Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 12:42 PM EDT

PDB ID	:	4JX4
Title	:	Structure of the carboxyl transferase domain from Rhizobium etli pyruvate carboxylase
Authors	:	Lietzan, A.D.; St Maurice, M.
Deposited on	:	2013-03-27
Resolution	:	2.98 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

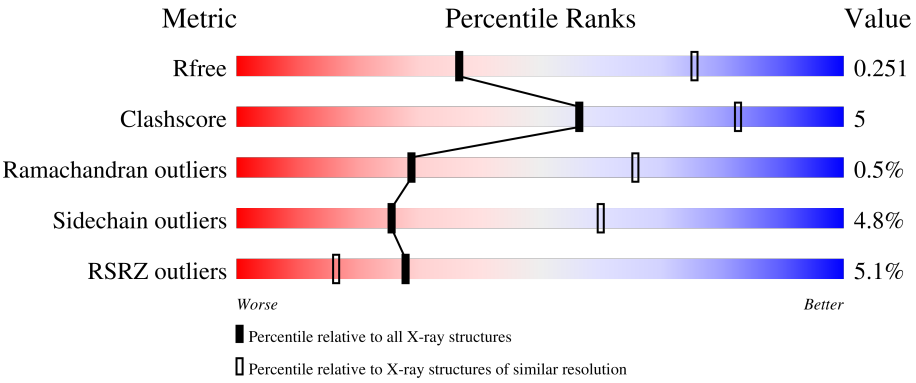
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

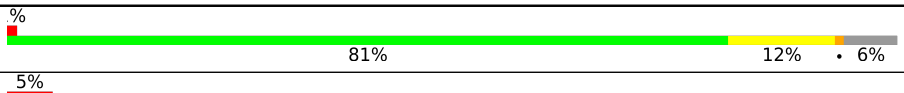
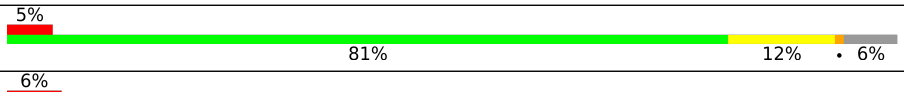
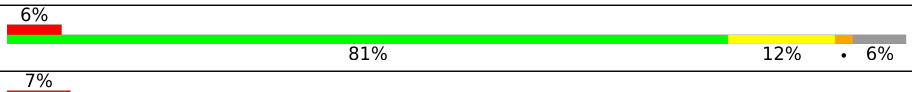
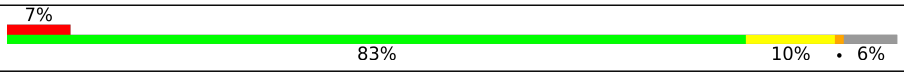
The reported resolution of this entry is 2.98 Å.

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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	632	
1	B	632	
1	C	632	
1	D	632	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17166 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	1	0
			4450	2831	740	856	23			
1	B	595	Total	C	N	O	S	0	0	0
			4268	2699	716	831	22			
1	C	595	Total	C	N	O	S	0	0	0
			4325	2730	730	843	22			
1	D	594	Total	C	N	O	S	0	0	0
			4117	2573	704	818	22			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	-	expression tag	UNP Q2K340
A	437	GLY	-	expression tag	UNP Q2K340
A	438	SER	-	expression tag	UNP Q2K340
A	439	SER	-	expression tag	UNP Q2K340
A	440	HIS	-	expression tag	UNP Q2K340
A	441	HIS	-	expression tag	UNP Q2K340
A	442	HIS	-	expression tag	UNP Q2K340
A	443	HIS	-	expression tag	UNP Q2K340
A	444	HIS	-	expression tag	UNP Q2K340
A	445	HIS	-	expression tag	UNP Q2K340
A	446	HIS	-	expression tag	UNP Q2K340
A	447	HIS	-	expression tag	UNP Q2K340
A	448	ASP	-	expression tag	UNP Q2K340
A	449	TYR	-	expression tag	UNP Q2K340
A	450	ASP	-	expression tag	UNP Q2K340
A	451	ILE	-	expression tag	UNP Q2K340
A	452	PRO	-	expression tag	UNP Q2K340
A	453	THR	-	expression tag	UNP Q2K340
A	454	SER	-	expression tag	UNP Q2K340
A	455	GLU	-	expression tag	UNP Q2K340
A	456	ASN	-	expression tag	UNP Q2K340

