Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:06 AM GMT

PDB ID	:	2ZI6
Title	:	C4S dCK variant of dCK in complex with D-dA+UDP
Authors	:	Sabini, E.; Lavie, A.
Deposited on	:	2008-02-13
Resolution	:	1.77 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:

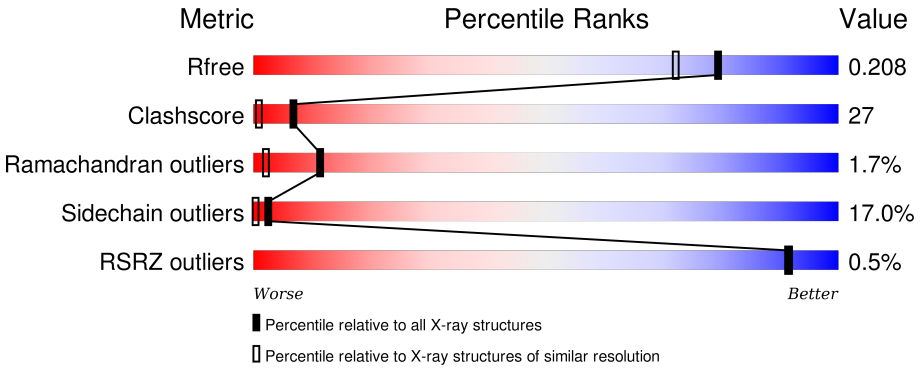
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.77 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	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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	279	% 33% 36% 8% • 22%
1	B	279	39% 32% 9% 19%
1	C	279	30% 37% 9% • 23%
1	D	279	35% 34% 9% • 22%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7616 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 Deoxycytidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	1	0
			1807	1165	299	337	6			
1	B	225	Total	C	N	O	S	0	1	0
			1867	1203	309	349	6			
1	C	216	Total	C	N	O	S	0	2	0
			1808	1167	300	335	6			
1	D	218	Total	C	N	O	S	0	0	0
			1797	1161	297	333	6			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	982	MET	-	EXPRESSION TAG	UNP P27707
A	983	GLY	-	EXPRESSION TAG	UNP P27707
A	984	SER	-	EXPRESSION TAG	UNP P27707
A	985	SER	-	EXPRESSION TAG	UNP P27707
A	986	HIS	-	EXPRESSION TAG	UNP P27707
A	987	HIS	-	EXPRESSION TAG	UNP P27707
A	988	HIS	-	EXPRESSION TAG	UNP P27707
A	989	HIS	-	EXPRESSION TAG	UNP P27707
A	990	HIS	-	EXPRESSION TAG	UNP P27707
A	991	HIS	-	EXPRESSION TAG	UNP P27707
A	992	SER	-	EXPRESSION TAG	UNP P27707
A	993	GLY	-	EXPRESSION TAG	UNP P27707
A	994	LEU	-	EXPRESSION TAG	UNP P27707
A	995	VAL	-	EXPRESSION TAG	UNP P27707
A	996	PRO	-	EXPRESSION TAG	UNP P27707
A	997	ARG	-	EXPRESSION TAG	UNP P27707
A	998	GLY	-	EXPRESSION TAG	UNP P27707
A	999	SER	-	EXPRESSION TAG	UNP P27707
A	1000	HIS	-	EXPRESSION TAG	UNP P27707
A	1009	SER	CYS	ENGINEERED	UNP P27707
A	1045	SER	CYS	ENGINEERED	UNP P27707

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1059	SER	CYS	ENGINEERED	UNP P27707
A	1146	SER	CYS	ENGINEERED	UNP P27707
B	1982	MET	-	EXPRESSION TAG	UNP P27707
B	1983	GLY	-	EXPRESSION TAG	UNP P27707
B	1984	SER	-	EXPRESSION TAG	UNP P27707
B	1985	SER	-	EXPRESSION TAG	UNP P27707
B	1986	HIS	-	EXPRESSION TAG	UNP P27707
B	1987	HIS	-	EXPRESSION TAG	UNP P27707
B	1988	HIS	-	EXPRESSION TAG	UNP P27707
B	1989	HIS	-	EXPRESSION TAG	UNP P27707
B	1990	HIS	-	EXPRESSION TAG	UNP P27707
B	1991	HIS	-	EXPRESSION TAG	UNP P27707
B	1992	SER	-	EXPRESSION TAG	UNP P27707
B	1993	GLY	-	EXPRESSION TAG	UNP P27707
B	1994	LEU	-	EXPRESSION TAG	UNP P27707
B	1995	VAL	-	EXPRESSION TAG	UNP P27707
B	1996	PRO	-	EXPRESSION TAG	UNP P27707
B	1997	ARG	-	EXPRESSION TAG	UNP P27707
B	1998	GLY	-	EXPRESSION TAG	UNP P27707
B	1999	SER	-	EXPRESSION TAG	UNP P27707
B	2000	HIS	-	EXPRESSION TAG	UNP P27707
B	2009	SER	CYS	ENGINEERED	UNP P27707
B	2045	SER	CYS	ENGINEERED	UNP P27707
B	2059	SER	CYS	ENGINEERED	UNP P27707
B	2146	SER	CYS	ENGINEERED	UNP P27707
C	2982	MET	-	EXPRESSION TAG	UNP P27707
C	2983	GLY	-	EXPRESSION TAG	UNP P27707
C	2984	SER	-	EXPRESSION TAG	UNP P27707
C	2985	SER	-	EXPRESSION TAG	UNP P27707
C	2986	HIS	-	EXPRESSION TAG	UNP P27707
C	2987	HIS	-	EXPRESSION TAG	UNP P27707
C	2988	HIS	-	EXPRESSION TAG	UNP P27707
C	2989	HIS	-	EXPRESSION TAG	UNP P27707
C	2990	HIS	-	EXPRESSION TAG	UNP P27707
C	2991	HIS	-	EXPRESSION TAG	UNP P27707
C	2992	SER	-	EXPRESSION TAG	UNP P27707
C	2993	GLY	-	EXPRESSION TAG	UNP P27707
C	2994	LEU	-	EXPRESSION TAG	UNP P27707
C	2995	VAL	-	EXPRESSION TAG	UNP P27707
C	2996	PRO	-	EXPRESSION TAG	UNP P27707
C	2997	ARG	-	EXPRESSION TAG	UNP P27707
C	2998	GLY	-	EXPRESSION TAG	UNP P27707

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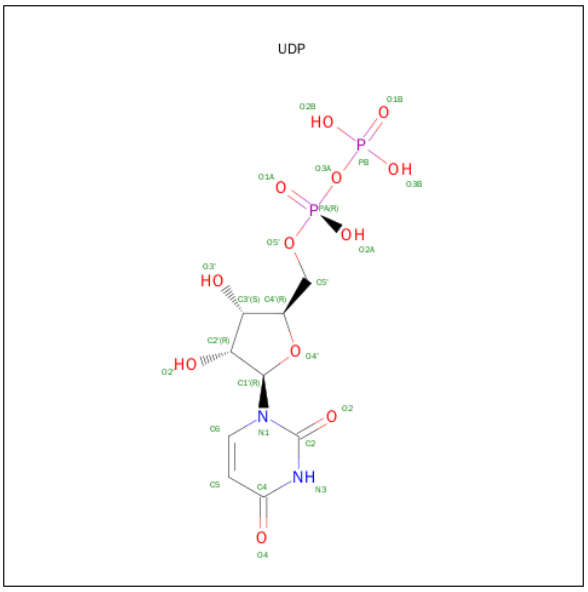
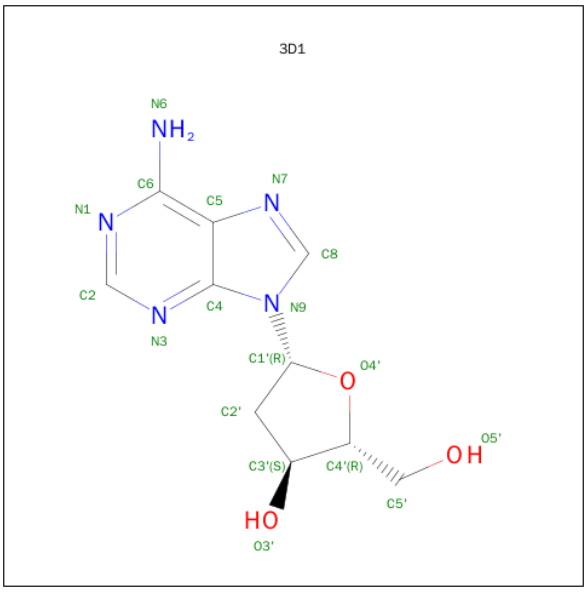
Chain	Residue	Modelled	Actual	Comment	Reference
C	2999	SER	-	EXPRESSION TAG	UNP P27707
C	3000	HIS	-	EXPRESSION TAG	UNP P27707
C	3009	SER	CYS	ENGINEERED	UNP P27707
C	3045	SER	CYS	ENGINEERED	UNP P27707
C	3059	SER	CYS	ENGINEERED	UNP P27707
C	3146	SER	CYS	ENGINEERED	UNP P27707
D	3982	MET	-	EXPRESSION TAG	UNP P27707
D	3983	GLY	-	EXPRESSION TAG	UNP P27707
D	3984	SER	-	EXPRESSION TAG	UNP P27707
D	3985	SER	-	EXPRESSION TAG	UNP P27707
D	3986	HIS	-	EXPRESSION TAG	UNP P27707
D	3987	HIS	-	EXPRESSION TAG	UNP P27707
D	3988	HIS	-	EXPRESSION TAG	UNP P27707
D	3989	HIS	-	EXPRESSION TAG	UNP P27707
D	3990	HIS	-	EXPRESSION TAG	UNP P27707
D	3991	HIS	-	EXPRESSION TAG	UNP P27707
D	3992	SER	-	EXPRESSION TAG	UNP P27707
D	3993	GLY	-	EXPRESSION TAG	UNP P27707
D	3994	LEU	-	EXPRESSION TAG	UNP P27707
D	3995	VAL	-	EXPRESSION TAG	UNP P27707
D	3996	PRO	-	EXPRESSION TAG	UNP P27707
D	3997	ARG	-	EXPRESSION TAG	UNP P27707
D	3998	GLY	-	EXPRESSION TAG	UNP P27707
D	3999	SER	-	EXPRESSION TAG	UNP P27707
D	4000	HIS	-	EXPRESSION TAG	UNP P27707
D	4009	SER	CYS	ENGINEERED	UNP P27707
D	4045	SER	CYS	ENGINEERED	UNP P27707
D	4059	SER	CYS	ENGINEERED	UNP P27707
D	4146	SER	CYS	ENGINEERED	UNP P27707

