Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:26 PM GMT

PDB ID	:	4LK3
Title	:	Crystal structure of Human UDP-xylose synthase R236A substitution
Authors	:	Walsh Jr., R.M.; Polizzi, S.J.; Wood, Z.A.
Deposited on	:	2013-07-05
Resolution	:	2.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

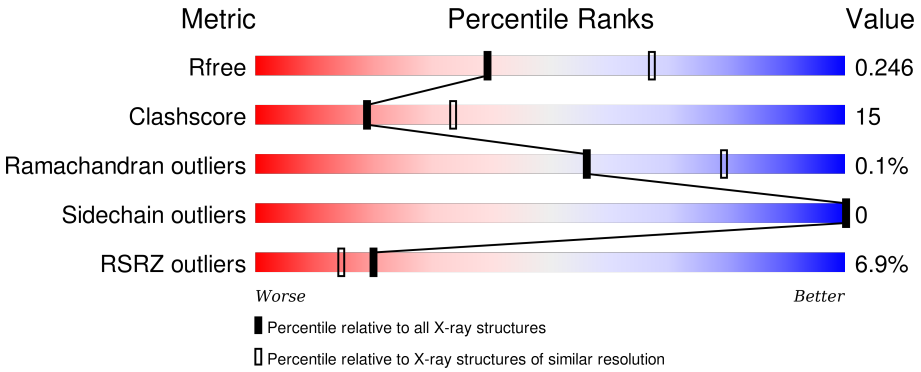
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.64 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	11% 53% 26% 21%
1	B	336	4% 65% 16% 18%
1	C	336	% 67% 14% 19%
1	D	336	% 61% 20% 19%
1	E	336	7% 61% 19% 20%

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Mol	Chain	Length	Quality of chain
1	F	336	8% 47% 31% 22%

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
5	SO4	A	505	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13434 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.

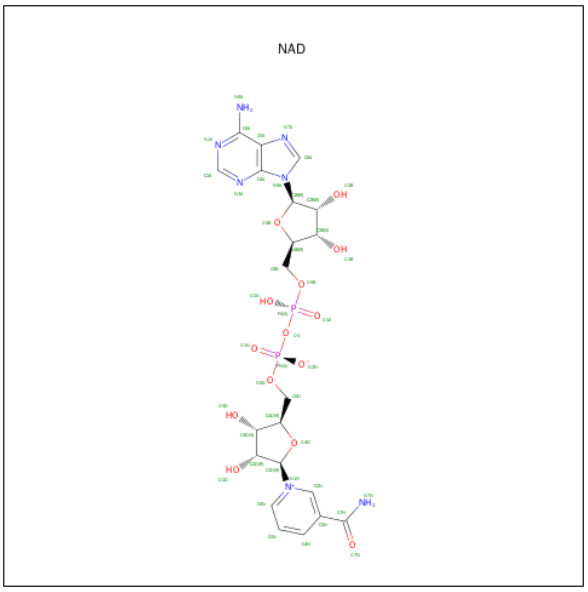
- Molecule 1 is a protein called UDP-glucuronic acid decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2113	1349	367	387	10			
1	B	274	Total	C	N	O	S	0	0	0
			2156	1375	374	396	11			
1	C	271	Total	C	N	O	S	0	0	0
			2130	1359	368	393	10			
1	D	273	Total	C	N	O	S	0	0	0
			2148	1370	373	395	10			
1	E	269	Total	C	N	O	S	0	0	0
			2118	1350	369	389	10			
1	F	261	Total	C	N	O	S	0	0	0
			2062	1314	360	378	10			

There are 6 discrepancies between the modelled and reference sequences:

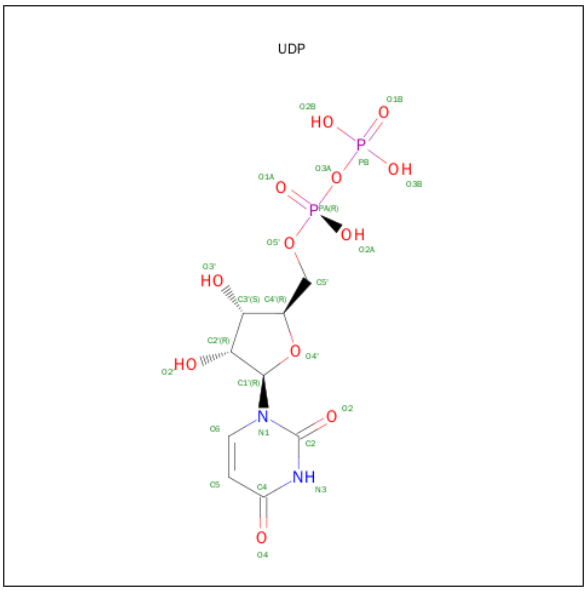
Chain	Residue	Modelled	Actual	Comment	Reference
A	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
B	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
C	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
D	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
E	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
F	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7

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



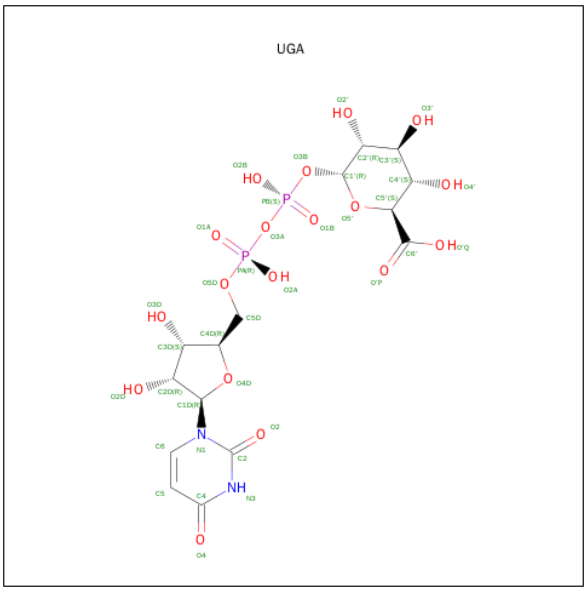
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



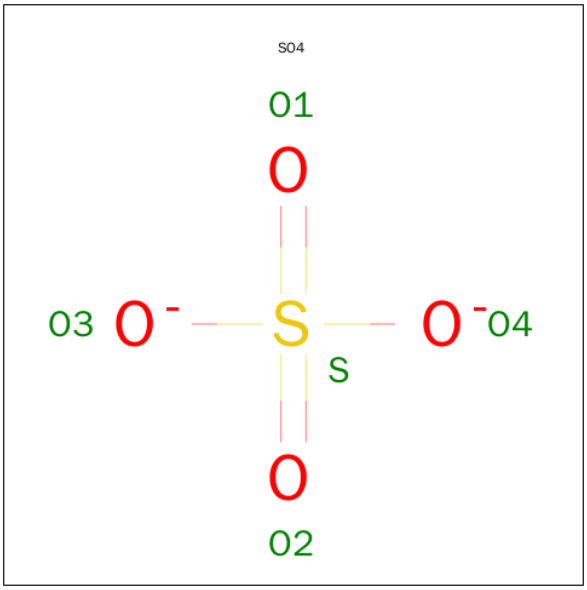
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (three-letter code: UGA) (formula: $C_{15}H_{22}N_2O_{18}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	B	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	C	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	D	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	E	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	F	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

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



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

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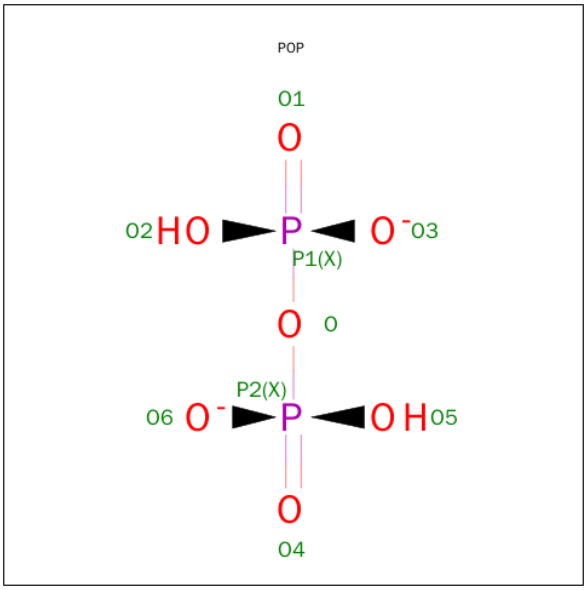
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O P 9 7 2	0	0
6	E	1	Total O P 9 7 2	0	0
6	F	1	Total O P 9 7 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	32	Total O 32 32	0	0
7	C	31	Total O 31 31	0	0
7	D	9	Total O 9 9	0	0