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	expression tag	UNP Q2K340
A	458	TYR	-	expression tag	UNP Q2K340
A	459	PHE	-	expression tag	UNP Q2K340
A	460	GLN	-	expression tag	UNP Q2K340
A	461	GLY	-	expression tag	UNP Q2K340
A	462	LEU	-	expression tag	UNP Q2K340
A	463	LEU	-	expression tag	UNP Q2K340
A	464	HIS	-	expression tag	UNP Q2K340
B	436	MET	-	expression tag	UNP Q2K340
B	437	GLY	-	expression tag	UNP Q2K340
B	438	SER	-	expression tag	UNP Q2K340
B	439	SER	-	expression tag	UNP Q2K340
B	440	HIS	-	expression tag	UNP Q2K340
B	441	HIS	-	expression tag	UNP Q2K340
B	442	HIS	-	expression tag	UNP Q2K340
B	443	HIS	-	expression tag	UNP Q2K340
B	444	HIS	-	expression tag	UNP Q2K340
B	445	HIS	-	expression tag	UNP Q2K340
B	446	HIS	-	expression tag	UNP Q2K340
B	447	HIS	-	expression tag	UNP Q2K340
B	448	ASP	-	expression tag	UNP Q2K340
B	449	TYR	-	expression tag	UNP Q2K340
B	450	ASP	-	expression tag	UNP Q2K340
B	451	ILE	-	expression tag	UNP Q2K340
B	452	PRO	-	expression tag	UNP Q2K340
B	453	THR	-	expression tag	UNP Q2K340
B	454	SER	-	expression tag	UNP Q2K340
B	455	GLU	-	expression tag	UNP Q2K340
B	456	ASN	-	expression tag	UNP Q2K340
B	457	LEU	-	expression tag	UNP Q2K340
B	458	TYR	-	expression tag	UNP Q2K340
B	459	PHE	-	expression tag	UNP Q2K340
B	460	GLN	-	expression tag	UNP Q2K340
B	461	GLY	-	expression tag	UNP Q2K340
B	462	LEU	-	expression tag	UNP Q2K340
B	463	LEU	-	expression tag	UNP Q2K340
B	464	HIS	-	expression tag	UNP Q2K340
C	436	MET	-	expression tag	UNP Q2K340
C	437	GLY	-	expression tag	UNP Q2K340
C	438	SER	-	expression tag	UNP Q2K340
C	439	SER	-	expression tag	UNP Q2K340
C	440	HIS	-	expression tag	UNP Q2K340

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	441	HIS	-	expression tag	UNP Q2K340
C	442	HIS	-	expression tag	UNP Q2K340
C	443	HIS	-	expression tag	UNP Q2K340
C	444	HIS	-	expression tag	UNP Q2K340
C	445	HIS	-	expression tag	UNP Q2K340
C	446	HIS	-	expression tag	UNP Q2K340
C	447	HIS	-	expression tag	UNP Q2K340
C	448	ASP	-	expression tag	UNP Q2K340
C	449	TYR	-	expression tag	UNP Q2K340
C	450	ASP	-	expression tag	UNP Q2K340
C	451	ILE	-	expression tag	UNP Q2K340
C	452	PRO	-	expression tag	UNP Q2K340
C	453	THR	-	expression tag	UNP Q2K340
C	454	SER	-	expression tag	UNP Q2K340
C	455	GLU	-	expression tag	UNP Q2K340
C	456	ASN	-	expression tag	UNP Q2K340
C	457	LEU	-	expression tag	UNP Q2K340
C	458	TYR	-	expression tag	UNP Q2K340
C	459	PHE	-	expression tag	UNP Q2K340
C	460	GLN	-	expression tag	UNP Q2K340
C	461	GLY	-	expression tag	UNP Q2K340
C	462	LEU	-	expression tag	UNP Q2K340
C	463	LEU	-	expression tag	UNP Q2K340
C	464	HIS	-	expression tag	UNP Q2K340
D	436	MET	-	expression tag	UNP Q2K340
D	437	GLY	-	expression tag	UNP Q2K340
D	438	SER	-	expression tag	UNP Q2K340
D	439	SER	-	expression tag	UNP Q2K340
D	440	HIS	-	expression tag	UNP Q2K340
D	441	HIS	-	expression tag	UNP Q2K340
D	442	HIS	-	expression tag	UNP Q2K340
D	443	HIS	-	expression tag	UNP Q2K340
D	444	HIS	-	expression tag	UNP Q2K340
D	445	HIS	-	expression tag	UNP Q2K340
D	446	HIS	-	expression tag	UNP Q2K340
D	447	HIS	-	expression tag	UNP Q2K340
D	448	ASP	-	expression tag	UNP Q2K340
D	449	TYR	-	expression tag	UNP Q2K340
D	450	ASP	-	expression tag	UNP Q2K340
D	451	ILE	-	expression tag	UNP Q2K340
D	452	PRO	-	expression tag	UNP Q2K340
D	453	THR	-	expression tag	UNP Q2K340

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	454	SER	-	expression tag	UNP Q2K340
D	455	GLU	-	expression tag	UNP Q2K340
D	456	ASN	-	expression tag	UNP Q2K340
D	457	LEU	-	expression tag	UNP Q2K340
D	458	TYR	-	expression tag	UNP Q2K340
D	459	PHE	-	expression tag	UNP Q2K340
D	460	GLN	-	expression tag	UNP Q2K340
D	461	GLY	-	expression tag	UNP Q2K340
D	462	LEU	-	expression tag	UNP Q2K340
D	463	LEU	-	expression tag	UNP Q2K340
D	464	HIS	-	expression tag	UNP Q2K340

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

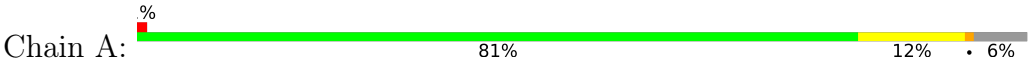
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