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	4	Total	C	N	O	P	0	0
			100	36	8	48	8		

- Molecule 3 is (2R,3S,5R)-5-(6-AMINO-9H-PURIN-9-YL)-TETRAHYDRO-2-(HYDROXY METHYL)FURAN-3-OL (three-letter code: 3D1) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	10	5	3		
3	B	1	Total	C	N	O	0	0
			18	10	5	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O 18 10 5 3	0	0
3	D	1	Total C N O 18 10 5 3	0	0

- Molecule 4 is water.

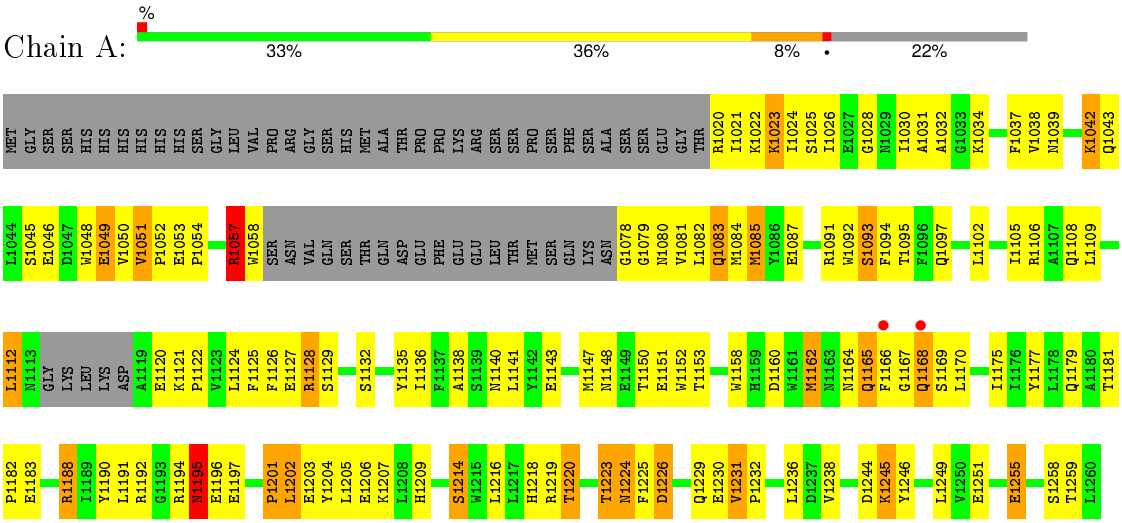
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	50	Total O 50 50	0	0
4	B	42	Total O 42 42	0	0
4	C	38	Total O 38 38	0	0
4	D	35	Total O 35 35	0	0

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.

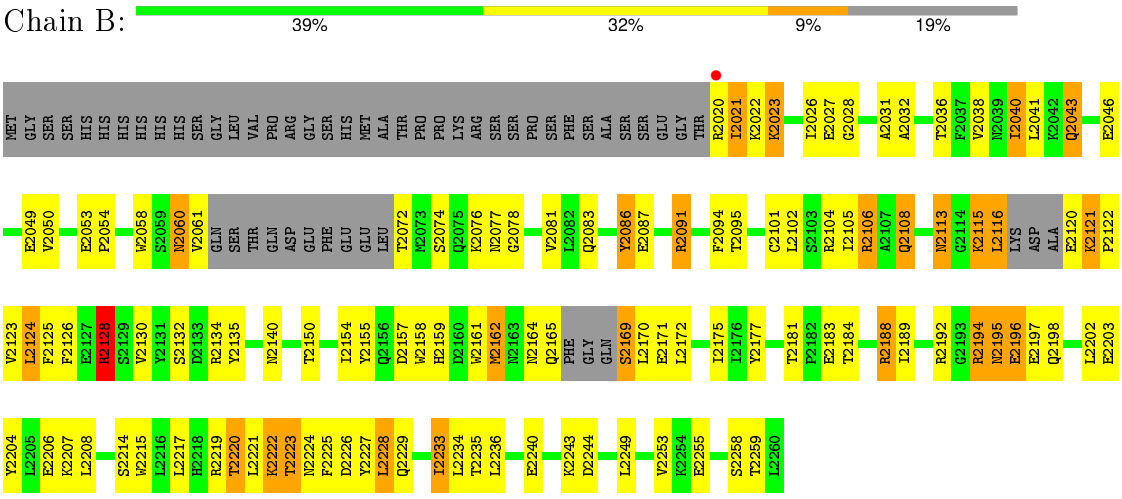
- Molecule 1: Deoxycytidine kinase

Chain A:



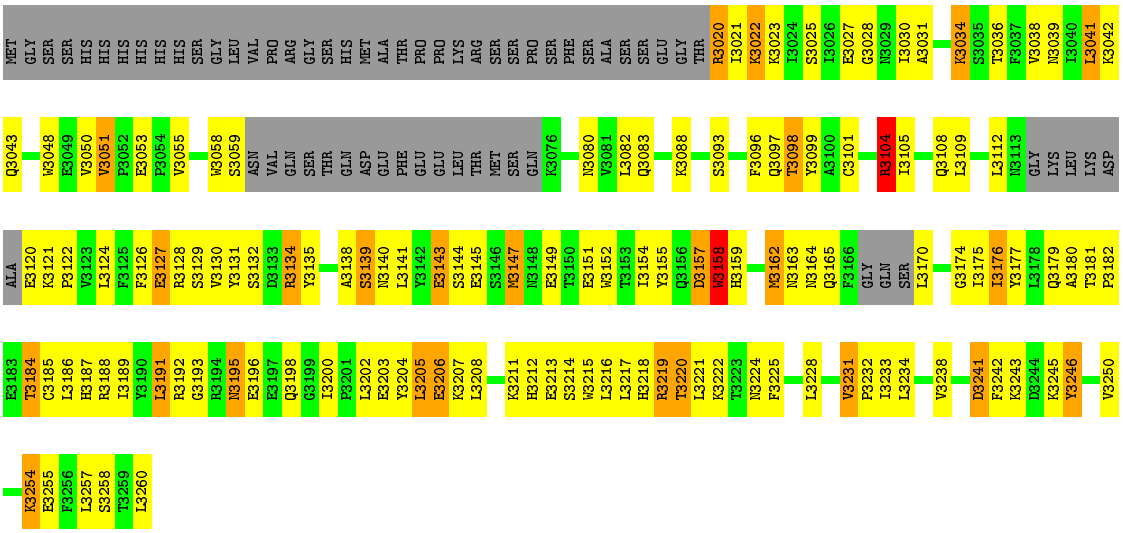
- Molecule 1: Deoxycytidine kinase

Chain B:



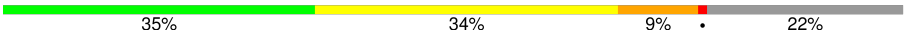
- Molecule 1: Deoxycytidine kinase

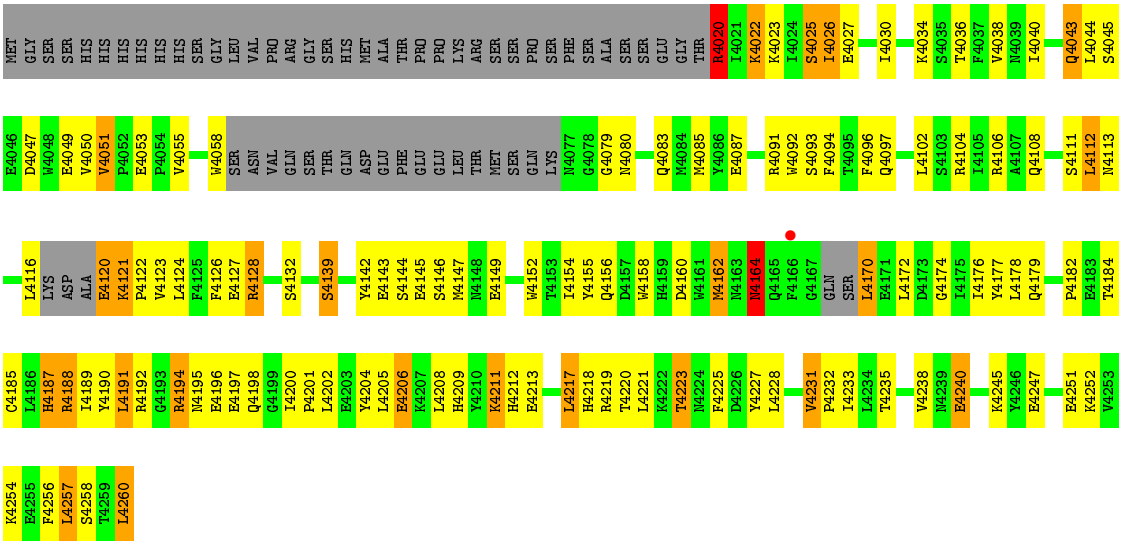
Chain C:



• Molecule 1: Deoxycytidine kinase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	138.25Å 138.51Å 118.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.77 29.96 – 1.77	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.77) 97.4 (29.96-1.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.77Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.208 , 0.283 0.209 , 0.208	Depositor DCC
R_{free} test set	10872 reflections (11.15%)	DCC
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.468 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 109957 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7616	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.04 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1957e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: UDP, 3D1

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	0.40	0/1855	1.25	11/2513 (0.4%)
1	B	0.41	0/1913	1.35	13/2590 (0.5%)
1	C	0.40	0/1854	1.30	14/2509 (0.6%)
1	D	0.40	0/1840	1.30	15/2492 (0.6%)
All	All	0.40	0/7462	1.30	53/10104 (0.5%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2091	ARG	NE-CZ-NH1	-15.12	112.74	120.30
1	C	3104	ARG	NE-CZ-NH1	-12.06	114.27	120.30
1	B	2091	ARG	NE-CZ-NH2	9.53	125.07	120.30
1	D	4020	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	D	4020	ARG	CD-NE-CZ	8.91	136.08	123.60
1	A	1057	ARG	CD-NE-CZ	8.80	135.92	123.60
1	B	2219	ARG	CD-NE-CZ	8.58	135.61	123.60
1	C	3192	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	C	3104	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	B	2128	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	1190	TYR	CB-CG-CD2	7.88	125.72	121.00
1	D	4128	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	D	4212	HIS	CA-CB-CG	7.85	126.94	113.60
1	D	4192	ARG	CD-NE-CZ	7.82	134.55	123.60
1	D	4128	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	C	3127	GLU	C-N-CA	7.16	139.60	121.70
1	A	1057	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	3241	ASP	CB-CG-OD2	7.07	124.67	118.30
1	D	4155	TYR	CB-CG-CD1	-7.02	116.79	121.00
1	D	4187	HIS	CA-CB-CG	6.85	125.24	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	4155	TYR	CB-CG-CD2	6.80	125.08	121.00
1	C	3104	ARG	CD-NE-CZ	-6.75	114.14	123.60
1	B	2219	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	3127	GLU	O-C-N	6.49	133.08	122.70
1	C	3158	TRP	CA-CB-CG	6.18	125.44	113.70
1	A	1128	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	1209	HIS	CA-CB-CG	6.02	123.83	113.60
1	D	4188	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	1128	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	2219	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	C	3192	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	2128	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	2106	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	C	3195	ASN	C-N-CA	5.58	135.66	121.70
1	A	1188	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	2155	TYR	CB-CG-CD1	-5.56	117.67	121.00
1	B	2188	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	4188	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	1190	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	B	2113	ASN	C-N-CA	5.51	133.87	122.30
1	B	2194	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	D	4145	GLU	CA-C-O	5.41	131.46	120.10
1	A	1167	GLY	C-N-CA	5.32	135.00	121.70
1	C	3128	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	1023	LYS	C-N-CA	5.26	134.86	121.70
1	C	3241	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	D	4094	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	C	3134	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	B	2155	TYR	CB-CG-CD2	5.09	124.06	121.00
1	C	3041	LEU	CA-CB-CG	5.05	126.92	115.30
1	D	4194	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	D	4192	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	1025	SER	C-N-CA	5.01	134.24	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1807	0	1739	113	0
1	B	1867	0	1819	99	0
1	C	1808	0	1752	92	0
1	D	1797	0	1731	97	0
2	A	100	0	44	9	0
3	A	18	0	13	1	0
3	B	18	0	13	0	0
3	C	18	0	13	1	0
3	D	18	0	13	0	0
4	A	50	0	0	1	0
4	B	42	0	0	3	0
4	C	38	0	0	1	0
4	D	35	0	0	1	0
All	All	7616	0	7137	391	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 27.