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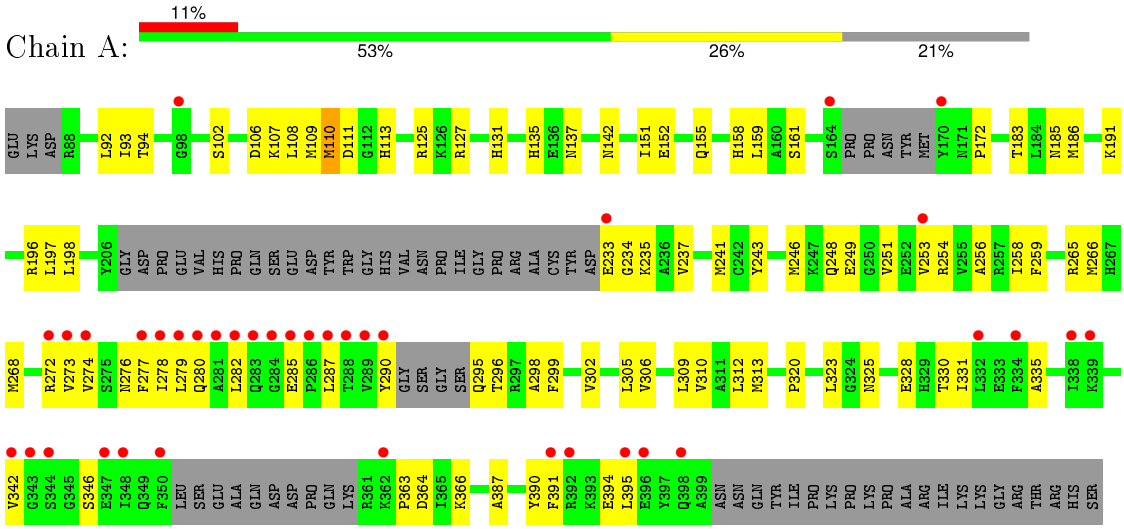
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	2	Total O 2 2	0	0

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.

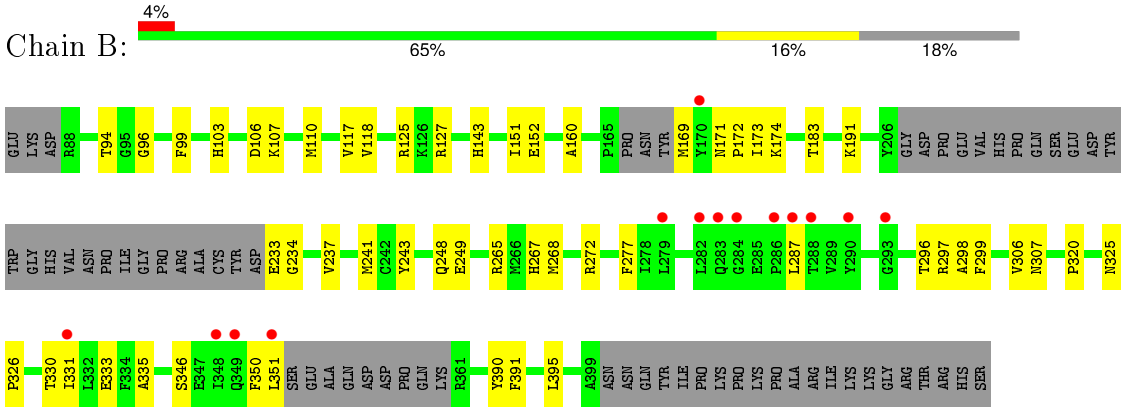
- Molecule 1: UDP-glucuronic acid decarboxylase 1

Chain A:



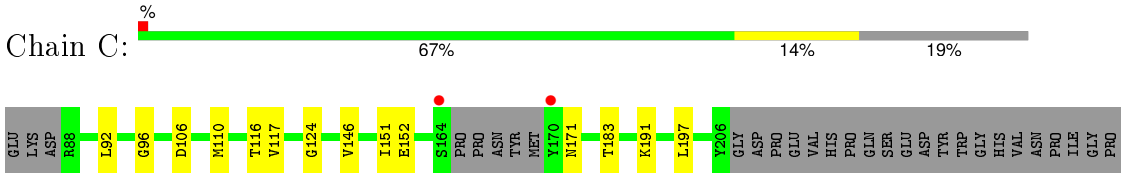
- Molecule 1: UDP-glucuronic acid decarboxylase 1

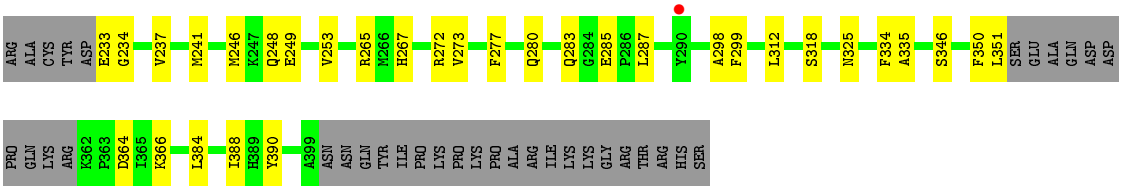
Chain B:



- Molecule 1: UDP-glucuronic acid decarboxylase 1

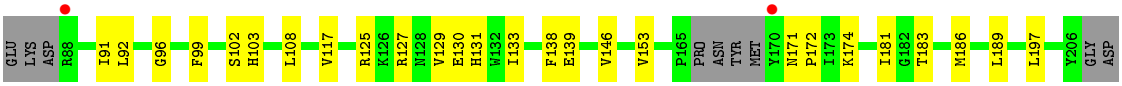
Chain C:

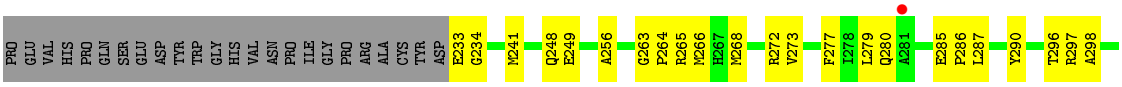


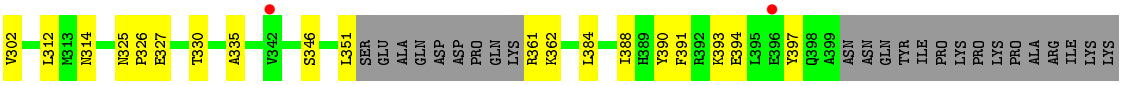


• Molecule 1: UDP-glucuronic acid decarboxylase 1

Chain D:

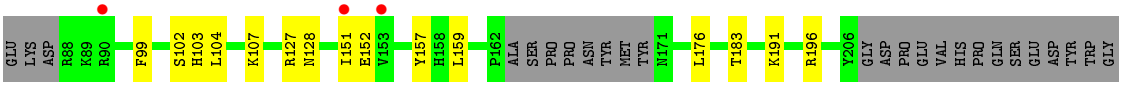






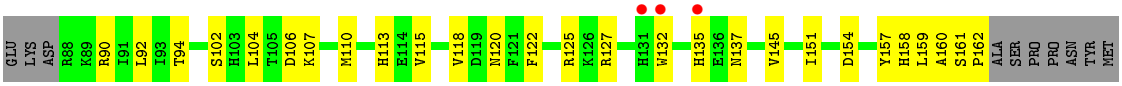
• Molecule 1: UDP-glucuronic acid decarboxylase 1

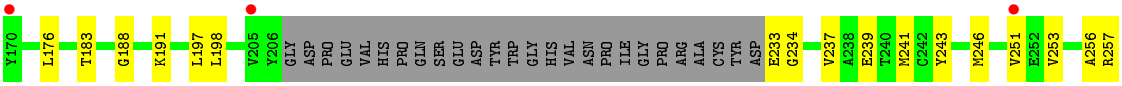
Chain E:

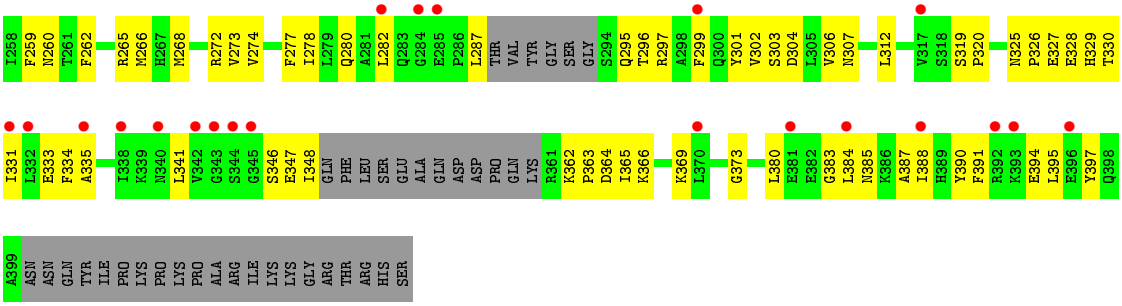


• Molecule 1: UDP-glucuronic acid decarboxylase 1

Chain F:






I258 F259 N260 T261 F262 R265 M266 H267 M268 R272 V273 V274 F277 I278 L279 Q280 A281 L282 Q283 G284 E285 P286 L287 THR VAL TYR GLY SER GLY S294 Q295 T296 R297 A298 F299 Q300 Y301 V302 S303 D304 L305 V306 N307 L312 V317 S318 S319 P320 N325 P326 E327 E328 H329 T330
I331 L332 E333 F334 A335 I338 K339 N340 L341 V342 G343 S344 G345 S346 E347 I348 GLN PHE LEU SER GLU ALA GLN ASP ASP PRO GLN LYS R361 K362 P363 D364 I365 K366 K369 L370 G373 L380 E381 E382 G383 L384 N385 K386 A387 I388 H389 Y390 F391 R392 K393 E394 L395 E396 Y397 Q398
A399 ASN ASN GLN TYR ILE PRO LYS PRO LYS PRO ALA ARG ILE LYS LYS GLY ARG THR ARG HIS SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.57Å 92.07Å 290.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.37 – 2.64 38.90 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.4 (36.37-2.64) 95.6 (38.90-2.64)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.65Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.198 , 0.245 0.204 , 0.246	Depositor DCC
R_{free} test set	3330 reflections (5.49%)	DCC
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	2 of 65871 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13434	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, UDP, UGA, NAD, POP

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	0.48	0/2152	0.67	0/2905
1	B	0.57	0/2197	0.73	0/2967
1	C	0.56	0/2170	0.72	0/2931
1	D	0.50	0/2189	0.67	1/2957 (0.0%)
1	E	0.48	0/2157	0.66	0/2912
1	F	0.47	0/2099	0.70	0/2832
All	All	0.51	0/12964	0.69	1/17504 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	314	ASN	O-C-N	-5.18	114.41	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2113	0	2123	88	0
1	B	2156	0	2167	47	0
1	C	2130	0	2138	46	0
1	D	2148	0	2158	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2118	0	2132	57	0
1	F	2062	0	2076	108	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	3	0
3	A	25	0	11	1	0
3	B	25	0	11	0	0
3	D	25	0	11	2	0
4	A	37	0	19	2	0
4	B	37	0	19	2	0
4	C	37	0	19	0	0
4	D	37	0	19	1	0
4	E	37	0	19	0	0
4	F	37	0	19	2	0
5	A	10	0	0	3	0
5	B	10	0	0	1	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
6	C	9	0	0	2	0
6	E	9	0	0	0	0
6	F	9	0	0	3	0
7	B	32	0	0	2	0
7	C	31	0	0	3	0
7	D	9	0	0	0	0
7	E	2	0	0	0	0
All	All	13434	0	13097	404	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 15.

