43:ALA:HB2	2.15	0.46
1:A:12:ILE:HD11	1:A:62:TRP:CZ3	2.51	0.46
1:B:37:ASN:O	1:B:43:ALA:HB2	2.16	0.46
1:C:26:LEU:HD23	1:C:507:VAL:HG21	1.98	0.46
1:A:12:ILE:O	1:A:39:ASP:HA	2.16	0.46
1:B:367:SER:HB3	1:B:436:ALA:HB3	1.98	0.46
1:B:110:PRO:HB2	1:D:497:GLY:HA2	1.97	0.45
1:A:524:ASN:O	1:A:528:THR:HG23	2.17	0.44
1:D:77:ASP:O	1:D:96:SER:HA	2.17	0.44
1:D:367:SER:HB3	1:D:436:ALA:HB3	1.98	0.44
1:C:371:GLU:HG3	1:C:375:LYS:HE3	2.00	0.44
1:C:272:ASN:HA	1:C:285:ARG:NH2	2.33	0.44
1:D:45:ASN:HB3	1:D:50:VAL:HB	1.99	0.44
1:C:219:LEU:HD11	1:C:251:LEU:HD21	2.00	0.44
1:A:131:GLN:HB3	1:A:132:MET:H	1.68	0.44
1:D:393:TRP:CH2	1:D:401:ILE:HD13	2.53	0.43
1:B:131:GLN:HB3	1:B:132:MET:H	1.70	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:396:MET:HB2	1:C:396:MET:HE2	1.88	0.43
1:C:131:GLN:HB3	1:C:132:MET:H	1.68	0.43
1:C:150:TYR:CZ	1:C:154:VAL:HG21	2.53	0.43
1:A:489:HIS:HB2	1:A:501:HIS:CE1	2.53	0.43
1:C:138:ILE:O	1:C:138:ILE:HG13	2.18	0.43
1:C:151:GLU:HG2	1:C:412:TRP:CD2	2.53	0.42
1:B:25:TRP:CD2	1:B:437:PRO:HG2	2.55	0.42
1:A:228:LYS:HE3	1:A:229:TYR:CE1	2.54	0.42
1:C:29:ALA:CB	1:C:507:VAL:CG1	2.98	0.42
1:C:188:LEU:O	1:C:396:MET:HE1	2.19	0.42
1:A:376:THR:O	1:A:380:VAL:HG23	2.19	0.42
1:B:392:ARG:HA	1:B:392:ARG:HD2	1.85	0.42
1:C:367:SER:HB3	1:C:436:ALA:HB3	2.02	0.42
1:B:504:MET:HE3	1:B:521:VAL:CG1	2.50	0.41
1:A:324:GLY:HA3	1:A:455:ARG:HD2	2.02	0.41
1:D:268:HIS:CD2	4:D:3001:NAD:O3D	2.73	0.41
1:A:518:ILE:HG23	1:A:522:LEU:HD12	2.03	0.41
1:C:383:LEU:HD22	1:C:420:LYS:HE2	2.02	0.41
1:A:103:ILE:O	1:A:487:SER:HA	2.21	0.41
1:A:12:ILE:HD11	1:A:62:TRP:HZ3	1.85	0.41
1:C:161:TYR:CD1	1:C:168:LYS:HE2	2.56	0.41
1:D:374:TYR:CE1	1:D:398:ARG:HG3	2.55	0.41
1:D:132:MET:CE	1:D:445:LEU:HD21	2.50	0.41
1:D:198:SER:O	1:D:241:HIS:HE1	2.04	0.41
1:B:439:VAL:HG12	1:B:507:VAL:HG22	2.02	0.41
1:D:132:MET:HE1	1:D:445:LEU:HD21	2.03	0.41
1:C:163:GLY:HA3	1:C:389:HIS:CE1	2.55	0.41
1:A:497:GLY:HA2	1:C:110:PRO:HB2	2.03	0.41
1:B:261:VAL:HG23	1:B:318:VAL:HG11	2.03	0.41
1:B:12:ILE:O	1:B:39:ASP:HA	2.21	0.41
1:B:343:PRO:HG3	3:B:1563:GOL:H32	2.04	0.40
1:A:202:ARG:O	1:A:206:ARG:HD2	2.22	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	551/557 (99%)	535 (97%)	16 (3%)	0	100	100
1	B	551/557 (99%)	531 (96%)	20 (4%)	0	100	100
1	C	551/557 (99%)	539 (98%)	11 (2%)	1 (0%)	56	51
1	D	551/557 (99%)	536 (97%)	14 (2%)	1 (0%)	56	51
All	All	2204/2228 (99%)	2141 (97%)	61 (3%)	2 (0%)	59	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	138	ILE
1	D	138	ILE

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	435/439 (99%)	428 (98%)	7 (2%)	75	77