All (391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:LYS:HD3	1:A:1169:SER:O	1.53	1.08
1:A:1023:LYS:CD	1:A:1169:SER:O	2.09	1.00
1:A:1166:PHE:HA	1:A:1168:GLN:HG2	1.54	0.88
1:A:1051:VAL:HG21	1:A:1108:GLN:HG2	1.55	0.86
1:D:4123:VAL:HG21	1:D:4257:LEU:HD11	1.59	0.85
1:D:4194:ARG:HB2	1:D:4197:GLU:HG3	1.61	0.82
1:D:4178:LEU:HD22	1:D:4238:VAL:HG11	1.63	0.78
1:D:4020:ARG:HB2	1:D:4020:ARG:HH11	1.49	0.78
1:C:3038:VAL:HG13	1:C:3050:VAL:HG21	1.67	0.77
1:D:4102:LEU:O	1:D:4106:ARG:HG3	1.84	0.76
1:A:1021:ILE:HA	1:A:1122:PRO:HB2	1.66	0.76
1:D:4040:ILE:HA	1:D:4043:GLN:OE1	1.86	0.75
2:A:2301:UDP:H5'1	1:B:2192:ARG:HD3	1.69	0.75
1:C:3162:MET:O	1:C:3165[B]:GLN:HB2	1.87	0.75
1:A:1057:ARG:HH11	1:A:1057:ARG:HG3	1.50	0.74
1:D:4185:CYS:O	1:D:4189:ILE:HG13	1.87	0.74
1:C:3109:LEU:HA	1:C:3112:LEU:HD12	1.70	0.73
1:C:3202:LEU:HG	1:C:3206:GLU:OE2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4201:PRO:HG2	1:D:4204:TYR:HB2	1.69	0.72
1:A:1188:ARG:HA	1:A:1191:LEU:HB2	1.71	0.72
1:C:3188:ARG:HA	1:C:3191:LEU:HB2	1.72	0.72
1:B:2175:ILE:HB	1:B:2233:ILE:HG23	1.72	0.71
1:A:1158:TRP:O	1:A:1162:MET:HB2	1.90	0.71
1:C:3021:ILE:HA	1:C:3122:PRO:HB2	1.73	0.70
1:D:4139:SER:O	1:D:4143:GLU:HG3	1.92	0.69
1:C:3022:LYS:HD2	1:C:3260:LEU:HD12	1.73	0.69
1:B:2078:GLY:O	1:B:2081:VAL:HG12	1.92	0.69
1:D:4079:GLY:O	1:D:4083:GLN:HG2	1.92	0.69
1:D:4179:GLN:O	1:D:4238:VAL:HG22	1.93	0.68
1:D:4120:GLU:HG3	1:D:4121:LYS:HG2	1.76	0.67
1:D:4112:LEU:HD23	1:D:4124:LEU:HD22	1.77	0.67
1:D:4139:SER:OG	1:D:4211:LYS:HE3	1.96	0.66
1:B:2104:ARG:HD2	1:B:2130:VAL:HG12	1.78	0.66
1:B:2060:ASN:HA	1:B:2061:VAL:O	1.94	0.66
1:D:4225:PHE:HB2	1:D:4228:LEU:HG	1.76	0.66
1:B:2115:LYS:HG2	1:B:2116:LEU:HD23	1.76	0.66
1:D:4023:LYS:HD3	1:D:4112:LEU:HD11	1.77	0.66
1:C:3020:ARG:HH12	1:C:3120:GLU:N	1.94	0.66
1:B:2140:ASN:HD21	1:B:2207:LYS:NZ	1.93	0.65
1:D:4221:LEU:HG	1:D:4223:THR:HG22	1.78	0.65
1:B:2181:THR:HB	1:B:2183:GLU:OE1	1.97	0.64
1:A:1202:LEU:O	1:A:1206:GLU:HG2	1.97	0.64
1:D:4188:ARG:HA	1:D:4191:LEU:HG	1.79	0.64
1:B:2102:LEU:HD13	1:B:2162:MET:HE3	1.78	0.64
1:D:4080:ASN:O	1:D:4083:GLN:HG3	1.98	0.63
1:D:4049:GLU:HB2	1:D:4124:LEU:HD12	1.80	0.63
1:A:1094:PHE:CE2	1:B:2095:THR:HG23	2.34	0.63
1:C:3036:THR:HG23	1:C:3243:LYS:HE3	1.79	0.63
1:A:1135:TYR:CZ	1:A:1223:THR:HB	2.34	0.63
1:D:4055:VAL:HG23	4:D:7001:HOH:O	1.97	0.63
1:C:3028:GLY:O	1:C:3034:LYS:HE3	1.99	0.63
1:D:4116:LEU:HB3	1:D:4122:PRO:HB3	1.81	0.62
1:A:1082:LEU:O	1:A:1085:MET:HB3	1.98	0.62
1:A:1153:THR:HG22	1:B:2077:ASN:HD21	1.64	0.62
1:C:3187:HIS:HD2	1:C:3191:LEU:HD12	1.64	0.61
1:D:4174:GLY:HA2	1:D:4231:VAL:HG22	1.82	0.61
1:A:1112:LEU:HD23	1:A:1170:LEU:HD23	1.81	0.61
1:B:2104:ARG:O	1:B:2108:GLN:HB2	2.01	0.60
1:C:3176:ILE:HD12	1:C:3234:LEU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1177:TYR:CE2	1:A:1179:GLN:HB2	2.37	0.59
1:A:1093:SER:O	1:A:1097:GLN:HG2	2.02	0.59
1:C:3134:ARG:HA	1:C:3138:ALA:HB3	1.84	0.59
1:B:2060:ASN:OD1	1:B:2061:VAL:HG22	2.01	0.59
1:A:1223:THR:HG1	1:A:1225:PHE:HD1	1.49	0.59
1:A:1042:LYS:HG3	1:A:1042:LYS:O	2.02	0.59
1:B:2116:LEU:HD12	1:B:2122:PRO:HB3	1.85	0.58
1:B:2049:GLU:HB3	1:B:2124:LEU:CD1	2.34	0.58
1:D:4182:PRO:HB2	1:D:4202:LEU:HD11	1.85	0.58
1:A:1255:GLU:O	1:A:1259:THR:HG23	2.03	0.58
1:D:4232:PRO:HB2	1:D:4256:PHE:HE2	1.69	0.58
1:D:4022:LYS:HE3	1:D:4260:LEU:O	2.03	0.58
1:A:1182:PRO:HD2	1:A:1183:GLU:OE2	2.04	0.58
1:C:3231:VAL:HG22	1:C:3232:PRO:HD2	1.84	0.58
1:A:1112:LEU:HD21	1:A:1169:SER:O	2.03	0.58
1:A:1026:ILE:HG13	1:A:1038:VAL:HG23	1.84	0.58
1:B:2204:TYR:HA	1:B:2207:LYS:HE3	1.85	0.57
1:A:1202:LEU:HD12	1:A:1206:GLU:OE2	2.03	0.57
1:A:1158:TRP:CE2	1:A:1162:MET:HG2	2.38	0.57
1:A:1158:TRP:HE1	1:A:1162:MET:CE	2.17	0.57
1:D:4093:SER:O	1:D:4097:GLN:HG2	2.05	0.57
1:D:4160:ASP:O	1:D:4164:ASN:HB2	2.04	0.57
1:B:2225:PHE:O	1:B:2228:LEU:HB2	2.04	0.56
1:C:3255:GLU:O	1:C:3255:GLU:HG2	2.06	0.56
1:A:1023:LYS:NZ	1:A:1169:SER:HA	2.21	0.56
1:D:4191:LEU:H	1:D:4191:LEU:HD23	1.69	0.56
1:C:3022:LYS:HE3	1:C:3257:LEU:HD22	1.87	0.56
1:B:2049:GLU:HB3	1:B:2124:LEU:HD12	1.88	0.56
1:A:1083:GLN:NE2	1:C:3245:LYS:HD2	2.21	0.56
1:D:4201:PRO:HG2	1:D:4204:TYR:CB	2.35	0.56
1:D:4049:GLU:HG3	1:D:4116:LEU:HG	1.88	0.56
1:D:4152:TRP:O	1:D:4156:GLN:HG3	2.05	0.56
1:D:4158:TRP:O	1:D:4162:MET:HB3	2.06	0.55
1:A:1052:PRO:HB2	1:A:1057:ARG:NH2	2.22	0.55
1:A:1150:THR:OG1	1:D:4247:GLU:HG2	2.06	0.55
1:A:1078:GLY:HA2	1:A:1081:VAL:HG12	1.89	0.55
1:D:4022:LYS:HE2	1:D:4257:LEU:HD22	1.89	0.55
1:C:3250:VAL:O	1:C:3254:LYS:HG3	2.06	0.54
1:C:3164:ASN:HD21	1:C:3225:PHE:HE2	1.54	0.54
1:A:1214:SER:OG	1:A:1220:THR:HG23	2.07	0.54
1:D:4116:LEU:HD22	1:D:4122:PRO:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4047:ASP:O	1:D:4122:PRO:HA	2.08	0.54
1:C:3053:GLU:HB2	1:C:3127:GLU:O	2.08	0.54
1:A:1050:VAL:HG12	1:A:1052:PRO:HD3	1.88	0.54
1:A:1165:GLN:N	1:A:1165:GLN:HE21	2.06	0.54
1:B:2022:LYS:HB2	1:B:2123:VAL:HG22	1.91	0.53
1:C:3174:GLY:HA2	1:C:3232:PRO:HG2	1.90	0.53
1:C:3082:LEU:HA	1:C:3096:PHE:HE1	1.73	0.53
1:B:2038:VAL:HG13	1:B:2050:VAL:CG2	2.39	0.53
1:D:4091:ARG:HG3	1:D:4092:TRP:NE1	2.23	0.53
1:C:3130:VAL:HB	1:C:3159:HIS:HE2	1.73	0.53
1:B:2101:CYS:HB3	1:B:2158:TRP:HH2	1.72	0.53
1:C:3204:TYR:CE1	1:C:3208:LEU:HD11	2.44	0.53
1:A:1203:GLU:HA	1:A:1206:GLU:HG3	1.91	0.53
1:A:1031:ALA:HA	2:A:1301:UDP:PB	2.49	0.53
1:D:4038:VAL:HG22	1:D:4050:VAL:HG22	1.91	0.52
1:D:4053:GLU:H	1:D:4127:GLU:HB3	1.74	0.52
1:D:4219:ARG:CZ	1:D:4233:ILE:HD11	2.39	0.52
1:C:3246:TYR:O	1:C:3250:VAL:HG23	2.10	0.52
1:B:2054:PRO:HD2	4:B:7003:HOH:O	2.09	0.52
1:B:2053:GLU:OE1	1:B:2128:ARG:HD2	2.09	0.52
1:A:1031:ALA:HA	2:A:1301:UDP:O3A	2.10	0.52
1:A:1166:PHE:CA	1:A:1168:GLN:HG2	2.35	0.52
1:C:3036:THR:CG2	1:C:3243:LYS:HE3	2.40	0.52
1:B:2202:LEU:HG	1:B:2202:LEU:O	2.10	0.52
1:A:1105:ILE:O	1:A:1109:LEU:HG	2.10	0.52
1:A:1024:ILE:O	1:A:1125:PHE:HA	2.10	0.52
1:A:1023:LYS:CE	1:A:1169:SER:O	2.58	0.51
1:D:4178:LEU:HD22	1:D:4238:VAL:CG1	2.35	0.51
1:D:4043:GLN:HE21	1:D:4044:LEU:CD2	2.23	0.51
1:B:2102:LEU:HD13	1:B:2162:MET:CE	2.40	0.51
1:A:1132:SER:O	1:A:1136:ILE:HB	2.11	0.51