All (404) 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:F:262:PHE:HE2	1:F:299:PHE:CD1	1.43	1.37
1:F:262:PHE:CE2	1:F:299:PHE:CD1	2.34	1.15
1:B:233:GLU:HG2	1:B:234:GLY:H	1.05	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:GLU:HG2	1:F:234:GLY:H	0.94	1.06
1:F:262:PHE:CZ	1:F:272:ARG:HD3	1.90	1.06
1:C:233:GLU:HG2	1:C:234:GLY:H	0.95	1.06
1:E:233:GLU:HG2	1:E:234:GLY:H	0.89	1.05
1:E:233:GLU:CG	1:E:234:GLY:H	1.71	1.01
1:D:130:GLU:HG3	1:D:133:ILE:HD12	1.40	1.00
1:E:233:GLU:HG2	1:E:234:GLY:N	1.74	0.99
1:A:387:ALA:O	1:A:391:PHE:HD1	1.46	0.98
1:F:233:GLU:HG2	1:F:234:GLY:N	1.79	0.97
1:F:233:GLU:CG	1:F:234:GLY:H	1.77	0.97
1:C:233:GLU:HG2	1:C:234:GLY:N	1.78	0.96
1:D:233:GLU:HG2	1:D:234:GLY:H	1.28	0.96
1:F:92:LEU:HD22	1:F:151:ILE:HD11	1.46	0.95
1:E:350:PHE:C	1:E:351:LEU:HD12	1.87	0.95
1:C:233:GLU:CG	1:C:234:GLY:H	1.79	0.94
1:E:280:GLN:OE1	1:E:287:LEU:HA	1.67	0.94
1:C:183:THR:HB	1:C:241:MET:HE1	1.50	0.92
1:C:272:ARG:HG3	6:C:503:POP:O1	1.70	0.92
1:B:183:THR:HB	1:B:241:MET:HE1	1.49	0.92
1:F:243:TYR:OH	1:F:320:PRO:HD3	1.69	0.91
1:A:387:ALA:O	1:A:391:PHE:CD1	2.22	0.91
1:B:183:THR:HB	1:B:241:MET:CE	2.02	0.89
1:D:287:LEU:CD1	1:D:346:SER:HB3	2.05	0.87
1:D:125:ARG:HD3	1:D:127:ARG:NE	1.88	0.87
1:A:155:GLN:HB3	1:A:313:MET:CE	2.05	0.86
1:A:268:MET:HG2	1:A:391:PHE:CE2	2.10	0.85
1:B:233:GLU:HG2	1:B:234:GLY:N	1.89	0.85
1:B:233:GLU:CG	1:B:234:GLY:H	1.87	0.83
1:F:273:VAL:HG12	6:F:503:POP:O1	1.79	0.82
1:A:155:GLN:HB3	1:A:313:MET:HE2	1.62	0.82
1:A:390:TYR:O	1:A:394:GLU:HG2	1.80	0.82
1:B:350:PHE:C	1:B:351:LEU:HD12	1.99	0.81
1:F:328:GLU:OE2	1:F:362:LYS:HB2	1.80	0.81
1:E:270:ASP:OD2	1:E:272:ARG:HG3	1.81	0.81
1:B:107:LYS:HD3	1:B:306:VAL:HG12	1.64	0.80
1:A:243:TYR:OH	1:A:320:PRO:HD3	1.83	0.79
1:F:260:ASN:HB3	1:F:272:ARG:NH1	1.98	0.79
1:C:350:PHE:C	1:C:351:LEU:HD12	2.03	0.79
1:D:393:LYS:NZ	1:E:399:ALA:C	2.37	0.78
1:F:262:PHE:CZ	1:F:272:ARG:CD	2.67	0.78
1:F:260:ASN:HB3	1:F:272:ARG:HH12	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:HB3	5:A:505:SO4:O1	1.85	0.77
1:A:280:GLN:OE1	1:A:287:LEU:HA	1.84	0.76
1:A:183:THR:HB	1:A:241:MET:HE1	1.66	0.76
1:E:183:THR:HB	1:E:241:MET:HE1	1.67	0.76
1:E:384:LEU:O	1:E:388:ILE:HG13	1.86	0.76
1:C:246:MET:HE3	1:C:318:SER:HB2	1.66	0.75
1:F:262:PHE:HE2	1:F:299:PHE:CE1	2.04	0.74
4:F:502:UGA:O2'	4:F:502:UGA:O3A	2.03	0.74
1:E:350:PHE:O	1:E:351:LEU:HD12	1.88	0.73
1:A:233:GLU:CG	1:A:234:GLY:H	2.01	0.72
1:F:260:ASN:CB	1:F:272:ARG:HH12	2.03	0.72
1:E:328:GLU:OE2	1:E:362:LYS:HB2	1.89	0.71
1:D:125:ARG:HD3	1:D:127:ARG:CZ	2.21	0.71
1:D:125:ARG:HG2	1:D:125:ARG:HH11	1.54	0.71
1:A:161:SER:OG	1:A:235:LYS:NZ	2.21	0.70
1:B:125:ARG:HD3	1:B:127:ARG:NH2	2.06	0.70
1:D:287:LEU:HD11	1:D:346:SER:HB3	1.74	0.69
1:A:268:MET:HG2	1:A:391:PHE:CD2	2.27	0.69
1:F:369:LYS:O	1:F:373:GLY:HA2	1.92	0.69
1:D:393:LYS:HZ2	1:E:399:ALA:C	1.94	0.69
1:F:132:TRP:HA	1:F:135:HIS:HD2	1.56	0.69
1:F:391:PHE:O	1:F:395:LEU:HG	1.93	0.69
1:D:186:MET:HE3	1:D:189:LEU:HD23	1.76	0.68
1:C:272:ARG:CG	6:C:503:POP:O1	2.41	0.68
4:A:503:UGA:H2'1	1:B:173:ILE:HG21	1.75	0.68
1:A:285:GLU:O	1:A:346:SER:HB3	1.94	0.67
1:F:262:PHE:CE1	1:F:272:ARG:HD2	2.30	0.67
1:F:132:TRP:HA	1:F:135:HIS:CD2	2.30	0.67
1:C:299:PHE:HD2	1:C:334:PHE:CZ	2.12	0.66
1:A:266:MET:SD	1:A:391:PHE:HZ	2.19	0.66
1:F:262:PHE:CE2	1:F:299:PHE:CE1	2.81	0.66
1:D:361:ARG:NH1	1:D:362:LYS:O	2.28	0.66
1:F:287:LEU:CD1	1:F:346:SER:HB3	2.25	0.66
1:F:262:PHE:CE1	1:F:272:ARG:CD	2.78	0.66
1:F:262:PHE:CE1	1:F:274:VAL:HB	2.31	0.65
1:F:268:MET:HE2	1:F:391:PHE:CD2	2.32	0.65
1:E:328:GLU:CD	1:E:362:LYS:HB2	2.16	0.65
1:B:277:PHE:CE2	1:B:335:ALA:HB2	2.32	0.65
1:A:233:GLU:CD	1:A:234:GLY:H	2.00	0.64
1:F:243:TYR:OH	1:F:320:PRO:CD	2.44	0.64
1:D:125:ARG:HD3	1:D:127:ARG:HE	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:HG12	1:A:152:GLU:H	1.63	0.64
1:F:107:LYS:HE3	1:F:307:ASN:OD1	1.97	0.64
1:A:102:SER:CB	1:A:265:ARG:HH11	2.11	0.64
1:E:107:LYS:HE3	1:E:307:ASN:OD1	1.98	0.64
1:F:273:VAL:CG1	6:F:503:POP:O1	2.46	0.63
1:E:183:THR:HB	1:E:241:MET:CE	2.28	0.63
1:D:233:GLU:HG2	1:D:234:GLY:N	2.09	0.63
1:C:237:VAL:O	1:C:241:MET:HG3	1.98	0.63
1:C:183:THR:HB	1:C:241:MET:CE	2.25	0.63
1:D:183:THR:HB	1:D:241:MET:HE1	1.80	0.63
1:D:287:LEU:HD12	1:D:346:SER:HB3	1.78	0.62
1:F:301:TYR:CE1	1:F:302:VAL:HG12	2.33	0.62
1:F:239:GLU:OE1	1:F:257:ARG:NH2	2.30	0.62
1:F:262:PHE:CD1	1:F:266:MET:CE	2.83	0.62
1:C:298:ALA:HB1	1:C:325:ASN:O	1.99	0.62
1:E:332:LEU:HD13	1:E:350:PHE:HE1	1.64	0.62
1:E:243:TYR:OH	1:E:320:PRO:HD3	1.99	0.62
1:A:159:LEU:HD12	1:A:159:LEU:N	2.15	0.61
1:B:107:LYS:NZ	1:B:307:ASN:HA	2.15	0.61
5:A:505:SO4:O2	1:F:125:ARG:HB3	1.99	0.61
1:A:198:LEU:HD23	1:A:198:LEU:C	2.20	0.61
1:B:350:PHE:O	1:B:351:LEU:HD12	2.01	0.61
1:F:301:TYR:O	1:F:304:ASP:HB2	2.01	0.61
1:E:104:LEU:CD1	1:E:306:VAL:HG13	2.31	0.61
1:A:93:ILE:HD11	1:A:108:LEU:HD12	1.83	0.60
1:F:262:PHE:HE2	1:F:299:PHE:HD1	1.33	0.60
1:C:246:MET:CE	1:C:318:SER:HB2	2.30	0.60
1:D:326:PRO:O	1:D:362:LYS:HE2	2.02	0.60
1:C:280:GLN:OE1	1:C:287:LEU:HA	2.01	0.59
1:C:248:GLN:OE1	1:D:172:PRO:HG2	2.02	0.59
1:D:393:LYS:HZ1	1:E:399:ALA:C	2.05	0.58
1:E:237:VAL:O	1:E:241:MET:HG3	2.02	0.58
1:F:302:VAL:O	1:F:306:VAL:HG23	2.02	0.58
1:F:259:PHE:CE2	1:F:363:PRO:HB3	2.38	0.58
1:D:91:ILE:HD13	1:D:108:LEU:HD13	1.84	0.58
1:A:151:ILE:HG12	1:A:152:GLU:N	2.18	0.58
1:A:285:GLU:O	1:A:346:SER:CB	2.51	0.58
1:A:282:LEU:HD23	1:A:342:VAL:HG13	1.84	0.58
1:F:329:HIS:CD2	1:F:380:LEU:HD22	2.39	0.57
1:E:260:ASN:HB3	1:E:299:PHE:CE1	2.39	0.57
1:B:249:GLU:OE2	4:B:503:UGA:O3'	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:LEU:HD11	1:F:312:LEU:HD23	1.85	0.57
1:C:287:LEU:N	1:C:287:LEU:HD12	2.19	0.57
1:A:233:GLU:CG	1:A:234:GLY:N	2.67	0.57
1:F:159:LEU:HD12	1:F:159:LEU:N	2.20	0.56
1:F:183:THR:HB	1:F:241:MET:HE1	1.87	0.56
1:D:268:MET:HG2	1:D:391:PHE:CE2	2.40	0.56
1:D:130:GLU:HG3	1:D:133:ILE:CD1	2.27	0.56
1:A:237:VAL:O	1:A:241:MET:HG3	2.05	0.56
1:E:328:GLU:OE1	1:E:362:LYS:HE3	2.06	0.56
1:B:125:ARG:HD3	1:B:127:ARG:CZ	2.36	0.56
1:D:92:LEU:HD21	1:D:186:MET:HE1	1.88	0.56
1:F:183:THR:HB	1:F:241:MET:CE	2.36	0.56
1:A:131:HIS:O	1:A:135:HIS:CE1	2.58	0.56
1:A:155:GLN:HB3	1:A:313:MET:HE3	1.88	0.55
1:F:325:ASN:OD1	1:F:327:GLU:HB3	2.06	0.55
1:A:107:LYS:O	1:A:107:LYS:HG3	2.04	0.55
1:A:233:GLU:HG2	1:A:234:GLY:H	1.71	0.55
1:B:267:HIS:HB3	5:B:504:SO4:O1	2.06	0.55
1:F:301:TYR:HD1	1:F:303:SER:H	1.53	0.55
1:E:298:ALA:HB1	1:E:325:ASN:O	2.07	0.55
1:F:259:PHE:CZ	1:F:363:PRO:HB3	2.42	0.55
1:A:273:VAL:HG21	1:A:331:ILE:HD12	1.87	0.55
1:C:312:LEU:HD11	7:C:606:HOH:O	2.06	0.55
1:D:297:ARG:NE	3:D:502:UDP:H5'1	2.21	0.55
1:F:262:PHE:HD1	1:F:266:MET:CE	2.20	0.54
1:D:277:PHE:CE2	1:D:335:ALA:HB2	2.41	0.54
1:E:240:THR:HG22	1:F:176:LEU:HD11	1.87	0.54
1:F:287:LEU:N	1:F:347:GLU:O	2.24	0.54
1:D:189:LEU:HD12	1:D:189:LEU:O	2.06	0.54
1:E:330:THR:OG1	1:E:333:GLU:HB2	2.08	0.54
1:B:330:THR:OG1	1:B:333:GLU:HB2	2.06	0.54
1:C:106:ASP:O	1:C:110:MET:HG2	2.08	0.54
1:D:280:GLN:OE1	1:D:287:LEU:HA	2.07	0.54
4:B:503:UGA:H1'1	4:B:503:UGA:O2A	2.08	0.54
1:D:102:SER:HB2	1:D:265:ARG:NH1	2.23	0.54
1:B:298:ALA:HB1	1:B:325:ASN:O	2.07	0.54
1:F:282:LEU:CD1	1:F:391:PHE:HB3	2.38	0.54
1:E:325:ASN:OD1	1:E:327:GLU:HB3	2.08	0.54
1:A:277:PHE:CE2	1:A:335:ALA:HB2	2.43	0.53
1:C:364:ASP:OD2	1:C:366:LYS:HE2	2.07	0.53
1:C:350:PHE:O	1:C:351:LEU:HD12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:TYR:CE1	1:F:394:GLU:OE2	2.61	0.53
1:F:104:LEU:HD21	1:F:157:TYR:CD2	2.43	0.53
1:F:280:GLN:OE1	1:F:287:LEU:HA	2.09	0.53
1:A:364:ASP:OD2	1:A:366:LYS:HE2	2.08	0.53
1:F:296:THR:O	1:F:297:ARG:HD3	2.09	0.53
1:F:295:GLN:O	1:F:330:THR:HA	2.08	0.53
1:D:290:TYR:CD1	1:D:351:LEU:HD22	2.44	0.53
1:F:125:ARG:HB3	1:F:127:ARG:HG2	1.91	0.53
1:E:104:LEU:HD12	1:E:306:VAL:HG13	1.91	0.53
1:F:287:LEU:HD13	1:F:346:SER:HB3	1.92	0.52
1:D:183:THR:HB	1:D:241:MET:CE	2.38	0.52
1:A:248:GLN:NE2	1:B:171:ASN:OD1	2.42	0.52
1:C:171:ASN:OD1	1:D:248:GLN:NE2	2.40	0.52
1:F:102:SER:CB	1:F:265:ARG:HH11	2.22	0.52
1:F:277:PHE:CE2	1:F:335:ALA:HB2	2.43	0.52
1:B:107:LYS:HD3	1:B:306:VAL:CG1	2.37	0.52
1:D:183:THR:CG2	1:D:241:MET:CE	2.87	0.52
1:F:301:TYR:CD1	1:F:302:VAL:N	2.77	0.52
1:C:248:GLN:OE1	1:D:172:PRO:HD2	2.09	0.52
1:D:96:GLY:HA3	1:D:117:VAL:HG13	1.91	0.52
1:F:92:LEU:HD11	1:F:118:VAL:HG23	1.90	0.52
1:E:332:LEU:HD13	1:E:350:PHE:CE1	2.45	0.52
1:F:256:ALA:HB2	1:F:312:LEU:CD2	2.40	0.52
1:C:151:ILE:HG12	1:C:152:GLU:N	2.24	0.52
1:B:106:ASP:O	1:B:110:MET:HG2	2.09	0.52
1:F:262:PHE:HZ	1:F:272:ARG:HD3	1.64	0.52
1:E:104:LEU:HA	1:E:306:VAL:CG1	2.40	0.52
1:A:158:HIS:C	1:A:159:LEU:HD12	2.31	0.52
1:F:132:TRP:CA	1:F:135:HIS:HD2	2.23	0.51
1:A:391:PHE:O	1:A:395:LEU:HG	2.10	0.51
1:B:237:VAL:O	1:B:241:MET:HG3	2.10	0.51
1:F:102:SER:OG	1:F:265:ARG:NH1	2.41	0.51
1:D:130:GLU:CG	1:D:133:ILE:HD12	2.26	0.51
1:B:191:LYS:HE3	1:B:249:GLU:OE1	2.10	0.51
1:E:290:TYR:N	1:E:290:TYR:CD1	2.77	0.51
1:D:287:LEU:HD11	1:D:346:SER:CB	2.40	0.51
1:A:161:SER:CB	1:A:235:LYS:HZ3	2.23	0.51
1:A:387:ALA:HB1	1:A:391:PHE:HE1	1.75	0.51
1:A:298:ALA:HB1	1:A:325:ASN:O	2.11	0.51