1	B	435/439 (99%)	430 (99%)	5 (1%)	84	86
1	C	435/439 (99%)	429 (99%)	6 (1%)	78	81
1	D	435/439 (99%)	429 (99%)	6 (1%)	78	81
All	All	1740/1756 (99%)	1716 (99%)	24 (1%)	78	81

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	205	PHE
1	A	206	ARG
1	A	308	GLN
1	A	409	ARG
1	A	504	MET
1	A	532	ARG

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Mol	Chain	Res	Type
1	B	93	LYS
1	B	205	PHE
1	B	206	ARG
1	B	332	LYS
1	B	532	ARG
1	C	82	LEU
1	C	282	GLU
1	C	322	ASP
1	C	323	TYR
1	C	504	MET
1	C	532	ARG
1	D	223	LEU
1	D	323	TYR
1	D	411	CYS
1	D	458	GLU
1	D	504	MET
1	D	532	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	160	HIS
1	A	308	GLN
1	B	18	ASN
1	B	241	HIS
1	C	5	ASN
1	C	119	ASN
1	C	268	HIS
1	C	389	HIS
1	C	454	ASN
1	D	18	ASN
1	D	241	HIS
1	D	268	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

20 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	ACT	A	1558	-	1,3,3	1.40	0	0,3,3	0.00	-
2	ACT	A	1559	-	1,3,3	1.26	0	0,3,3	0.00	-
3	GOL	A	1560	-	5,5,5	0.49	0	5,5,5	0.55	0
3	GOL	A	1561	-	5,5,5	0.30	0	5,5,5	0.51	0
4	NAD	A	3001	-	48,48,48	1.21	3 (6%)	73,73,73	1.86	11 (15%)
2	ACT	B	1558	-	1,3,3	1.29	0	0,3,3	0.00	-
2	ACT	B	1559	-	1,3,3	1.24	0	0,3,3	0.00	-
2	ACT	B	1560	-	1,3,3	1.44	0	0,3,3	0.00	-
3	GOL	B	1561	-	5,5,5	0.27	0	5,5,5	0.33	0
3	GOL	B	1562	-	5,5,5	0.37	0	5,5,5	0.56	0
3	GOL	B	1563	-	5,5,5	0.25	0	5,5,5	0.57	0
4	NAD	B	3001	-	48,48,48	1.14	4 (8%)	73,73,73	1.89	13 (17%)
2	ACT	C	1558	-	1,3,3	1.25	0	0,3,3	0.00	-
2	ACT	C	1559	-	1,3,3	1.44	0	0,3,3	0.00	-
4	NAD	C	3001	-	48,48,48	1.16	5 (10%)	73,73,73	1.70	10 (13%)
3	GOL	D	1558	-	5,5,5	0.37	0	5,5,5	0.32	0
3	GOL	D	1559	-	5,5,5	0.35	0	5,5,5	0.19	0
3	GOL	D	1560	-	5,5,5	0.32	0	5,5,5	0.14	0
3	GOL	D	1561	-	5,5,5	0.35	0	5,5,5	0.48	0
4	NAD	D	3001	-	48,48,48	1.07	3 (6%)	73,73,73	1.66	10 (13%)

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	ACT	A	1558	-	-	0/0/0/0	0/0/0/0
2	ACT	A	1559	-	-	0/0/0/0	0/0/0/0
3	GOL	A	1560	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1561	-	-	0/4/4/4	0/0/0/0
4	NAD	A	3001	-	-	0/30/62/62	0/3/5/5
2	ACT	B	1558	-	-	0/0/0/0	0/0/0/0
2	ACT	B	1559	-	-	0/0/0/0	0/0/0/0
2	ACT	B	1560	-	-	0/0/0/0	0/0/0/0
3	GOL	B	1561	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1562	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1563	-	-	0/4/4/4	0/0/0/0
4	NAD	B	3001	-	-	0/30/62/62	0/3/5/5
2	ACT	C	1558	-	-	0/0/0/0	0/0/0/0
2	ACT	C	1559	-	-	0/0/0/0	0/0/0/0
4	NAD	C	3001	-	-	0/30/62/62	0/3/5/5