1:C:3022:LYS:HD2	1:C:3260:LEU:CD1	2.38	0.51
1:C:3041:LEU:O	1:C:3048:TRP:HE3	1.93	0.51
1:D:4030:ILE:O	1:D:4185:CYS:HB3	2.10	0.51
1:C:3202:LEU:O	1:C:3205:LEU:HB2	2.11	0.51
1:A:1080:ASN:ND2	1:C:3245:LYS:HG3	2.26	0.51
1:D:4240:GLU:OE2	1:D:4245:LYS:HE3	2.11	0.51
1:C:3093:SER:O	1:C:3097:GLN:HG2	2.11	0.51
1:B:2086:TYR:HE1	1:B:2196:GLU:OE2	1.93	0.51
1:D:4197:GLU:O	1:D:4200:ILE:HG13	2.10	0.50
1:D:4043:GLN:HE21	1:D:4044:LEU:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:PRO:C	1:A:1057:ARG:HH22	2.15	0.50
1:A:1042:LYS:HZ1	1:A:1049:GLU:HA	1.76	0.50
1:A:1127:GLU:O	1:A:1128:ARG:HB2	2.12	0.50
1:B:2060:ASN:OD1	1:B:2061:VAL:HA	2.11	0.50
1:C:3202:LEU:O	1:C:3206:GLU:OE2	2.29	0.50
1:B:2108:GLN:HB3	1:B:2170:LEU:CD1	2.41	0.50
1:B:2038:VAL:HG13	1:B:2050:VAL:HG22	1.94	0.50
1:D:4091:ARG:HG3	1:D:4092:TRP:CD1	2.47	0.50
1:D:4195:ASN:HA	1:D:4198:GLN:HG2	1.94	0.50
1:A:1192:ARG:HD3	2:A:1301:UDP:H5'1	1.93	0.50
1:C:3038:VAL:HG22	1:C:3050:VAL:HG22	1.94	0.50
1:D:4116:LEU:HD13	1:D:4122:PRO:HB3	1.94	0.50
1:A:1181:THR:HB	1:A:1183:GLU:OE2	2.11	0.50
1:B:2184:THR:O	1:B:2188:ARG:HG3	2.12	0.50
1:C:3139:SER:HB2	1:C:3152:TRP:CZ2	2.47	0.50
1:D:4139:SER:O	1:D:4142:TYR:HB3	2.12	0.50
1:C:3139:SER:O	1:C:3143:GLU:OE1	2.30	0.49
1:C:3129:SER:HB2	4:C:7005:HOH:O	2.12	0.49
1:D:4184:THR:HG22	1:D:4188:ARG:HD2	1.95	0.49
1:C:3179:GLN:NE2	1:C:3217:LEU:HD22	2.27	0.49
1:C:3185:CYS:HB2	1:C:3205:LEU:CD1	2.41	0.49
1:D:4112:LEU:HD23	1:D:4124:LEU:CD2	2.41	0.49
1:A:1164:ASN:C	1:A:1165:GLN:HE21	2.16	0.49
1:A:1084:MET:HB3	1:A:1092:TRP:CD1	2.47	0.49
1:C:3027:GLU:OE2	1:C:3132:SER:OG	2.28	0.49
1:B:2108:GLN:HB3	1:B:2170:LEU:HD13	1.93	0.49
1:A:1244:ASP:O	1:A:1245:LYS:HB2	2.13	0.49
1:B:2021:ILE:HG13	1:B:2122:PRO:HB2	1.95	0.49
1:D:4053:GLU:OE1	1:D:4128:ARG:HD2	2.12	0.49
1:A:1175:ILE:HG21	1:A:1216:LEU:HD22	1.95	0.49
1:A:1112:LEU:HD23	1:A:1170:LEU:CD2	2.42	0.49
1:B:2021:ILE:HG22	1:B:2021:ILE:O	2.13	0.49
1:B:2116:LEU:CD1	1:B:2122:PRO:HB3	2.42	0.49
1:C:3082:LEU:HA	1:C:3096:PHE:CE1	2.48	0.49
1:C:3093:SER:HB3	1:C:3141:LEU:HD13	1.94	0.49
1:B:2086:TYR:OH	1:B:2197:GLU:HG2	2.13	0.48
1:C:3038:VAL:HG12	1:C:3039:ASN:ND2	2.27	0.48
1:D:4040:ILE:O	1:D:4044:LEU:HG	2.13	0.48
1:A:1030:ILE:HD12	1:A:1205:LEU:HD21	1.96	0.48
1:D:4204:TYR:CZ	1:D:4208:LEU:HD11	2.49	0.48
1:C:3215:TRP:CD1	1:C:3221:LEU:HD23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3108:GLN:O	1:C:3112:LEU:HD12	2.12	0.48
1:D:4232:PRO:HG2	1:D:4260:LEU:HD21	1.96	0.48
1:B:2140:ASN:HD21	1:B:2207:LYS:HZ1	1.62	0.48
1:C:3175:ILE:O	1:C:3233:ILE:HA	2.14	0.48
1:C:3154:ILE:O	1:C:3157:ASP:HB2	2.13	0.48
1:D:4209:HIS:O	1:D:4213:GLU:HG2	2.14	0.48
1:C:3163:ASN:C	1:C:3164:ASN:HD22	2.17	0.48
1:D:4194:ARG:HB3	1:D:4196:GLU:OE2	2.13	0.48
1:D:4116:LEU:HD13	1:D:4122:PRO:CB	2.44	0.48
1:C:3144:SER:O	1:C:3145:GLU:HB2	2.13	0.48
1:B:2134:ARG:HG2	1:B:2135:TYR:CE1	2.49	0.47
1:A:1194:ARG:HB3	1:A:1197:GLU:HB2	1.96	0.47
1:A:1204:TYR:O	1:A:1207:LYS:HB2	2.13	0.47
1:B:2130:VAL:HG13	4:B:7080:HOH:O	2.13	0.47
1:C:3025:SER:HA	1:C:3126:PHE:HB2	1.96	0.47
1:A:1158:TRP:NE1	1:A:1162:MET:HG2	2.30	0.47
1:B:2204:TYR:CE2	1:B:2208:LEU:HD11	2.50	0.47
1:D:4202:LEU:O	1:D:4206:GLU:HG3	2.14	0.47
1:A:1203:GLU:HA	1:A:1206:GLU:CG	2.44	0.47
1:A:1079:GLY:O	1:A:1083:GLN:HB2	2.15	0.47
1:D:4038:VAL:HG21	1:D:4050:VAL:HG13	1.96	0.47
1:D:4123:VAL:CG2	1:D:4257:LEU:HD11	2.35	0.47
1:D:4177:TYR:CE2	1:D:4179:GLN:HB2	2.50	0.47
1:D:4187:HIS:O	1:D:4191:LEU:HD23	2.14	0.47
1:C:3101:CYS:O	1:C:3105:ILE:HD12	2.13	0.47
1:B:2196:GLU:HG3	1:B:2196:GLU:H	1.41	0.47
1:C:3180:ALA:HB2	1:C:3238:VAL:HG23	1.97	0.47
1:D:4172:LEU:HB2	1:D:4227:TYR:CE1	2.50	0.47
1:A:1223:THR:OG1	1:A:1225:PHE:HD1	1.98	0.47
1:B:2171:GLU:HA	1:B:2227:TYR:OH	2.14	0.47
1:B:2215:TRP:HB2	1:B:2221:LEU:HD23	1.97	0.47
1:C:3214:SER:HB2	1:C:3220:THR:OG1	2.15	0.47
1:C:3130:VAL:HG11	1:C:3163:ASN:HD21	1.80	0.46
1:B:2083:GLN:OE1	1:D:4245:LYS:HE2	2.15	0.46
1:A:1026:ILE:HG13	1:A:1038:VAL:CG2	2.44	0.46
1:A:1052:PRO:HB2	1:A:1057:ARG:HH22	1.79	0.46
1:C:3051:VAL:O	1:C:3051:VAL:HG22	2.15	0.46
1:B:2026:ILE:HD11	1:B:2125:PHE:HD2	1.81	0.46
1:D:4025:SER:OG	1:D:4027:GLU:OE1	2.31	0.46
1:A:1095:THR:HG23	1:B:2094:PHE:CE2	2.50	0.46
1:A:1021:ILE:HG22	1:A:1021:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2171:GLU:HB3	1:B:2227:TYR:CZ	2.51	0.46
1:B:2050:VAL:HG12	1:B:2050:VAL:O	2.16	0.46
1:A:1218:HIS:HB2	1:A:1220:THR:HG22	1.98	0.46
1:A:1032:ALA:O	1:A:1238:VAL:HG21	2.16	0.46
1:A:1153:THR:CG2	1:B:2077:ASN:HD21	2.27	0.46
1:B:2134:ARG:HD3	1:B:2159:HIS:ND1	2.31	0.46
1:B:2150:THR:HG22	1:B:2154:ILE:HD12	1.97	0.46
1:A:1140:ASN:HB3	4:A:7133:HOH:O	2.15	0.46
1:A:1053:GLU:O	1:A:1057:ARG:NH1	2.49	0.45
1:C:3112:LEU:HD11	1:C:3170:LEU:CD2	2.45	0.45
1:B:2021:ILE:HG23	1:B:2022:LYS:O	2.16	0.45
1:B:2175:ILE:CB	1:B:2233:ILE:HG23	2.45	0.45
1:A:1214:SER:O	1:A:1220:THR:HG23	2.17	0.45
1:C:3214:SER:O	1:C:3220:THR:N	2.49	0.45
1:C:3055:VAL:HG22	1:C:3058:TRP:CE3	2.52	0.45
1:D:4051:VAL:HG22	1:D:4051:VAL:O	2.15	0.45
1:B:2121:LYS:HB2	1:B:2121:LYS:HE3	1.35	0.45
1:C:3215:TRP:HA	1:C:3221:LEU:HB3	1.98	0.45
1:D:4213:GLU:CD	1:D:4217:LEU:HD23	2.37	0.45
1:C:3155:TYR:O	1:C:3158:TRP:HB3	2.16	0.45
1:D:4232:PRO:HG2	1:D:4260:LEU:CD2	2.46	0.45
1:A:1226:ASP:N	1:A:1226:ASP:OD2	2.50	0.45
1:D:4251:GLU:OE2	1:D:4254:LYS:NZ	2.50	0.45
1:D:4202:LEU:HD12	1:D:4205:LEU:HB2	1.98	0.45
1:D:4038:VAL:HG22	1:D:4050:VAL:CG2	2.47	0.45
1:D:4213:GLU:OE1	1:D:4217:LEU:HD23	2.17	0.45
1:B:2194:ARG:O	1:B:2198:GLN:NE2	2.49	0.45
1:D:4049:GLU:HB2	1:D:4124:LEU:CD1	2.45	0.45
1:A:1097:GLN:HA	1:A:1097:GLN:OE1	2.17	0.45
1:C:3164:ASN:ND2	1:C:3225:PHE:HE2	2.15	0.45
1:A:1045:SER:HB3	1:A:1048:TRP:CG	2.52	0.45
1:B:2105:ILE:HG22	1:B:2106:ARG:N	2.31	0.45
1:B:2121:LYS:N	1:B:2122:PRO:HD3	2.32	0.45
1:D:4026:ILE:HD13	1:D:4026:ILE:N	2.32	0.45
1:A:1038:VAL:HG13	1:A:1050:VAL:HG21	1.98	0.44
1:A:1053:GLU:OE2	3:A:1302:3D1:H2	2.17	0.44
1:B:2120:GLU:C	1:B:2122:PRO:HD3	2.38	0.44
1:C:3112:LEU:HD11	1:C:3170:LEU:HD23	1.99	0.44
1:A:1177:TYR:CZ	1:A:1179:GLN:HB2	2.53	0.44
1:B:2225:PHE:O	1:B:2227:TYR:N	2.50	0.44