1:B:107:LYS:HZ3	1:B:307:ASN:HA	1.76	0.50
1:A:102:SER:CB	1:A:265:ARG:NH1	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD21	1:A:186:MET:HE1	1.94	0.50
1:B:265:ARG:HA	1:B:390:TYR:CZ	2.47	0.50
1:D:285:GLU:HB3	1:D:286:PRO:HD2	1.93	0.50
1:C:96:GLY:HA3	1:C:117:VAL:HG13	1.94	0.50
1:A:268:MET:HG2	1:A:391:PHE:HE2	1.72	0.50
1:F:107:LYS:CE	1:F:307:ASN:OD1	2.59	0.50
1:E:259:PHE:CE2	1:E:363:PRO:HB3	2.46	0.50
1:A:268:MET:O	1:A:279:LEU:HD11	2.12	0.50
1:A:191:LYS:HE3	1:A:249:GLU:OE1	2.11	0.50
1:D:298:ALA:HB1	1:D:325:ASN:O	2.11	0.50
1:A:185:ASN:HA	4:A:503:UGA:O4D	2.12	0.50
1:F:301:TYR:CE2	1:F:383:GLY:HA2	2.47	0.50
1:E:246:MET:HA	1:E:251:VAL:O	2.11	0.50
1:A:309:LEU:HD23	1:A:323:LEU:CD1	2.42	0.50
1:A:258:ILE:HG12	1:A:305:LEU:HD11	1.94	0.50
1:F:262:PHE:CD1	1:F:266:MET:HE1	2.46	0.49
1:D:125:ARG:CG	1:D:125:ARG:HH11	2.19	0.49
1:A:106:ASP:O	1:A:110:MET:HG2	2.11	0.49
1:A:102:SER:HB2	1:A:265:ARG:NH1	2.28	0.49
1:D:390:TYR:O	1:D:394:GLU:HG2	2.12	0.49
1:B:243:TYR:OH	1:B:320:PRO:HD3	2.12	0.49
1:E:260:ASN:HB3	1:E:299:PHE:CD1	2.47	0.49
1:F:102:SER:HB2	1:F:265:ARG:NH1	2.28	0.49
1:A:92:LEU:HD21	1:A:186:MET:CE	2.43	0.49
1:A:113:HIS:O	1:A:137:ASN:HB3	2.11	0.49
1:F:94:THR:HB	1:F:160:ALA:HB2	1.95	0.49
1:E:259:PHE:CD2	1:E:363:PRO:HB3	2.48	0.49
1:F:102:SER:CB	1:F:265:ARG:NH1	2.76	0.49
1:A:302:VAL:O	1:A:306:VAL:HG23	2.12	0.49
1:A:197:LEU:O	1:A:253:VAL:HA	2.12	0.49
1:A:285:GLU:O	1:A:346:SER:OG	2.30	0.49
1:C:384:LEU:O	1:C:388:ILE:HG13	2.13	0.48
1:F:158:HIS:C	1:F:159:LEU:HD12	2.34	0.48
1:D:272:ARG:HG2	1:D:273:VAL:N	2.28	0.48
1:E:233:GLU:CG	1:E:234:GLY:N	2.46	0.48
1:F:278:ILE:O	1:F:282:LEU:HG	2.14	0.48
1:C:277:PHE:CE2	1:C:335:ALA:HB2	2.48	0.48
1:B:169:MET:HE2	1:B:172:PRO:HB3	1.96	0.48
1:F:106:ASP:O	1:F:110:MET:HG2	2.13	0.48
1:D:146:VAL:HG13	1:D:181:ILE:HG21	1.95	0.48
1:C:233:GLU:CG	1:C:234:GLY:N	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:502:UGA:PA	4:F:502:UGA:HO'2	2.36	0.47
1:A:296:THR:HB	1:A:328:GLU:HB3	1.95	0.47
1:E:107:LYS:CE	1:E:307:ASN:OD1	2.62	0.47
1:C:146:VAL:O	1:C:146:VAL:HG12	2.14	0.47
1:A:256:ALA:HB2	1:A:312:LEU:CD2	2.43	0.47
1:F:92:LEU:HD11	1:F:118:VAL:CG2	2.45	0.47
1:E:104:LEU:HD13	1:E:306:VAL:HG13	1.95	0.47
1:E:285:GLU:O	1:E:346:SER:HB3	2.15	0.47
1:B:297:ARG:HG2	1:B:331:ILE:HD11	1.96	0.47
1:A:125:ARG:HD3	1:A:127:ARG:NH2	2.30	0.47
1:A:295:GLN:OE1	1:A:295:GLN:N	2.48	0.47
1:A:125:ARG:HD3	1:A:127:ARG:CZ	2.45	0.47
1:F:390:TYR:O	1:F:394:GLU:HG2	2.15	0.47
1:F:273:VAL:HG13	1:F:274:VAL:N	2.29	0.47
1:A:233:GLU:HG2	1:A:234:GLY:N	2.30	0.47
1:A:390:TYR:CE1	1:A:394:GLU:OE2	2.68	0.46
1:F:237:VAL:O	1:F:241:MET:N	2.43	0.46
1:F:384:LEU:O	1:F:388:ILE:HG13	2.15	0.46
1:F:268:MET:HB3	1:F:268:MET:HE2	1.72	0.46
1:F:325:ASN:HA	1:F:326:PRO:HD2	1.81	0.46
1:A:259:PHE:CD2	1:A:363:PRO:HB3	2.51	0.46
1:F:90:ARG:NH2	1:F:154:ASP:OD1	2.33	0.46
1:E:196:ARG:CZ	1:E:254:ARG:NH2	2.79	0.46
1:B:151:ILE:HG12	1:B:152:GLU:H	1.79	0.46
1:D:268:MET:HG2	1:D:391:PHE:CZ	2.51	0.46
1:C:151:ILE:HG12	1:C:152:GLU:H	1.79	0.46
1:B:183:THR:CB	1:B:241:MET:CE	2.84	0.46
1:A:131:HIS:O	1:A:135:HIS:HE1	1.99	0.46
1:D:263:GLY:O	1:D:266:MET:HG2	2.16	0.46
6:F:503:POP:O6	6:F:503:POP:O2	2.34	0.46
1:F:326:PRO:HG3	1:F:365:ILE:HD11	1.98	0.46
1:A:259:PHE:CE2	1:A:363:PRO:HB3	2.51	0.46
1:E:369:LYS:O	1:E:373:GLY:HA2	2.15	0.46
1:E:277:PHE:CE2	1:E:335:ALA:HB2	2.51	0.46
1:C:267:HIS:HD2	7:C:607:HOH:O	1.99	0.46
1:D:297:ARG:HE	3:D:502:UDP:H5'1	1.80	0.45
1:D:138:PHE:CG	1:D:139:GLU:N	2.84	0.45
1:B:94:THR:HB	1:B:160:ALA:HB2	1.99	0.45
1:C:265:ARG:HA	1:C:390:TYR:CZ	2.51	0.45
1:E:151:ILE:HG12	1:E:152:GLU:H	1.81	0.45
1:F:297:ARG:HG2	1:F:331:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:PHE:O	1:E:103:HIS:HD2	1.98	0.45
1:A:276:ASN:ND2	3:A:502:UDP:O4	2.49	0.45
1:F:246:MET:HA	1:F:251:VAL:O	2.17	0.45
1:A:183:THR:HB	1:A:241:MET:CE	2.41	0.45
1:D:327:GLU:O	1:D:327:GLU:HG2	2.17	0.45
1:B:125:ARG:HD3	1:B:127:ARG:HH21	1.80	0.45
1:F:197:LEU:O	1:F:253:VAL:HA	2.17	0.45
1:D:249:GLU:OE2	4:D:503:UGA:O3'	2.31	0.45
1:D:197:LEU:C	1:D:197:LEU:HD23	2.37	0.45
1:F:113:HIS:O	1:F:137:ASN:HB3	2.16	0.45
1:F:297:ARG:CG	1:F:331:ILE:HD11	2.47	0.45
1:D:129:VAL:O	1:D:131:HIS:N	2.50	0.45
1:F:299:PHE:HD2	1:F:334:PHE:CZ	2.35	0.44
1:A:266:MET:CG	1:A:391:PHE:HZ	2.30	0.44
1:F:260:ASN:CG	1:F:272:ARG:HH12	2.21	0.44
1:F:330:THR:OG1	1:F:333:GLU:HB2	2.16	0.44
1:D:290:TYR:N	1:D:290:TYR:CD1	2.85	0.44
1:F:319:SER:HB2	1:F:320:PRO:HD2	1.99	0.44
1:C:366:LYS:NZ	7:C:610:HOH:O	2.49	0.44
1:A:172:PRO:HD2	1:B:248:GLN:OE1	2.17	0.44
1:C:246:MET:CE	1:C:318:SER:CB	2.95	0.44
1:C:248:GLN:OE1	1:D:172:PRO:CD	2.65	0.44
1:B:151:ILE:HG12	1:B:152:GLU:N	2.32	0.44
1:E:296:THR:O	1:E:297:ARG:HD3	2.17	0.44
1:D:92:LEU:HB2	1:D:153:VAL:HG11	2.00	0.44
1:B:268:MET:HG2	1:B:391:PHE:CZ	2.52	0.44
1:B:272:ARG:HH11	1:B:299:PHE:HE1	1.64	0.44
1:D:102:SER:CB	1:D:265:ARG:HH11	2.31	0.44
1:D:129:VAL:O	1:D:130:GLU:C	2.56	0.43
1:B:325:ASN:HA	1:B:326:PRO:HD3	1.84	0.43
1:A:306:VAL:O	1:A:310:VAL:HG23	2.18	0.43
1:B:287:LEU:CD1	1:B:346:SER:HB3	2.48	0.43
1:D:171:ASN:ND2	1:D:174:LYS:HB2	2.33	0.43
1:C:124:GLY:HA3	2:C:501:NAD:O3B	2.18	0.43
1:A:161:SER:CB	1:A:235:LYS:NZ	2.80	0.43
1:E:304:ASP:CG	1:E:376:PRO:HA	2.39	0.43
1:A:394:GLU:OE1	1:F:397:TYR:HE1	2.01	0.43
1:A:159:LEU:N	1:A:159:LEU:CD1	2.81	0.43
1:B:169:MET:CE	1:B:172:PRO:HB3	2.48	0.43
1:F:145:VAL:HG22	2:F:501:NAD:N1A	2.34	0.43
1:A:394:GLU:HA	1:A:394:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:THR:O	1:B:297:ARG:HD3	2.19	0.43
1:B:118:VAL:HG13	1:B:143:HIS:HB3	2.00	0.43
1:B:233:GLU:CG	1:B:234:GLY:N	2.60	0.43
1:F:394:GLU:HA	1:F:394:GLU:OE1	2.18	0.43
1:B:174:LYS:CE	7:B:616:HOH:O	2.66	0.43
1:F:273:VAL:HG21	1:F:331:ILE:HD12	2.01	0.43
1:D:256:ALA:HB2	1:D:312:LEU:HD23	2.01	0.43
1:E:104:LEU:HA	1:E:306:VAL:HG11	1.99	0.43
1:A:295:GLN:O	1:A:330:THR:HA	2.19	0.43
1:F:188:GLY:O	1:F:191:LYS:HB3	2.19	0.43
1:A:256:ALA:HB2	1:A:312:LEU:HD23	2.00	0.43
1:E:157:TYR:HB3	1:E:159:LEU:CD1	2.48	0.43
1:D:287:LEU:N	1:D:287:LEU:HD12	2.34	0.43
1:E:243:TYR:OH	1:E:320:PRO:CD	2.65	0.43
1:D:103:HIS:HE1	1:D:264:PRO:O	2.02	0.43
1:D:265:ARG:HA	1:D:390:TYR:CZ	2.52	0.43
1:E:191:LYS:HE3	1:E:249:GLU:OE1	2.18	0.43
1:B:96:GLY:HA3	1:B:117:VAL:HG13	2.00	0.42
1:A:246:MET:HA	1:A:251:VAL:O	2.19	0.42
1:C:283:GLN:C	1:C:285:GLU:H	2.23	0.42
1:E:176:LEU:HD13	1:F:241:MET:HA	2.02	0.42
1:D:125:ARG:HG2	1:D:125:ARG:NH1	2.30	0.42
1:F:301:TYR:CD2	1:F:383:GLY:HA2	2.54	0.42
1:E:102:SER:HB3	1:E:128:ASN:HB3	2.02	0.42
1:A:102:SER:HB2	1:A:265:ARG:HH11	1.84	0.42
1:D:125:ARG:HD3	1:D:127:ARG:NH2	2.35	0.42
1:D:103:HIS:CE1	1:D:265:ARG:HD2	2.54	0.42
1:A:274:VAL:O	1:A:278:ILE:HG13	2.20	0.42
1:E:268:MET:HG2	1:E:391:PHE:CE2	2.55	0.42
1:F:262:PHE:HD1	1:F:266:MET:SD	2.43	0.42
1:A:243:TYR:OH	1:A:320:PRO:CD	2.61	0.42
1:F:282:LEU:HD21	1:F:388:ILE:HG23	2.02	0.42
1:F:347:GLU:CG	1:F:348:ILE:N	2.83	0.42
1:C:287:LEU:N	1:C:287:LEU:CD1	2.83	0.42
1:F:161:SER:HB3	2:F:501:NAD:O3D	2.20	0.42
1:D:130:GLU:HA	1:D:133:ILE:CD1	2.50	0.41
1:A:272:ARG:HH11	1:A:299:PHE:HE1	1.67	0.41
1:D:99:PHE:CZ	1:D:302:VAL:HB	2.54	0.41
1:A:290:TYR:N	1:A:290:TYR:CD1	2.86	0.41
1:B:99:PHE:O	1:B:103:HIS:HD2	2.03	0.41
1:D:397:TYR:OH	1:E:127:ARG:NH1	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:MET:SD	1:A:391:PHE:CZ	3.07	0.41
1:C:191:LYS:HE3	1:C:249:GLU:OE1	2.20	0.41
1:C:272:ARG:HG2	1:C:273:VAL:N	2.35	0.41
1:F:122:PHE:HD2	1:F:162:PRO:HB3	1.84	0.41
1:B:174:LYS:HE2	7:B:616:HOH:O	2.20	0.41
1:C:285:GLU:O	1:C:346:SER:HB3	2.21	0.41
1:A:109:MET:C	1:A:111:ASP:N	2.74	0.41
1:C:92:LEU:HD12	1:C:116:THR:O	2.20	0.41
1:C:299:PHE:CD2	1:C:334:PHE:CZ	3.00	0.41
1:E:104:LEU:HA	1:E:306:VAL:HG13	2.02	0.41
1:C:151:ILE:CG1	1:C:152:GLU:H	2.34	0.41
1:C:151:ILE:CG1	1:C:152:GLU:N	2.84	0.41
1:E:151:ILE:HG12	1:E:152:GLU:N	2.36	0.41
1:C:197:LEU:O	1:C:253:VAL:HA	2.20	0.41
1:B:395:LEU:HA	1:B:395:LEU:HD23	1.74	0.41
1:D:384:LEU:O	1:D:388:ILE:HG13	2.21	0.41
1:E:104:LEU:HD12	1:E:306:VAL:CG1	2.51	0.41
1:D:296:THR:HG22	1:D:330:THR:HG22	2.03	0.41
1:F:145:VAL:HG22	2:F:501:NAD:C6A	2.52	0.40
1:F:364:ASP:OD2	1:F:366:LYS:HE2	2.21	0.40
1:F:387:ALA:O	1:F:391:PHE:HD1	2.04	0.40
1:A:106:ASP:OD2	1:A:265:ARG:NH2	2.39	0.40
1:C:287:LEU:CD1	1:C:346:SER:HB3	2.51	0.40
1:B:297:ARG:HD3	1:B:297:ARG:HA	1.80	0.40
1:A:142:ASN:ND2	1:F:120:ASN:O	2.51	0.40
1:A:94:THR:O	1:A:159:LEU:HB2	2.21	0.40
1:A:127:ARG:NH2	5:A:505:SO4:O4	2.52	0.40
1:E:325:ASN:HA	1:E:326:PRO:HD2	1.89	0.40
1:F:115:VAL:N	1:F:137:ASN:O	2.53	0.40
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.78	0.40
1:F:341:LEU:HD22	1:F:385:ASN:OD1	2.21	0.40
1:A:196:ARG:CZ	1:A:254:ARG:NH2	2.85	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	257/336 (76%)	249 (97%)	7 (3%)	1 (0%)	39 63
1	B	266/336 (79%)	260 (98%)	6 (2%)	0	100 100
1	C	263/336 (78%)	254 (97%)	9 (3%)	0	100 100
1	D	265/336 (79%)	252 (95%)	13 (5%)	0	100 100
1	E	261/336 (78%)	255 (98%)	6 (2%)	0	100 100
1	F	251/336 (75%)	242 (96%)	9 (4%)	0	100 100
All	All	1563/2016 (78%)	1512 (97%)	50 (3%)	1 (0%)	56 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	MET