3	GOL	D	1558	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1559	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1560	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1561	-	-	0/4/4/4	0/0/0/0
4	NAD	D	3001	-	-	0/30/62/62	0/3/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3001	NAD	C2N-N1N	5.17	1.41	1.35
4	B	3001	NAD	C2N-N1N	4.43	1.41	1.35
4	D	3001	NAD	C2N-N1N	4.02	1.40	1.35
4	C	3001	NAD	C2N-N1N	4.01	1.40	1.35
4	C	3001	NAD	O4D-C1D	3.28	1.46	1.41
4	A	3001	NAD	O4D-C1D	3.10	1.46	1.41
4	B	3001	NAD	C4A-N9A	-3.07	1.33	1.37
4	A	3001	NAD	C4A-N9A	-2.99	1.33	1.37
4	C	3001	NAD	O4B-C1B	2.95	1.45	1.41
4	C	3001	NAD	C4A-N9A	-2.77	1.33	1.37
4	D	3001	NAD	C4A-N9A	-2.70	1.33	1.37
4	D	3001	NAD	O4D-C1D	2.52	1.45	1.41
4	B	3001	NAD	O4B-C1B	2.46	1.45	1.41
4	C	3001	NAD	C6N-N1N	2.22	1.41	1.35
4	B	3001	NAD	C6N-N1N	2.01	1.41	1.35

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	NAD	N3A-C2A-N1A	-8.85	121.31	128.71
4	D	3001	NAD	N3A-C2A-N1A	-8.81	121.34	128.71
4	C	3001	NAD	N3A-C2A-N1A	-8.73	121.41	128.71
4	B	3001	NAD	N3A-C2A-N1A	-8.72	121.42	128.71
4	B	3001	NAD	O4D-C1D-N1N	-6.75	101.04	107.95
4	A	3001	NAD	O4D-C1D-N1N	-6.25	101.56	107.95
4	A	3001	NAD	C4B-O4B-C1B	-5.18	104.13	109.75
4	B	3001	NAD	C4B-O4B-C1B	-5.10	104.21	109.75
4	C	3001	NAD	O4B-C1B-N9A	-5.08	103.71	108.44
4	B	3001	NAD	N3A-C4A-N9A	4.60	133.74	125.43
4	A	3001	NAD	N3A-C4A-N9A	4.41	133.40	125.43
4	C	3001	NAD	N3A-C4A-N9A	4.25	133.11	125.43
4	D	3001	NAD	N3A-C4A-N9A	4.17	132.96	125.43
4	D	3001	NAD	C4B-O4B-C1B	-3.89	105.53	109.75
4	D	3001	NAD	O4B-C1B-N9A	-3.56	105.13	108.44
4	A	3001	NAD	O4B-C1B-N9A	-3.40	105.28	108.44
4	D	3001	NAD	C3N-C7N-N7N	-3.32	113.99	117.77
4	B	3001	NAD	O4B-C1B-N9A	-3.14	105.52	108.44
4	B	3001	NAD	O4B-C1B-C2B	-3.10	102.02	106.77
4	C	3001	NAD	C4B-O4B-C1B	-3.02	106.47	109.75
4	D	3001	NAD	O4B-C1B-C2B	-2.83	102.43	106.77
4	A	3001	NAD	O4D-C1D-C2D	-2.82	102.45	106.77
4	C	3001	NAD	C5A-C4A-N3A	-2.81	119.59	125.70
4	D	3001	NAD	C5A-C4A-N3A	-2.80	119.60	125.70
4	C	3001	NAD	O4B-C1B-C2B	-2.79	102.50	106.77
4	B	3001	NAD	O4D-C1D-C2D	-2.77	102.53	106.77
4	B	3001	NAD	C5A-C4A-N3A	-2.73	119.76	125.70
4	B	3001	NAD	C4D-O4D-C1D	-2.62	106.91	109.75
4	A	3001	NAD	C5A-C4A-N3A	-2.60	120.04	125.70
4	D	3001	NAD	C4A-C5A-N7A	-2.49	107.39	109.52
4	C	3001	NAD	C4A-C5A-N7A	-2.47	107.41	109.52
4	A	3001	NAD	C4D-O4D-C1D	-2.44	107.10	109.75
4	B	3001	NAD	C8A-N9A-C4A	2.31	108.67	106.90
4	C	3001	NAD	C3N-C7N-N7N	-2.27	115.19	117.77
4	C	3001	NAD	C2A-N3A-C4A	2.26	120.44	114.01
4	D	3001	NAD	C2A-N3A-C4A	2.22	120.32	114.01
4	C	3001	NAD	C5B-C4B-C3B	-2.19	106.45	115.21
4	B	3001	NAD	C2A-N3A-C4A	2.17	120.19	114.01