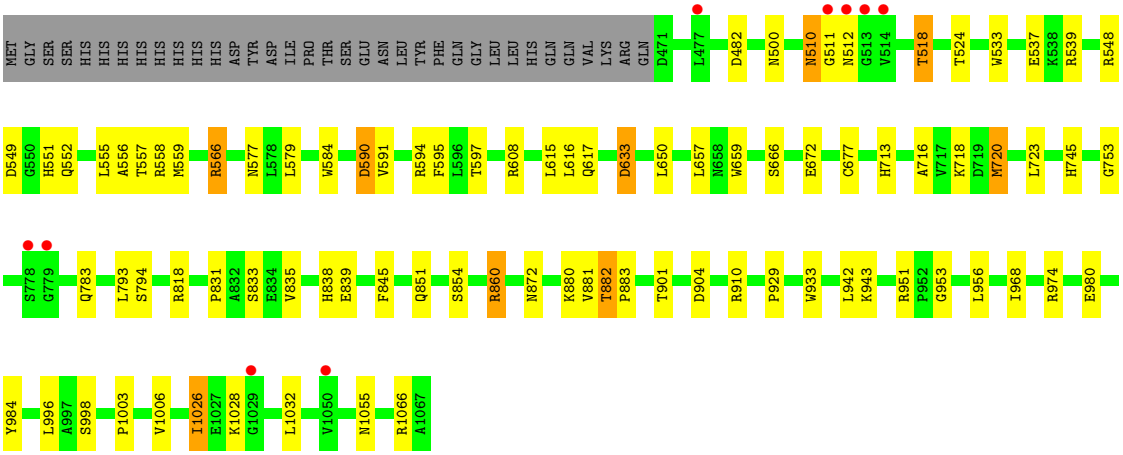
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pyruvate carboxylase

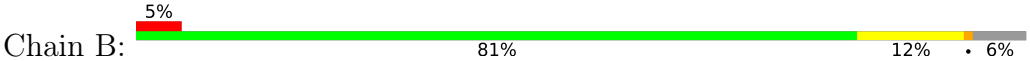
Chain A:

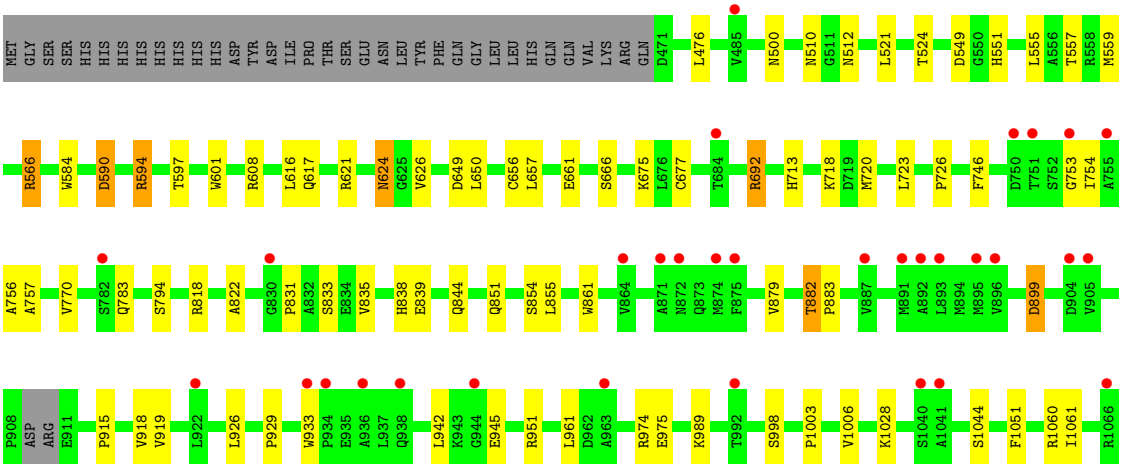




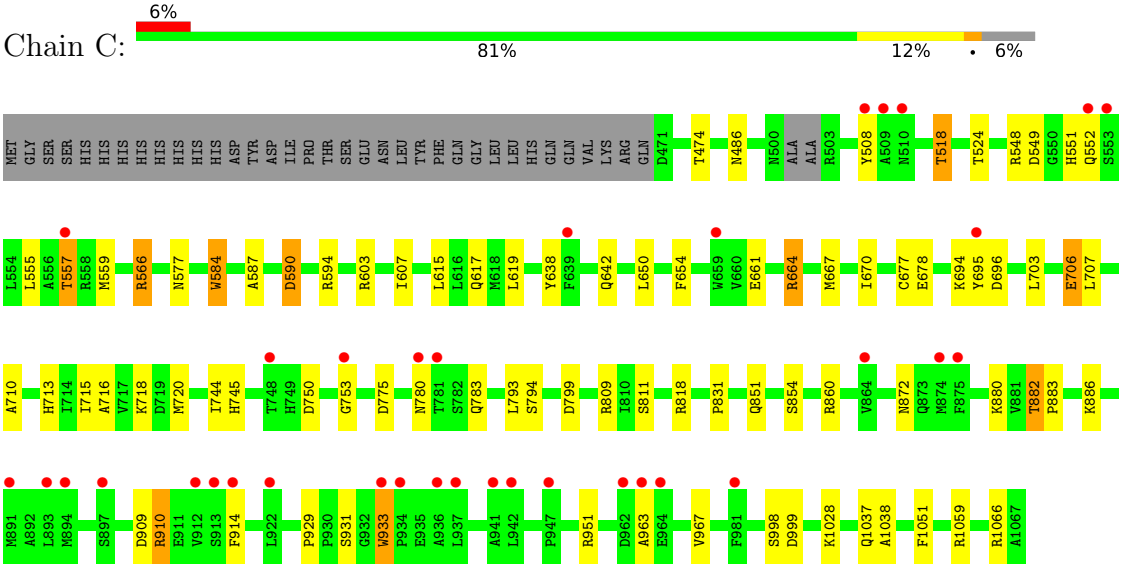
• Molecule 1: Pyruvate carboxylase

Chain B:

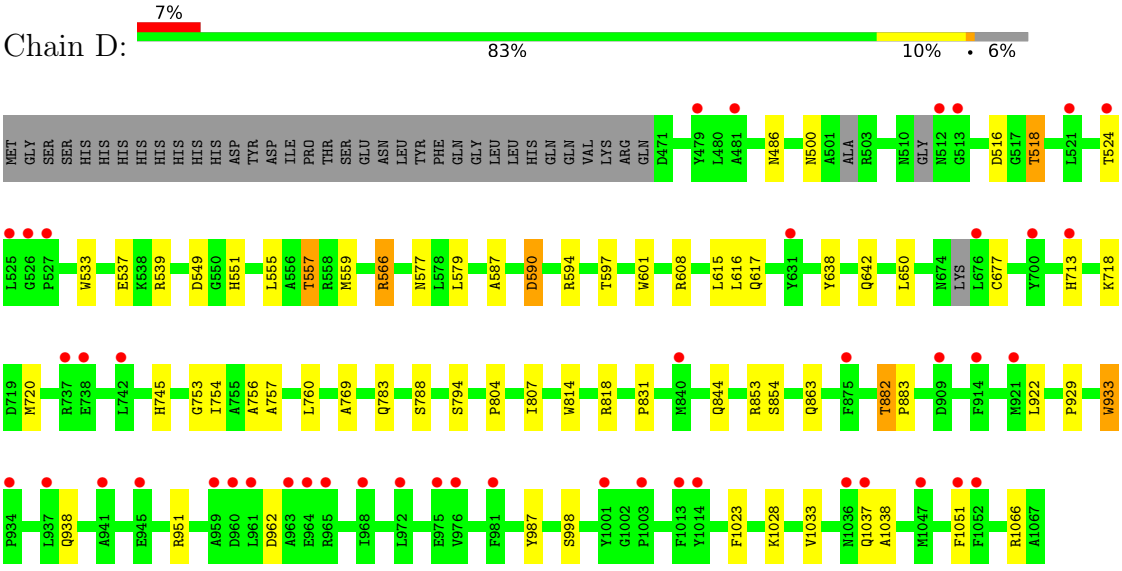




• Molecule 1: Pyruvate carboxylase



• Molecule 1: Pyruvate carboxylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.21Å 157.23Å 245.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.98 46.81 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.98) 99.8 (46.81-2.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.59 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.214 , 0.248 0.217 , 0.251	Depositor DCC
R_{free} test set	3471 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	79.0	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17166	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, KCX, CL

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	0.71	2/4536 (0.0%)	0.85	4/6189 (0.1%)
1	B	0.63	3/4349 (0.1%)	0.77	6/5957 (0.1%)
1	C	0.71	4/4409 (0.1%)	0.77	6/6026 (0.1%)
1	D	0.56	4/4193 (0.1%)	0.65	2/5743 (0.0%)
All	All	0.66	13/17487 (0.1%)	0.76	18/23915 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	659	TRP	CD2-CE2	6.58	1.49	1.41
1	D	814	TRP	CD2-CE2	5.91	1.48	1.41
1	C	933	TRP	CD2-CE2	5.62	1.48	1.41
1	D	601	TRP	CD2-CE2	5.28	1.47	1.41
1	B	601	TRP	CD2-CE2	5.25	1.47	1.41
1	B	861	TRP	CD2-CE2	5.25	1.47	1.41
1	C	678	GLU	CG-CD	5.20	1.59	1.51
1	D	533	TRP	CD2-CE2	5.10	1.47	1.41
1	D	933	TRP	CD2-CE2	5.06	1.47	1.41
1	B	899	ASP	CG-OD1	5.05	1.36	1.25
1	A	533	TRP	CD2-CE2	5.05	1.47	1.41
1	C	914	PHE	CE2-CZ	5.05	1.47	1.37
1	C	584	TRP	CD2-CE2	5.04	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	951	ARG	NE-CZ-NH2	16.46	128.53	120.30
1	B	594	ARG	NE-CZ-NH2	-15.09	112.76	120.30
1	B	594	ARG	NE-CZ-NH1	14.76	127.68	120.30
1	A	951	ARG	NE-CZ-NH1	-14.35	113.12	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	951	ARG	CD-NE-CZ	7.70	134.39	123.60
1	D	951	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	951	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	594	ARG	CD-NE-CZ	6.47	132.66	123.60
1	D	951	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	C	799	ASP	CB-CG-OD2	-6.23	112.70	118.30
1	C	951	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	C	951	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	692	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	C	696	ASP	CB-CG-OD1	5.26	123.03	118.30
1	B	951	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	707	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	C	799	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	860	ARG	NE-CZ-NH2	5.01	122.80	120.30