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	229/289 (79%)	229 (100%)	0	100 100
1	B	234/289 (81%)	234 (100%)	0	100 100
1	C	231/289 (80%)	231 (100%)	0	100 100
1	D	233/289 (81%)	233 (100%)	0	100 100
1	E	230/289 (80%)	230 (100%)	0	100 100
1	F	224/289 (78%)	224 (100%)	0	100 100
All	All	1381/1734 (80%)	1381 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	295	GLN
1	F	135	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

27 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	501	-	38,48,48	0.79	1 (2%)	47,73,73	1.67	6 (12%)
3	UDP	A	502	-	18,26,26	0.72	0	26,40,40	1.82	2 (7%)
4	UGA	A	503	-	27,39,39	0.55	0	41,60,60	1.33	3 (7%)
5	SO4	A	504	-	4,4,4	0.11	0	6,6,6	0.31	0
5	SO4	A	505	-	4,4,4	0.32	0	6,6,6	0.18	0
2	NAD	B	501	-	38,48,48	0.93	3 (7%)	47,73,73	1.64	4 (8%)
3	UDP	B	502	-	18,26,26	0.72	1 (5%)	26,40,40	1.80	3 (11%)
4	UGA	B	503	-	27,39,39	0.62	0	41,60,60	1.65	2 (4%)
5	SO4	B	504	-	4,4,4	0.26	0	6,6,6	0.65	0
5	SO4	B	505	-	4,4,4	0.25	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	C	501	-	38,48,48	0.94	1 (2%)	47,73,73	1.69	8 (17%)
4	UGA	C	502	-	27,39,39	0.58	0	41,60,60	1.49	3 (7%)
6	POP	C	503	-	8,8,8	0.63	0	13,13,13	1.23	1 (7%)
5	SO4	C	504	-	4,4,4	0.15	0	6,6,6	0.42	0
2	NAD	D	501	-	38,48,48	0.79	1 (2%)	47,73,73	1.69	4 (8%)
3	UDP	D	502	-	18,26,26	0.74	0	26,40,40	1.60	2 (7%)
4	UGA	D	503	-	27,39,39	0.62	0	41,60,60	1.46	1 (2%)
5	SO4	D	504	-	4,4,4	0.11	0	6,6,6	0.57	0
5	SO4	D	505	-	4,4,4	0.80	0	6,6,6	0.49	0
2	NAD	E	501	-	38,48,48	0.78	1 (2%)	47,73,73	1.85	8 (17%)
6	POP	E	502	-	8,8,8	0.99	0	13,13,13	2.06	2 (15%)
4	UGA	E	503	-	27,39,39	0.63	0	41,60,60	1.56	3 (7%)
5	SO4	E	504	-	4,4,4	0.39	0	6,6,6	0.33	0
2	NAD	F	501	-	38,48,48	0.84	1 (2%)	47,73,73	1.71	3 (6%)
4	UGA	F	502	-	27,39,39	0.60	0	41,60,60	1.49	4 (9%)
6	POP	F	503	-	8,8,8	0.58	0	13,13,13	1.27	1 (7%)
5	SO4	F	504	-	4,4,4	0.20	0	6,6,6	0.20	0