4	A	3001	NAD	C2A-N3A-C4A	2.13	120.06	114.01
4	A	3001	NAD	C5B-C4B-C3B	-2.07	106.90	115.21
4	A	3001	NAD	O4B-C1B-C2B	-2.07	103.60	106.77
4	D	3001	NAD	O7N-C7N-C3N	2.06	121.90	119.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3001	NAD	C4A-C5A-N7A	-2.06	107.76	109.52
4	B	3001	NAD	C3N-C7N-N7N	-2.05	115.44	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	553/557 (99%)	0.11	5 (0%) 81 82	21, 25, 30, 40	0
1	B	553/557 (99%)	0.03	6 (1%) 77 78	21, 25, 29, 35	0
1	C	553/557 (99%)	0.11	17 (3%) 47 46	19, 24, 32, 44	0
1	D	553/557 (99%)	0.20	27 (4%) 28 28	18, 24, 33, 40	0
All	All	2212/2228 (99%)	0.11	55 (2%) 54 54	18, 24, 31, 44	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	337	ALA	4.7
1	C	386	ASP	4.2
1	D	430	ARG	3.6
1	D	431	SER	3.4
1	D	386	ASP	3.3
1	D	5	ASN	3.3
1	C	9	ASP	3.1
1	C	399	GLU	3.1
1	D	285	ARG	3.0
1	D	371	GLU	3.0
1	D	385	PRO	3.0
1	C	10	VAL	2.9
1	A	5	ASN	2.8
1	C	282	GLU	2.8
1	D	289	GLN	2.8
1	D	427	GLU	2.8
1	D	217	THR	2.7
1	C	337	ALA	2.7
1	C	289	GLN	2.6
1	D	210	ARG	2.6
1	D	231	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	388	ALA	2.6
1	D	556	THR	2.5
1	C	19	LYS	2.5
1	D	10	VAL	2.5
1	D	224	VAL	2.5
1	B	282	GLU	2.4
1	B	144	GLY	2.4
1	D	9	ASP	2.4
1	D	399	GLU	2.4
1	D	505	VAL	2.4
1	C	103	ILE	2.4
1	A	145	ILE	2.3
1	B	145	ILE	2.3
1	A	104	ALA	2.3
1	A	134	ALA	2.3
1	C	265	THR	2.3
1	C	7	TYR	2.3
1	C	411	CYS	2.2
1	D	205	PHE	2.2
1	D	233	GLY	2.2
1	D	432	GLY	2.2
1	D	395	ASP	2.2
1	A	133	THR	2.2
1	C	21	THR	2.2
1	B	228	LYS	2.1
1	B	138	ILE	2.1
1	C	201	SER	2.1
1	C	208	GLU	2.1
1	D	382	GLU	2.1
1	D	557	GLY	2.1
1	C	18	ASN	2.0
1	B	253	LYS	2.0
1	C	382	GLU	2.0
1	D	208	GLU	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	D	1559	6/6	0.21	10.90	58,59,59,59	0
3	GOL	B	1561	6/6	0.24	9.24	44,46,46,48	0
2	ACT	A	1559	4/4	0.21	8.27	53,53,53,53	0
3	GOL	A	1560	6/6	0.29	7.65	36,36,38,39	0
3	GOL	B	1563	6/6	0.26	6.75	46,47,47,48	0
3	GOL	A	1561	6/6	0.20	5.30	42,43,43,43	0
2	ACT	B	1558	4/4	0.22	1.87	53,54,54,54	0
3	GOL	D	1560	6/6	0.20	1.49	38,42,43,44	0
3	GOL	B	1562	6/6	0.16	1.28	40,43,44,44	0
3	GOL	D	1558	6/6	0.18	1.02	37,39,40,40	0
2	ACT	B	1559	4/4	0.19	0.92	64,64,64,64	0
3	GOL	D	1561	6/6	0.15	0.54	46,46,47,47	0
2	ACT	C	1558	4/4	0.11	0.09	33,33,34,34	0
2	ACT	C	1559	4/4	0.09	-1.02	24,24,24,24	0
4	NAD	C	3001	44/44	0.08	-1.11	19,20,22,24	0
4	NAD	D	3001	44/44	0.08	-1.22	18,21,23,24	0
4	NAD	B	3001	44/44	0.08	-1.67	13,16,21,25	0
4	NAD	A	3001	44/44	0.09	-1.82	14,15,20,22	0
2	ACT	B	1560	4/4	0.10	-3.29	17,17,17,18	0
2	ACT	A	1558	4/4	0.08	-5.00	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.