1:A:1168:GLN:O	1:A:1168:GLN:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2086:TYR:CE1	1:B:2196:GLU:HB2	2.52	0.44
1:B:2031:ALA:HB1	1:B:2188:ARG:CB	2.47	0.44
1:C:3215:TRP:CG	1:C:3221:LEU:HD23	2.52	0.44
1:C:3213:GLU:O	1:C:3218:HIS:N	2.50	0.44
1:C:3080:ASN:O	1:C:3083:GLN:HB2	2.18	0.44
1:A:1021:ILE:CG2	1:A:1124:LEU:HB2	2.47	0.44
1:B:2204:TYR:O	1:B:2207:LYS:N	2.50	0.44
1:A:1039:ASN:O	1:A:1042:LYS:HB3	2.17	0.44
2:A:4301:UDP:O2A	1:D:4036:THR:N	2.50	0.44
1:D:4023:LYS:HB2	1:D:4023:LYS:HE3	1.62	0.44
1:B:2101:CYS:HB3	1:B:2158:TRP:CH2	2.52	0.44
1:D:4172:LEU:HB2	1:D:4227:TYR:HE1	1.83	0.44
1:A:1028:GLY:N	1:A:1034:LYS:HD3	2.33	0.44
1:C:3193:GLY:HA2	1:C:3198:GLN:NE2	2.32	0.44
1:D:4051:VAL:HG13	1:D:4126:PHE:CD2	2.52	0.44
1:B:2102:LEU:O	1:B:2102:LEU:HD12	2.17	0.44
1:A:1129:SER:O	1:A:1132:SER:HB2	2.17	0.44
1:B:2207:LYS:NZ	4:B:7102:HOH:O	2.49	0.44
1:C:3219:ARG:NH2	1:C:3231:VAL:O	2.50	0.44
1:A:1102:LEU:HD11	1:B:2161:TRP:CZ3	2.53	0.44
2:A:3301:UDP:N3	1:C:3241:ASP:OD1	2.49	0.44
1:C:3176:ILE:N	1:C:3176:ILE:HD13	2.33	0.44
1:A:1097:GLN:HE21	1:A:1141:LEU:CD1	2.31	0.44
1:B:2220:THR:HG22	1:B:2221:LEU:N	2.32	0.44
1:A:1219:ARG:NH1	1:A:1229:GLN:O	2.50	0.44
1:D:4201:PRO:O	1:D:4204:TYR:HB3	2.17	0.43
1:B:2220:THR:O	1:B:2222:LYS:HD2	2.18	0.43
1:A:1034:LYS:HE2	1:A:1034:LYS:HB2	1.86	0.43
1:C:3182:PRO:O	1:C:3205:LEU:HD12	2.18	0.43
1:B:2058:TRP:CD2	1:B:2078:GLY:HA3	2.52	0.43
1:D:4187:HIS:O	1:D:4190:TYR:HB3	2.18	0.43
1:C:3030:ILE:O	1:C:3031:ALA:HB3	2.19	0.43
1:B:2177:TYR:HD2	1:B:2235:THR:OG1	2.01	0.43
1:B:2223:THR:OG1	1:B:2224:ASN:N	2.50	0.43
1:B:2040:ILE:HG22	1:B:2041:LEU:N	2.33	0.43
1:A:1249:LEU:HD23	1:A:1249:LEU:HA	1.87	0.43
1:C:3131:TYR:O	1:C:3135:TYR:HB2	2.19	0.43
1:D:4108:GLN:HB3	1:D:4170:LEU:HD21	2.00	0.43
1:C:3215:TRP:CE2	1:C:3216:LEU:HD21	2.54	0.43
1:C:3213:GLU:HA	1:C:3213:GLU:OE2	2.18	0.43
1:D:4034:LYS:H	1:D:4034:LYS:HG3	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2255:GLU:O	1:B:2258:SER:OG	2.30	0.43
1:B:2249:LEU:O	1:B:2253:VAL:HG23	2.18	0.43
1:C:3165[A]:GLN:NE2	1:C:3165[A]:GLN:HA	2.34	0.43
1:C:3241:ASP:OD1	1:C:3242:PHE:N	2.51	0.43
1:B:2108:GLN:HG2	1:B:2126:PHE:CE2	2.53	0.43
1:A:1236:LEU:HD13	1:A:1249:LEU:HD22	1.99	0.43
1:C:3098:THR:HG22	1:C:3099:TYR:N	2.34	0.43
1:A:1045:SER:HB3	1:A:1048:TRP:CD2	2.53	0.43
1:C:3030:ILE:O	1:C:3185:CYS:HB3	2.19	0.43
1:A:1188:ARG:NH1	1:A:1238:VAL:O	2.50	0.43
2:A:3301:UDP:O4'	1:C:3188:ARG:HB3	2.18	0.43
1:D:4120:GLU:HG3	1:D:4121:LYS:CG	2.44	0.43
1:D:4055:VAL:O	1:D:4058:TRP:HB2	2.18	0.43
1:A:1165:GLN:HG2	1:A:1165:GLN:H	1.44	0.43
1:A:1037:PHE:CZ	1:A:1249:LEU:HB3	2.53	0.43
1:B:2255:GLU:O	1:B:2259:THR:HG23	2.19	0.43
1:B:2027:GLU:HG3	1:B:2175:ILE:HG23	2.01	0.42
1:B:2049:GLU:HG3	1:B:2050:VAL:H	1.84	0.42
1:B:2028:GLY:O	1:B:2128:ARG:NH2	2.49	0.42
1:A:1246:TYR:O	1:A:1249:LEU:HB2	2.19	0.42
1:A:1112:LEU:O	1:A:1112:LEU:HD12	2.19	0.42
1:A:1188:ARG:NH2	1:A:1238:VAL:O	2.53	0.42
1:B:2078:GLY:HA2	1:B:2081:VAL:HG12	2.01	0.42
1:B:2053:GLU:HA	1:B:2054:PRO:HD3	1.89	0.42
1:A:1021:ILE:HG21	1:A:1124:LEU:HD22	2.00	0.42
1:A:1091:ARG:HG3	1:A:1092:TRP:CE2	2.55	0.42
1:C:3104:ARG:HH11	1:C:3104:ARG:HD2	1.50	0.42
1:C:3181:THR:O	1:C:3184:THR:OG1	2.30	0.42
1:C:3204:TYR:CZ	1:C:3208:LEU:HD11	2.54	0.42
1:A:1058:TRP:CD2	1:A:1078:GLY:HA3	2.55	0.42
2:A:3301:UDP:O4	1:C:3241:ASP:OD1	2.37	0.42
1:A:1140:ASN:O	1:A:1143:GLU:HB2	2.19	0.42
1:A:1054:PRO:HA	1:A:1057:ARG:CZ	2.50	0.42
1:D:4124:LEU:HD23	1:D:4126:PHE:HE2	1.84	0.42
1:B:2115:LYS:HG3	1:B:2116:LEU:H	1.85	0.42
1:B:2091:ARG:HD2	1:B:2091:ARG:HH11	1.52	0.42
1:C:3141:LEU:HA	1:C:3144:SER:HB2	2.01	0.42
1:C:3140:ASN:O	1:C:3143:GLU:HB2	2.20	0.42
1:B:2189:ILE:HG22	1:B:2189:ILE:O	2.19	0.42
1:A:1148:ASN:N	1:A:1151:GLU:OE1	2.50	0.42
1:D:4096:PHE:HD2	1:D:4097:GLN:NE2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2202:LEU:O	1:B:2206:GLU:HG3	2.20	0.41
1:B:2032:ALA:O	1:B:2188:ARG:NH1	2.53	0.41
1:B:2043:GLN:H	1:B:2043:GLN:HG2	1.58	0.41
1:D:4154:ILE:HD13	1:D:4154:ILE:HG21	1.84	0.41
1:A:1201:PRO:HB3	1:A:1203:GLU:OE1	2.20	0.41
1:A:1140:ASN:O	1:A:1143:GLU:N	2.53	0.41
1:D:4177:TYR:CD2	1:D:4235:THR:HG23	2.54	0.41
1:B:2161:TRP:CE2	1:B:2165:GLN:HG3	2.55	0.41
1:B:2023:LYS:HE2	1:B:2169:SER:O	2.19	0.41
1:A:1138:ALA:HB1	1:A:1152:TRP:HZ3	1.84	0.41
1:B:2134:ARG:HD3	1:B:2159:HIS:CE1	2.56	0.41
1:C:3147:MET:HG2	1:C:3151:GLU:CB	2.50	0.41
1:B:2164:ASN:O	1:B:2164:ASN:ND2	2.53	0.41
1:B:2234:LEU:HD21	1:B:2236:LEU:HD21	2.01	0.41
1:B:2026:ILE:HD11	1:B:2125:PHE:CD2	2.55	0.41
1:D:4026:ILE:HD12	1:D:4176:ILE:HB	2.02	0.41
1:A:1093:SER:OG	1:A:1141:LEU:HD22	2.20	0.41
1:A:1106:ARG:NH1	1:B:2157:ASP:OD1	2.50	0.41
1:A:1231:VAL:HA	1:A:1232:PRO:HD3	1.75	0.41
1:D:4051:VAL:HG13	1:D:4126:PHE:HD2	1.86	0.41
1:A:1102:LEU:HG	1:A:1102:LEU:O	2.20	0.41
1:B:2161:TRP:CZ2	1:B:2165:GLN:HG3	2.55	0.41
1:D:4120:GLU:CG	1:D:4121:LYS:HG2	2.49	0.41
1:A:1192:ARG:NH2	1:A:1197:GLU:OE1	2.53	0.41
1:B:2031:ALA:HB1	1:B:2188:ARG:HB2	2.03	0.41
1:A:1195:ASN:HB3	1:A:1196:GLU:H	1.56	0.41
1:C:3177:TYR:CE1	1:C:3212:HIS:HB3	2.56	0.41
1:A:1120:GLU:C	1:A:1122:PRO:HD3	2.41	0.41
1:B:2203:GLU:O	1:B:2207:LYS:HG3	2.21	0.41
1:A:1223:THR:OG1	1:A:1224:ASN:N	2.52	0.41
1:A:1147:MET:HA	1:A:1151:GLU:OE1	2.21	0.41
1:C:3203:GLU:HA	1:C:3203:GLU:OE2	2.21	0.41
1:C:3147:MET:HG2	1:C:3151:GLU:HB3	2.02	0.40
1:D:4218:HIS:N	1:D:4218:HIS:ND1	2.69	0.40
1:D:4116:LEU:HA	1:D:4116:LEU:HD23	1.93	0.40
1:C:3200:ILE:HG23	1:C:3204:TYR:HD2	1.85	0.40
1:D:4240:GLU:CD	1:D:4245:LYS:HZ1	2.25	0.40
2:A:2301:UDP:O2A	1:B:2036:THR:OG1	2.39	0.40
1:A:1024:ILE:O	1:A:1126:PHE:N	2.50	0.40
1:B:2198:GLN:NE2	1:B:2198:GLN:N	2.70	0.40
1:A:1158:TRP:HE1	1:A:1162:MET:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3051:VAL:HG13	1:C:3126:PHE:HD2	1.85	0.40
1:C:3055:VAL:HG11	3:C:3302:3D1:N3	2.36	0.40
1:B:2091:ARG:O	1:B:2091:ARG:HG3	2.21	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	212/279 (76%)	193 (91%)	13 (6%)	6 (3%)	6 1
1	B	218/279 (78%)	195 (89%)	19 (9%)	4 (2%)	11 2
1	C	210/279 (75%)	185 (88%)	23 (11%)	2 (1%)	19 5
1	D	210/279 (75%)	191 (91%)	17 (8%)	2 (1%)	19 5
All	All	850/1116 (76%)	764 (90%)	72 (8%)	14 (2%)	11 2