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	501	-	-	0/22/62/62	0/5/5/5
3	UDP	A	502	-	-	0/12/32/32	0/2/2/2
4	UGA	A	503	-	-	0/17/61/61	0/3/3/3
5	SO4	A	504	-	-	0/0/0/0	0/0/0/0
5	SO4	A	505	-	-	0/0/0/0	0/0/0/0
2	NAD	B	501	-	-	0/22/62/62	0/5/5/5
3	UDP	B	502	-	-	0/12/32/32	0/2/2/2
4	UGA	B	503	-	-	0/17/61/61	0/3/3/3
5	SO4	B	504	-	-	0/0/0/0	0/0/0/0
5	SO4	B	505	-	-	0/0/0/0	0/0/0/0
2	NAD	C	501	-	-	0/22/62/62	0/5/5/5
4	UGA	C	502	-	-	0/17/61/61	0/3/3/3
6	POP	C	503	-	-	0/6/6/6	0/0/0/0
5	SO4	C	504	-	-	0/0/0/0	0/0/0/0
2	NAD	D	501	-	-	0/22/62/62	0/5/5/5
3	UDP	D	502	-	-	0/12/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UGA	D	503	-	-	0/17/61/61	0/3/3/3
5	SO4	D	504	-	-	0/0/0/0	0/0/0/0
5	SO4	D	505	-	-	0/0/0/0	0/0/0/0
2	NAD	E	501	-	-	0/22/62/62	0/5/5/5
6	POP	E	502	-	-	0/6/6/6	0/0/0/0
4	UGA	E	503	-	-	0/17/61/61	0/3/3/3
5	SO4	E	504	-	-	0/0/0/0	0/0/0/0
2	NAD	F	501	-	-	0/22/62/62	0/5/5/5
4	UGA	F	502	-	-	0/17/61/61	0/3/3/3
6	POP	F	503	-	-	0/6/6/6	0/0/0/0
5	SO4	F	504	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	C5A-N7A	-2.22	1.31	1.39
3	B	502	UDP	O4'-C1'	2.04	1.43	1.41
2	D	501	NAD	C5A-C4A	2.34	1.45	1.40
2	E	501	NAD	C5A-C4A	2.49	1.46	1.40
2	B	501	NAD	C5A-C4A	2.72	1.46	1.40
2	C	501	NAD	C5A-C4A	2.87	1.47	1.40
2	F	501	NAD	C5A-C4A	2.90	1.47	1.40
2	B	501	NAD	O4B-C1B	2.94	1.44	1.41
2	A	501	NAD	C5A-C4A	2.98	1.47	1.40