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	4450	0	4252	45	1
1	B	4268	0	3879	42	0
1	C	4325	0	3932	47	0
1	D	4117	0	3500	43	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
All	All	17166	0	15563	165	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (165) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:677:CYS:H	1:C:713:HIS:HD2	0.97	0.97
1:D:677:CYS:H	1:D:713:HIS:HD2	0.95	0.95
1:A:723:LEU:HD11	1:A:839:GLU:HG2	1.51	0.92
1:B:677:CYS:H	1:B:713:HIS:HD2	0.96	0.92
1:C:664:ARG:HH11	1:C:664:ARG:HG3	1.33	0.92
1:A:677:CYS:H	1:A:713:HIS:HD2	1.00	0.91
1:D:677:CYS:H	1:D:713:HIS:CD2	1.88	0.91
1:C:664:ARG:HH11	1:C:664:ARG:CG	1.83	0.90
1:B:677:CYS:H	1:B:713:HIS:CD2	1.89	0.89
1:C:677:CYS:H	1:C:713:HIS:CD2	1.90	0.84
1:A:677:CYS:H	1:A:713:HIS:CD2	1.92	0.83
1:D:590:ASP:OD1	1:D:594:ARG:NH2	2.17	0.78
1:A:590:ASP:OD1	1:A:594:ARG:NH2	2.18	0.77
1:B:677:CYS:N	1:B:713:HIS:HD2	1.81	0.74
1:A:723:LEU:CD1	1:A:839:GLU:HG2	2.17	0.74
1:B:656:CYS:O	1:B:879:VAL:HG13	1.88	0.73
1:C:664:ARG:HG3	1:C:664:ARG:NH1	2.02	0.73
1:B:915:PRO:HB2	1:B:918:VAL:HG23	1.71	0.73
1:C:590:ASP:OD1	1:C:594:ARG:NH2	2.21	0.72
1:C:1037:GLN:HB3	1:D:1051:PHE:HZ	1.54	0.72
1:C:1037:GLN:HB3	1:D:1051:PHE:CZ	2.25	0.70
1:B:590:ASP:OD1	1:B:594:ARG:NH2	2.24	0.70
1:C:619:LEU:HD11	1:C:654:PHE:CD2	2.29	0.67
1:A:677:CYS:N	1:A:713:HIS:HD2	1.84	0.66
1:C:677:CYS:N	1:C:713:HIS:HD2	1.83	0.65
1:B:1051:PHE:CE1	1:B:1060:ARG:HD2	2.33	0.63
1:A:953:GLY:HA2	1:A:956:LEU:HD12	1.81	0.63
1:D:677:CYS:N	1:D:713:HIS:HD2	1.80	0.61
1:A:482:ASP:OD2	1:A:1066:ARG:NH2	2.35	0.60
1:C:667:MET:HA	1:C:670:ILE:HD12	1.84	0.59
1:A:1032:LEU:HA	1:A:1055:ASN:HD21	1.67	0.59
1:C:694:LYS:HG2	1:C:695:TYR:CE2	2.38	0.59
1:C:549:ASP:HB3	1:C:783:GLN:HE22	1.68	0.58
1:A:753:GLY:HA3	1:A:831:PRO:HB3	1.85	0.58
1:C:566:ARG:CG	1:C:566:ARG:HH11	2.16	0.58
1:C:775:ASP:HB2	1:C:811:SER:OG	2.04	0.57
1:D:549:ASP:HB3	1:D:783:GLN:HE22	1.71	0.56
1:D:617:GLN:HG3	1:D:650:LEU:HB3	1.88	0.56
1:C:1051:PHE:CZ	1:D:1037:GLN:HB3	2.41	0.55
1:B:754:ILE:HG22	1:D:756:ALA:CB	2.36	0.55
1:C:716:ALA:HA	1:C:745:HIS:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:GLN:HG3	1:B:650:LEU:HD22	1.88	0.55
1:A:851:GLN:O	1:A:854:SER:HB2	2.07	0.54
1:A:566:ARG:CG	1:A:566:ARG:HH11	2.20	0.54
1:A:1026:ILE:HD13	1:A:1026:ILE:O	2.07	0.54
1:B:566:ARG:HH11	1:B:566:ARG:HG3	1.72	0.54
1:C:664:ARG:HH22	1:C:710:ALA:HA	1.73	0.54
1:A:566:ARG:HH11	1:A:566:ARG:HG3	1.74	0.53
1:B:1003:PRO:O	1:B:1006:VAL:HG22	2.08	0.53
1:A:901:THR:O	1:A:904:ASP:HB2	2.09	0.53
1:B:915:PRO:O	1:B:919:VAL:HG23	2.09	0.53