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1168	GLN
1	A	1195	ASN
1	B	2113	ASN
1	B	2195	ASN
1	B	2226	ASP
1	C	3158	TRP
1	D	4113	ASN
1	D	4164	ASN
1	A	1231	VAL
1	A	1201	PRO
1	A	1230	GLU
1	A	1245	LYS

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Mol	Chain	Res	Type
1	C	3104	ARG
1	B	2128	ARG

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	195/255 (76%)	168 (86%)	27 (14%)	4	1
1	B	205/255 (80%)	171 (83%)	34 (17%)	3	0
1	C	197/255 (77%)	158 (80%)	39 (20%)	1	0
1	D	193/255 (76%)	158 (82%)	35 (18%)	2	0
All	All	790/1020 (78%)	655 (83%)	135 (17%)	2	0

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1020	ARG
1	A	1022	LYS
1	A	1042	LYS
1	A	1043	GLN
1	A	1046	GLU
1	A	1049	GLU
1	A	1051	VAL
1	A	1057	ARG
1	A	1083	GLN
1	A	1085	MET
1	A	1087	GLU
1	A	1093	SER
1	A	1112	LEU
1	A	1121	LYS
1	A	1160	ASP
1	A	1162	MET
1	A	1165	GLN
1	A	1195	ASN
1	A	1202	LEU

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Mol	Chain	Res	Type
1	A	1214	SER
1	A	1220	THR
1	A	1223	THR
1	A	1224	ASN
1	A	1226	ASP
1	A	1251	GLU
1	A	1255	GLU
1	A	1258	SER
1	B	2020	ARG
1	B	2021	ILE
1	B	2023	LYS
1	B	2040	ILE
1	B	2043	GLN
1	B	2046	GLU
1	B	2060	ASN
1	B	2072	THR
1	B	2074	SER
1	B	2076	LYS
1	B	2086	TYR
1	B	2087	GLU
1	B	2108	GLN
1	B	2115	LYS
1	B	2116	LEU
1	B	2121	LYS
1	B	2124	LEU
1	B	2132	SER
1	B	2162	MET
1	B	2169	SER
1	B	2172	LEU
1	B	2195	ASN
1	B	2196	GLU
1	B	2214	SER
1	B	2217	LEU
1	B	2220	THR
1	B	2222	LYS
1	B	2223	THR
1	B	2228	LEU
1	B	2229	GLN
1	B	2233	ILE
1	B	2240	GLU
1	B	2243	LYS
1	B	2244	ASP

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Mol	Chain	Res	Type
1	C	3020	ARG
1	C	3022	LYS
1	C	3023	LYS
1	C	3034	LYS
1	C	3043[A]	GLN
1	C	3043[B]	GLN
1	C	3051	VAL
1	C	3059	SER
1	C	3088	LYS
1	C	3098	THR
1	C	3104	ARG
1	C	3121	LYS
1	C	3124	LEU
1	C	3139	SER
1	C	3143	GLU
1	C	3147	MET
1	C	3149	GLU
1	C	3157	ASP
1	C	3162	MET
1	C	3176	ILE
1	C	3184	THR
1	C	3186	LEU
1	C	3189	ILE
1	C	3191	LEU
1	C	3195	ASN
1	C	3196	GLU
1	C	3205	LEU
1	C	3206	GLU
1	C	3207	LYS
1	C	3211	LYS
1	C	3219	ARG
1	C	3220	THR
1	C	3222	LYS
1	C	3224	ASN
1	C	3228	LEU
1	C	3231	VAL
1	C	3246	TYR
1	C	3254	LYS
1	C	3258	SER
1	D	4020	ARG
1	D	4022	LYS
1	D	4025	SER