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	NAD	N3A-C2A-N1A	-8.18	122.63	128.89
2	D	501	NAD	N3A-C2A-N1A	-7.34	123.28	128.89
2	E	501	NAD	N3A-C2A-N1A	-7.08	123.47	128.89
2	A	501	NAD	N3A-C2A-N1A	-6.46	123.95	128.89
2	B	501	NAD	N3A-C2A-N1A	-6.37	124.02	128.89
6	E	502	POP	P2-O-P1	-6.02	115.83	132.73
2	C	501	NAD	N3A-C2A-N1A	-5.69	124.53	128.89
2	C	501	NAD	C4A-C5A-N7A	-4.16	105.66	109.48
4	C	502	UGA	PA-O3A-PB	-3.99	121.53	132.73
4	E	503	UGA	PA-O3A-PB	-3.97	121.57	132.73
2	A	501	NAD	PN-O3-PA	-3.89	121.81	132.73
4	B	503	UGA	PA-O3A-PB	-3.87	121.86	132.73
4	F	502	UGA	O3A-PB-O3B	-3.83	92.60	103.63
2	D	501	NAD	PN-O3-PA	-3.65	122.47	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	503	POP	P2-O-P1	-3.55	122.75	132.73
2	E	501	NAD	PN-O3-PA	-3.47	122.99	132.73
6	C	503	POP	P2-O-P1	-3.44	123.06	132.73
3	A	502	UDP	PA-O3A-PB	-3.17	122.05	132.67
6	E	502	POP	O-P2-O4	-3.08	98.09	107.70
3	B	502	UDP	PA-O3A-PB	-3.01	122.56	132.67
2	C	501	NAD	PN-O3-PA	-3.00	124.31	132.73
2	F	501	NAD	C4A-C5A-N7A	-2.94	106.77	109.48
4	A	503	UGA	PA-O3A-PB	-2.91	124.55	132.73
2	E	501	NAD	C1B-N9A-C4A	-2.90	122.57	126.94
2	E	501	NAD	C4A-C5A-N7A	-2.77	106.93	109.48
3	D	502	UDP	PA-O3A-PB	-2.61	123.91	132.67
2	A	501	NAD	O3-PN-O5D	-2.58	96.10	102.94
2	D	501	NAD	O3-PN-O5D	-2.52	96.25	102.94
2	B	501	NAD	O3-PN-O5D	-2.50	96.31	102.94
2	C	501	NAD	C5B-C4B-C3B	-2.37	105.78	115.21
2	A	501	NAD	O3-PA-O5B	-2.26	96.93	102.94
2	A	501	NAD	C4A-C5A-N7A	-2.24	107.42	109.48
2	B	501	NAD	PN-O3-PA	-2.21	126.52	132.73
4	E	503	UGA	O5'-C1'-O3B	-2.20	108.46	111.36
4	F	502	UGA	PA-O3A-PB	-2.19	126.57	132.73
4	A	503	UGA	O3A-PB-O3B	-2.13	97.50	103.63
2	E	501	NAD	O3-PA-O5B	-2.12	97.31	102.94
2	C	501	NAD	C2B-C1B-N9A	-2.05	111.16	114.29
2	E	501	NAD	C2B-C1B-N9A	-2.00	111.23	114.29
2	E	501	NAD	O4B-C1B-N9A	2.01	112.30	108.10
4	F	502	UGA	O3B-C1'-C2'	2.06	112.24	108.39
2	C	501	NAD	O4D-C1D-N1N	2.43	110.81	108.13
4	C	502	UGA	O3B-C1'-C2'	2.48	113.02	108.39
3	B	502	UDP	O3B-PB-O2B	2.52	116.99	107.38
2	C	501	NAD	C2N-C3N-C4N	2.72	121.31	118.29
2	C	501	NAD	O4B-C1B-N9A	4.14	116.77	108.10
2	D	501	NAD	O4D-C1D-N1N	4.21	112.75	108.13
2	A	501	NAD	O4D-C1D-N1N	4.31	112.87	108.13
2	F	501	NAD	O4D-C1D-N1N	4.40	112.97	108.13
2	B	501	NAD	O4D-C1D-N1N	4.93	113.55	108.13
2	E	501	NAD	O4D-C1D-N1N	5.91	114.63	108.13
3	D	502	UDP	C4-N3-C2	5.98	120.06	114.14
4	C	502	UGA	C4-N3-C2	6.01	120.09	114.14
4	F	502	UGA	C4-N3-C2	6.07	120.16	114.14
4	A	503	UGA	C4-N3-C2	6.22	120.30	114.14
4	E	503	UGA	C4-N3-C2	6.79	120.87	114.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	UDP	C4-N3-C2	6.91	120.99	114.14
3	A	502	UDP	C4-N3-C2	7.01	121.09	114.14
4	D	503	UGA	C4-N3-C2	7.57	121.64	114.14
4	B	503	UGA	C4-N3-C2	7.84	121.91	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	UDP	1	0
4	A	503	UGA	2	0
5	A	505	SO4	3	0
4	B	503	UGA	2	0
5	B	504	SO4	1	0
2	C	501	NAD	1	0
6	C	503	POP	2	0
3	D	502	UDP	2	0
4	D	503	UGA	1	0
2	F	501	NAD	3	0
4	F	502	UGA	2	0
6	F	503	POP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	267/336 (79%)	0.58	38 (14%) 4 2	45, 83, 138, 167	0
1	B	274/336 (81%)	0.19	14 (5%) 32 25	33, 54, 104, 131	0
1	C	271/336 (80%)	-0.17	3 (1%) 82 80	38, 59, 95, 130	0
1	D	273/336 (81%)	0.03	5 (1%) 71 66	40, 65, 111, 126	0
1	E	269/336 (80%)	0.49	25 (9%) 11 7	57, 89, 127, 152	0
1	F	261/336 (77%)	0.59	27 (10%) 9 5	63, 105, 136, 168	0
All	All	1615/2016 (80%)	0.28	112 (6%) 20 14	33, 75, 126, 168	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	282	LEU	6.2
1	B	290	TYR	5.8
1	F	131	HIS	5.7
1	A	338	ILE	5.4
1	A	395	LEU	5.3
1	F	332	LEU	5.2
1	D	170	TYR	4.9
1	E	282	LEU	4.7
1	A	279	LEU	4.5
1	B	351	LEU	4.2
1	E	361	ARG	4.1
1	B	279	LEU	4.0
1	F	343	GLY	3.8
1	A	350	PHE	3.8
1	F	299	PHE	3.7
1	E	297	ARG	3.7
1	A	283	GLN	3.7
1	F	132	TRP	3.7
1	E	392	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	273	VAL	3.6
1	A	334	PHE	3.5
1	E	279	LEU	3.5
1	E	288	THR	3.5
1	A	339	LYS	3.5
1	A	332	LEU	3.5
1	F	381	GLU	3.5
1	F	335	ALA	3.3
1	F	338	ILE	3.3
1	A	342	VAL	3.3
1	B	348	ILE	3.2
1	A	392	ARG	3.2
1	A	287	LEU	3.2
1	A	277	PHE	3.2
1	F	388	ILE	3.1
1	E	273	VAL	3.1
1	A	286	PRO	3.1
1	A	282	LEU	3.1
1	E	90	ARG	3.0
1	F	345	GLY	3.0
1	B	331	ILE	3.0
1	B	282	LEU	2.9
1	A	398	GLN	2.9
1	E	331	ILE	2.9
1	E	151	ILE	2.9
1	B	286	PRO	2.9
1	C	164	SER	2.9
1	A	284	GLY	2.9
1	A	164	SER	2.8
1	F	392	ARG	2.8
1	B	293	GLY	2.8
1	A	343	GLY	2.8
1	E	347	GLU	2.7
1	C	290	TYR	2.7
1	F	317	VAL	2.7
1	A	391	PHE	2.6
1	F	344	SER	2.6
1	A	288	THR	2.6
1	E	290	TYR	2.6
1	E	343	GLY	2.6
1	A	272	ARG	2.6
1	A	348	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	272	ARG	2.5
1	E	396	GLU	2.5
1	E	345	GLY	2.5
1	A	253	VAL	2.5
1	E	397	TYR	2.5
1	A	396	GLU	2.5
1	F	285	GLU	2.5
1	A	281	ALA	2.5
1	F	331	ILE	2.5
1	E	287	LEU	2.5
1	F	170	TYR	2.5
1	B	287	LEU	2.5
1	E	289	VAL	2.4
1	D	88	ARG	2.4
1	F	393	LYS	2.4
1	A	285	GLU	2.4
1	B	288	THR	2.4
1	E	153	VAL	2.4
1	A	170	TYR	2.3
1	E	344	SER	2.3
1	A	274	VAL	2.3
1	F	370	LEU	2.3
1	D	342	VAL	2.3
1	F	205	VAL	2.3
1	A	347	GLU	2.3
1	E	340	ASN	2.3
1	A	98	GLY	2.3
1	E	281	ALA	2.2
1	A	289	VAL	2.2
1	F	135	HIS	2.2
1	F	340	ASN	2.2
1	F	342	VAL	2.2
1	A	280	GLN	2.2
1	F	251	VAL	2.2
1	F	396	GLU	2.2
1	F	284	GLY	2.2
1	F	384	LEU	2.2
1	A	362	LYS	2.2
1	A	233	GLU	2.1
1	B	349	GLN	2.1
1	A	278	ILE	2.1
1	A	290	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	283	GLN	2.1
1	D	281	ALA	2.1
1	B	284	GLY	2.0
1	A	344	SER	2.0
1	C	170	TYR	2.0
1	B	170	TYR	2.0
1	E	335	ALA	2.0
1	D	396	GLU	2.0
1	E	334	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SO4	C	504	5/5	0.92	0.23	1.47	79,90,95,100	0
3	UDP	D	502	25/25	0.82	0.23	0.80	84,100,120,147	0
3	UDP	B	502	25/25	0.82	0.35	0.75	81,108,119,173	0
5	SO4	D	504	5/5	0.96	0.33	0.74	75,83,84,87	0
5	SO4	E	504	5/5	0.86	0.24	0.40	109,118,119,123	0
4	UGA	A	503	37/37	0.94	0.18	0.40	70,87,112,114	0
5	SO4	D	505	5/5	0.92	0.22	0.24	88,96,98,107	0
2	NAD	A	501	44/44	0.97	0.22	0.10	47,67,76,84	0
4	UGA	E	503	37/37	0.95	0.19	0.06	60,81,112,120	0
6	POP	F	503	9/9	0.85	0.26	0.04	86,91,184,186	3
2	NAD	B	501	44/44	0.98	0.19	0.04	23,40,51,63	0
2	NAD	E	501	44/44	0.96	0.19	-0.02	51,67,89,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAD	C	501	44/44	0.98	0.18	-0.05	25,42,58,77	0
2	NAD	F	501	44/44	0.96	0.19	-0.10	54,76,103,105	0
2	NAD	D	501	44/44	0.97	0.19	-0.22	36,51,71,88	0
4	UGA	C	502	37/37	0.97	0.15	-0.26	45,63,114,118	0
4	UGA	B	503	37/37	0.96	0.16	-0.43	36,69,115,120	0
5	SO4	B	504	5/5	0.94	0.16	-0.53	77,78,85,97	0
4	UGA	F	502	37/37	0.93	0.17	-0.59	90,98,139,142	0
5	SO4	F	504	5/5	0.84	0.18	-0.68	121,123,127,128	0
4	UGA	D	503	37/37	0.96	0.13	-0.77	40,59,90,93	0
3	UDP	A	502	25/25	0.82	0.23	-0.88	100,124,141,142	0
6	POP	C	503	9/9	0.87	0.17	-0.89	64,95,130,200	1
6	POP	E	502	9/9	0.85	0.14	-1.35	71,81,135,148	3
5	SO4	A	505	5/5	0.95	0.17	-1.76	95,96,100,102	0
5	SO4	B	505	5/5	0.98	0.16	-2.06	56,62,73,75	0
5	SO4	A	504	5/5	0.86	0.14	-	132,135,137,140	0

6.5 Other polymers (i)

There are no such residues in this entry.