1:A:518:THR:HB	1:A:615:LEU:HG	1.92	0.52
1:B:566:ARG:HH11	1:B:566:ARG:CG	2.22	0.52
1:B:621:ARG:CB	1:B:624:ASN:OD1	2.57	0.52
1:D:566:ARG:HH11	1:D:566:ARG:CG	2.22	0.52
1:C:617:GLN:HG3	1:C:650:LEU:HB3	1.92	0.52
1:B:657:LEU:HA	1:B:879:VAL:CG1	2.40	0.52
1:C:566:ARG:CG	1:C:566:ARG:NH1	2.73	0.52
1:B:756:ALA:CB	1:D:754:ILE:HG22	2.40	0.52
1:B:851:GLN:O	1:B:854:SER:HB2	2.10	0.52
1:A:974:ARG:HH12	1:A:980:GLU:CD	2.13	0.51
1:A:633:ASP:N	1:A:633:ASP:OD1	2.44	0.51
1:C:1038:ALA:HB1	1:D:1038:ALA:HB1	1.94	0.50
1:A:617:GLN:HG3	1:A:650:LEU:HB3	1.93	0.50
1:D:551:HIS:CE1	1:D:559:MET:HB3	2.47	0.50
1:C:706:GLU:OE1	1:C:706:GLU:HA	2.12	0.50
1:C:566:ARG:HH11	1:C:566:ARG:HG3	1.76	0.50
1:D:566:ARG:HH11	1:D:566:ARG:HG3	1.76	0.50
1:B:726:PRO:HG2	1:D:760:LEU:HD13	1.94	0.49
1:D:590:ASP:HB2	1:D:987:TYR:CZ	2.48	0.49
1:C:909:ASP:O	1:C:910:ARG:C	2.51	0.48
1:B:746:PHE:HB3	1:B:770:VAL:HG12	1.95	0.48
1:C:664:ARG:CG	1:C:664:ARG:NH1	2.55	0.48
1:C:1051:PHE:HZ	1:D:1037:GLN:HB3	1.78	0.48
1:A:518:THR:HG21	1:A:579:LEU:HD12	1.95	0.48
1:A:537:GLU:HG3	1:A:539:ARG:HG2	1.94	0.48
1:C:851:GLN:O	1:C:854:SER:HB2	2.14	0.48
1:A:1032:LEU:HA	1:A:1055:ASN:ND2	2.29	0.48
1:A:555:LEU:HD11	1:A:818:ARG:HG3	1.95	0.47
1:B:549:ASP:HB3	1:B:783:GLN:HE22	1.78	0.47
1:B:974:ARG:NH1	1:B:975:GLU:O	2.45	0.47
1:D:518:THR:HB	1:D:615:LEU:HG	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:LEU:HD11	1:C:818:ARG:HG3	1.95	0.47
1:B:757:ALA:HB2	1:D:757:ALA:HA	1.95	0.47
1:D:555:LEU:HD11	1:D:818:ARG:HG3	1.96	0.47
1:B:608:ARG:HA	1:B:616:LEU:HD11	1.96	0.47
1:B:942:LEU:HD13	1:B:945:GLU:O	2.15	0.47
1:A:1003:PRO:O	1:A:1006:VAL:HG22	2.15	0.47
1:D:753:GLY:HA3	1:D:831:PRO:HB3	1.97	0.47
1:D:929:PRO:HD3	1:D:933:TRP:CZ2	2.49	0.47
1:A:566:ARG:CG	1:A:566:ARG:NH1	2.78	0.46
1:B:754:ILE:HG22	1:D:756:ALA:HB1	1.97	0.46
1:B:757:ALA:HA	1:D:757:ALA:HB2	1.96	0.46
1:A:617:GLN:HG3	1:A:650:LEU:HD22	1.97	0.46
1:B:753:GLY:HA3	1:B:831:PRO:HB3	1.96	0.46
1:A:591:VAL:HG13	1:A:595:PHE:HD2	1.81	0.46
1:C:664:ARG:HH11	1:C:664:ARG:HG2	1.77	0.46
1:D:844:GLN:O	1:D:844:GLN:CG	2.63	0.46
1:C:551:HIS:CE1	1:C:559:MET:HB3	2.50	0.46
1:C:557:THR:HG21	1:C:587:ALA:HB3	1.98	0.46
1:A:929:PRO:HD3	1:A:933:TRP:CZ2	2.51	0.46
1:A:872:ASN:HB2	1:A:880:LYS:HD3	1.97	0.45
1:D:486:ASN:HD21	1:D:1066:ARG:H	1.63	0.45
1:A:942:LEU:HA	1:A:942:LEU:HD23	1.68	0.45
1:D:566:ARG:CG	1:D:566:ARG:NH1	2.79	0.45
1:C:793:LEU:HA	1:C:793:LEU:HD23	1.74	0.45
1:C:753:GLY:HA3	1:C:831:PRO:HB3	1.98	0.45
1:A:720:MET:HG3	1:A:881:VAL:HG23	1.98	0.45
1:A:968:ILE:HD13	1:A:984:TYR:CD1	2.52	0.45