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Mol	Chain	Res	Type
1	D	4026	ILE
1	D	4043	GLN
1	D	4045	SER
1	D	4051	VAL
1	D	4085	MET
1	D	4087	GLU
1	D	4104	ARG
1	D	4111	SER
1	D	4112	LEU
1	D	4120	GLU
1	D	4121	LYS
1	D	4132	SER
1	D	4139	SER
1	D	4144	SER
1	D	4146	SER
1	D	4147	MET
1	D	4149	GLU
1	D	4162	MET
1	D	4164	ASN
1	D	4170	LEU
1	D	4191	LEU
1	D	4206	GLU
1	D	4211	LYS
1	D	4217	LEU
1	D	4220	THR
1	D	4223	THR
1	D	4231	VAL
1	D	4240	GLU
1	D	4252	LYS
1	D	4257	LEU
1	D	4258	SER
1	D	4260	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1080	ASN
1	A	1156	GLN
1	A	1165	GLN
1	A	1195	ASN
1	A	1224	ASN
1	B	2077	ASN

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Mol	Chain	Res	Type
1	B	2140	ASN
1	B	2156	GLN
1	B	2164	ASN
1	B	2165	GLN
1	B	2195	ASN
1	C	3039	ASN
1	C	3164	ASN
1	C	3187	HIS
1	C	3218	HIS
1	C	3224	ASN
1	D	4039	ASN
1	D	4043	GLN
1	D	4164	ASN
1	D	4179	GLN
1	D	4195	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	UDP	A	1301	-	18,26,26	1.36	2 (11%)	26,40,40	1.41	4 (15%)
3	3D1	A	1302	-	16,20,20	2.22	2 (12%)	17,29,29	5.03	5 (29%)
2	UDP	A	2301	-	18,26,26	1.25	2 (11%)	26,40,40	1.15	1 (3%)
2	UDP	A	3301	-	18,26,26	1.24	2 (11%)	26,40,40	1.57	5 (19%)
2	UDP	A	4301	-	18,26,26	1.31	3 (16%)	26,40,40	1.52	4 (15%)
3	3D1	B	2302	-	16,20,20	2.18	2 (12%)	17,29,29	4.80	4 (23%)
3	3D1	C	3302	-	16,20,20	2.20	2 (12%)	17,29,29	5.14	4 (23%)
3	3D1	D	4302	-	16,20,20	2.28	3 (18%)	17,29,29	5.10	7 (41%)

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	UDP	A	1301	-	-	0/12/32/32	0/2/2/2
3	3D1	A	1302	-	-	0/2/18/18	0/3/3/3
2	UDP	A	2301	-	-	0/12/32/32	0/2/2/2
2	UDP	A	3301	-	-	0/12/32/32	0/2/2/2
2	UDP	A	4301	-	-	0/12/32/32	0/2/2/2
3	3D1	B	2302	-	-	0/2/18/18	0/3/3/3
3	3D1	C	3302	-	-	0/2/18/18	0/3/3/3
3	3D1	D	4302	-	-	0/2/18/18	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	UDP	PB-O3B	-3.43	1.42	1.54
2	A	2301	UDP	PB-O3B	-2.29	1.46	1.54
2	A	4301	UDP	PB-O3B	-2.20	1.46	1.54
2	A	4301	UDP	PA-O2A	-2.10	1.46	1.54
3	D	4302	3D1	C6-N6	-2.05	1.28	1.34
2	A	3301	UDP	PB-O3B	-2.04	1.47	1.54
2	A	2301	UDP	C4-N3	2.58	1.37	1.33
2	A	4301	UDP	C4-N3	2.73	1.38	1.33
2	A	1301	UDP	C4-N3	2.77	1.38	1.33
2	A	3301	UDP	C4-N3	2.83	1.38	1.33
3	B	2302	3D1	C2-N1	4.04	1.41	1.33
3	C	3302	3D1	C2-N1	4.33	1.42	1.33
3	A	1302	3D1	C2-N1	4.44	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4302	3D1	C2-N1	4.54	1.42	1.33
3	A	1302	3D1	C2-N3	6.54	1.43	1.32
3	C	3302	3D1	C2-N3	6.58	1.43	1.32
3	B	2302	3D1	C2-N3	6.80	1.44	1.32
3	D	4302	3D1	C2-N3	6.92	1.44	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3302	3D1	N3-C2-N1	-19.69	113.82	128.89
3	D	4302	3D1	N3-C2-N1	-19.12	114.26	128.89
3	A	1302	3D1	N3-C2-N1	-19.07	114.29	128.89
3	B	2302	3D1	N3-C2-N1	-18.15	115.00	128.89
3	A	1302	3D1	C4-C5-N7	-3.86	105.93	109.48
3	B	2302	3D1	C4-C5-N7	-3.68	106.10	109.48
2	A	3301	UDP	O3'-C3'-C4'	-3.44	100.72	111.05
3	A	1302	3D1	O4'-C1'-N9	-2.78	102.90	107.72
3	C	3302	3D1	C4-C5-N7	-2.61	107.08	109.48
2	A	1301	UDP	PA-O3A-PB	-2.60	123.94	132.67
3	D	4302	3D1	C4-C5-N7	-2.39	107.28	109.48
2	A	1301	UDP	C5'-C4'-C3'	-2.34	105.94	115.21
2	A	4301	UDP	C5'-C4'-C3'	-2.08	106.95	115.21
2	A	3301	UDP	O3'-C3'-C2'	-2.07	105.11	111.83
3	B	2302	3D1	O4'-C1'-N9	-2.05	104.16	107.72
2	A	3301	UDP	C2'-C3'-C4'	-2.02	98.46	102.61
3	D	4302	3D1	O4'-C1'-C2'	2.02	110.31	106.27
3	A	1302	3D1	N6-C6-N1	2.10	123.70	119.20
2	A	3301	UDP	O5'-PA-O1A	2.16	118.00	109.62
2	A	1301	UDP	C4-N3-C2	2.46	116.58	114.14
2	A	4301	UDP	O5'-PA-O1A	2.51	119.35	109.62
3	D	4302	3D1	C2'-C1'-N9	2.58	120.43	114.16
3	C	3302	3D1	N6-C6-N1	2.88	125.39	119.20
2	A	4301	UDP	O3B-PB-O1B	2.93	120.03	110.58
3	D	4302	3D1	C1'-N9-C4	3.13	132.46	127.16
2	A	2301	UDP	C4-N3-C2	3.25	117.37	114.14
3	D	4302	3D1	N6-C6-N1	3.42	126.54	119.20
2	A	1301	UDP	O3B-PB-O1B	3.64	122.31	110.58
2	A	4301	UDP	C4-N3-C2	4.73	118.82	114.14
2	A	3301	UDP	C4-N3-C2	4.93	119.02	114.14
3	A	1302	3D1	C2-N1-C6	5.33	128.29	118.77
3	D	4302	3D1	C2-N1-C6	5.60	128.78	118.77
3	C	3302	3D1	C2-N1-C6	5.72	128.99	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2302	3D1	C2-N1-C6	5.90	129.31	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	UDP	3	0
3	A	1302	3D1	1	0
2	A	2301	UDP	2	0
2	A	3301	UDP	3	0
2	A	4301	UDP	1	0
3	C	3302	3D1	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	217/279 (77%)	-0.12	2 (0%) 85 85	14, 28, 46, 62	0
1	B	225/279 (80%)	-0.22	1 (0%) 93 92	11, 24, 41, 60	0
1	C	216/279 (77%)	-0.19	0 100 100	13, 29, 47, 56	0
1	D	218/279 (78%)	-0.22	1 (0%) 91 91	13, 25, 44, 61	0
All	All	876/1116 (78%)	-0.19	4 (0%) 91 91	11, 27, 46, 62	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1166	PHE	2.6
1	D	4166	PHE	2.5
1	B	2020	ARG	2.4
1	A	1168	GLN	2.2

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^{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
3	3D1	B	2302	18/18	0.96	0.08	0.37	15,17,20,24	0
2	UDP	A	2301	25/25	0.98	0.08	0.20	9,23,28,39	0
3	3D1	C	3302	18/18	0.92	0.09	0.20	26,29,33,34	0
2	UDP	A	1301	25/25	0.98	0.08	-0.36	4,25,33,36	0
2	UDP	A	3301	25/25	0.98	0.07	-0.40	13,24,33,33	0
2	UDP	A	4301	25/25	0.99	0.07	-0.58	17,22,28,33	0
3	3D1	D	4302	18/18	0.98	0.07	-0.69	13,20,21,22	0
3	3D1	A	1302	18/18	0.97	0.07	-1.40	11,23,27,27	0

6.5 Other polymers

There are no such residues in this entry.