1:A:882:THR:HA	1:A:883:PRO:HA	1.73	0.44
1:B:566:ARG:CG	1:B:566:ARG:NH1	2.79	0.44
1:A:548:ARG:NH2	1:A:552:GLN:OE1	2.49	0.44
1:B:551:HIS:CE1	1:B:559:MET:HB3	2.52	0.44
1:C:664:ARG:NH2	1:C:710:ALA:HA	2.32	0.44
1:C:548:ARG:HD2	1:C:548:ARG:C	2.38	0.44
1:C:929:PRO:HD3	1:C:933:TRP:CZ2	2.53	0.44
1:A:793:LEU:HD23	1:A:793:LEU:HA	1.78	0.43
1:B:617:GLN:HG3	1:B:650:LEU:HB3	2.00	0.43
1:B:961:LEU:HD23	1:B:961:LEU:HA	1.79	0.43
1:B:555:LEU:HD11	1:B:818:ARG:HG3	2.01	0.43
1:C:486:ASN:HD21	1:C:1066:ARG:H	1.65	0.43
1:A:482:ASP:CG	1:A:1066:ARG:HH21	2.21	0.43
1:C:963:ALA:O	1:C:967:VAL:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:THR:HG21	1:D:587:ALA:HB3	2.01	0.43
1:B:942:LEU:HD23	1:B:942:LEU:HA	1.78	0.43
1:D:882:THR:HA	1:D:883:PRO:HA	1.76	0.43
1:C:715:ILE:O	1:C:744:ILE:HA	2.19	0.42
1:D:804:PRO:HA	1:D:807:ILE:HD12	2.00	0.42
1:A:551:HIS:CE1	1:A:559:MET:HB3	2.54	0.42
1:A:716:ALA:HA	1:A:745:HIS:O	2.20	0.42
1:C:750:ASP:C	1:C:780:ASN:O	2.58	0.42
1:B:833:SER:HB3	1:D:788:SER:N	2.33	0.42
1:B:882:THR:HA	1:B:883:PRO:HA	1.76	0.42
1:C:882:THR:HA	1:C:883:PRO:HA	1.75	0.42
1:D:608:ARG:HA	1:D:616:LEU:HD11	2.02	0.42
1:B:723:LEU:HD11	1:B:839:GLU:HG2	2.01	0.41
1:B:1061:ILE:HD13	1:B:1061:ILE:HA	1.76	0.41
1:C:474:THR:HG23	1:C:1059:ARG:NH2	2.34	0.41
1:C:548:ARG:NH2	1:C:552:GLN:OE1	2.53	0.41
1:B:929:PRO:HD3	1:B:933:TRP:CZ2	2.55	0.41
1:C:872:ASN:HB2	1:C:880:LYS:HD3	2.01	0.41
1:D:745:HIS:HA	1:D:769:ALA:O	2.20	0.41
1:D:853:ARG:HG3	1:D:854:SER:N	2.35	0.41
1:D:1023:PHE:CD1	1:D:1033:VAL:HG22	2.55	0.41
1:A:657:LEU:HD23	1:A:657:LEU:HA	1.90	0.41
1:B:835:VAL:HA	1:B:838:HIS:CE1	2.56	0.41
1:D:922:LEU:O	1:D:938:GLN:NE2	2.54	0.41
1:B:844:GLN:O	1:B:844:GLN:CG	2.67	0.41
1:A:549:ASP:HB3	1:A:783:GLN:HE22	1.85	0.41
1:A:556:ALA:O	1:A:558:ARG:HD3	2.21	0.41
1:A:833:SER:C	1:A:835:VAL:N	2.74	0.41
1:A:996:LEU:HD23	1:A:996:LEU:HA	1.94	0.41
1:C:638:TYR:O	1:C:642:GLN:HG2	2.21	0.41
1:D:486:ASN:ND2	1:D:1066:ARG:H	2.19	0.41
1:D:638:TYR:O	1:D:642:GLN:HG2	2.21	0.41
1:D:844:GLN:O	1:D:844:GLN:HG2	2.19	0.41
1:A:835:VAL:HA	1:A:838:HIS:CE1	2.56	0.41
1:C:518:THR:HB	1:C:615:LEU:HG	2.03	0.41
1:D:537:GLU:HG3	1:D:539:ARG:HG2	2.03	0.41
1:B:649:ASP:HA	1:B:675:LYS:HD2	2.01	0.40
1:C:603:ARG:O	1:C:607:ILE:HG13	2.22	0.40
1:A:608:ARG:HA	1:A:616:LEU:HD11	2.03	0.40
1:D:518:THR:HG21	1:D:579:LEU:HD12	2.04	0.40
1:B:521:LEU:HD23	1:B:521:LEU:HA	1.96	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:549:ASP:HB3	1:D:783:GLN:NE2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ASN:O	1:D:516:ASP:OD2[3_344]	1.76	0.44

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	595/632 (94%)	559 (94%)	31 (5%)	5 (1%)	19	55
1	B	590/632 (93%)	555 (94%)	31 (5%)	4 (1%)	22	58
1	C	590/632 (93%)	554 (94%)	35 (6%)	1 (0%)	47	80
1	D	585/632 (93%)	554 (95%)	29 (5%)	2 (0%)	41	74
All	All	2360/2528 (93%)	2222 (94%)	126 (5%)	12 (0%)	29	66

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1028	LYS
1	B	1028	LYS
1	C	1028	LYS
1	D	1028	LYS
1	A	500	ASN
1	D	500	ASN
1	B	512	ASN
1	A	510	ASN
1	A	511	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	845	PHE
1	B	500	ASN
1	B	822	ALA

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	443/519 (85%)	423 (96%)	20 (4%)	27	62
1	B	398/519 (77%)	376 (94%)	22 (6%)	21	55
1	C	406/519 (78%)	384 (95%)	22 (5%)	22	55
1	D	349/519 (67%)	336 (96%)	13 (4%)	34	68
All	All	1596/2076 (77%)	1519 (95%)	77 (5%)	25	60

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	510	ASN
1	A	518	THR
1	A	524	THR
1	A	557	THR
1	A	566	ARG
1	A	577	ASN
1	A	584	TRP
1	A	590	ASP
1	A	597	THR
1	A	633	ASP
1	A	666	SER
1	A	672	GLU
1	A	720	MET
1	A	794	SER
1	A	860	ARG
1	A	882	THR
1	A	910	ARG
1	A	943	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	998	SER
1	A	1026	ILE
1	B	476	LEU
1	B	510	ASN
1	B	524	THR
1	B	557	THR
1	B	566	ARG
1	B	584	TRP
1	B	590	ASP
1	B	597	THR
1	B	624	ASN
1	B	626	VAL
1	B	661	GLU
1	B	666	SER
1	B	692	ARG
1	B	720	MET
1	B	794	SER
1	B	855	LEU
1	B	882	THR
1	B	899	ASP
1	B	926	LEU
1	B	989	LYS
1	B	998	SER
1	B	1044	SER
1	C	508	TYR
1	C	518	THR
1	C	524	THR
1	C	557	THR
1	C	566	ARG
1	C	577	ASN
1	C	584	TRP
1	C	590	ASP
1	C	661	GLU
1	C	664	ARG
1	C	703	LEU
1	C	706	GLU
1	C	720	MET
1	C	794	SER
1	C	809	ARG
1	C	860	ARG
1	C	882	THR
1	C	886	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	910	ARG
1	C	931	SER
1	C	998	SER
1	C	999	ASP
1	D	518	THR
1	D	524	THR
1	D	557	THR
1	D	566	ARG
1	D	577	ASN
1	D	590	ASP
1	D	597	THR
1	D	720	MET
1	D	794	SER
1	D	863	GLN
1	D	882	THR
1	D	962	ASP
1	D	998	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	630	ASN
1	A	713	HIS
1	A	783	GLN
1	A	820	GLN
1	A	1055	ASN
1	B	486	ASN
1	B	630	ASN
1	B	713	HIS
1	B	783	GLN
1	C	486	ASN
1	C	577	ASN
1	C	630	ASN
1	C	713	HIS
1	C	783	GLN
1	C	873	GLN
1	D	486	ASN
1	D	630	ASN
1	D	713	HIS
1	D	783	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KCX	C	718	1,2	9,11,12	0.86	0	5,12,14	8.85	2 (40%)
1	KCX	D	718	1,2	9,11,12	0.72	0	5,12,14	3.00	1 (20%)
1	KCX	B	718	1,2	9,11,12	0.58	0	5,12,14	4.08	2 (40%)
1	KCX	A	718	1,2	9,11,12	0.46	0	5,12,14	4.39	3 (60%)

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
1	KCX	C	718	1,2	-	2/9/10/12	-
1	KCX	D	718	1,2	-	1/9/10/12	-
1	KCX	B	718	1,2	-	1/9/10/12	-
1	KCX	A	718	1,2	-	1/9/10/12	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	718	KCX	CE-NZ-CX	18.00	150.78	121.89
1	A	718	KCX	CE-NZ-CX	8.76	135.95	121.89
1	B	718	KCX	CE-NZ-CX	8.46	135.47	121.89
1	C	718	KCX	OQ1-CX-NZ	-8.12	112.38	124.96
1	D	718	KCX	CE-NZ-CX	6.41	132.17	121.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	718	KCX	OQ1-CX-NZ	3.16	129.86	124.96
1	A	718	KCX	CD-CE-NZ	3.08	121.02	112.21
1	B	718	KCX	CD-CE-NZ	2.88	120.44	112.21

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	718	KCX	O-C-CA-CB
1	B	718	KCX	O-C-CA-CB
1	C	718	KCX	O-C-CA-CB
1	D	718	KCX	O-C-CA-CB
1	C	718	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	596/632 (94%)	-0.15	9 (1%) 73 54	43, 65, 95, 159	19 (3%)
1	B	594/632 (93%)	0.10	33 (5%) 24 13	51, 89, 157, 239	13 (2%)
1	C	594/632 (93%)	0.24	35 (5%) 22 12	44, 91, 166, 216	20 (3%)
1	D	593/632 (93%)	0.39	45 (7%) 13 6	75, 111, 155, 195	12 (2%)
All	All	2377/2528 (94%)	0.14	122 (5%) 28 16	43, 88, 154, 239	64 (2%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	510	ASN	5.9
1	D	941	ALA	5.0
1	D	968	ILE	5.0
1	B	874	MET	5.0
1	D	713	HIS	4.9
1	B	893	LEU	4.7
1	B	875	PHE	4.3
1	D	964	GLU	4.2
1	D	963	ALA	4.1
1	C	914	PHE	4.0
1	A	511	GLY	4.0
1	D	700	TYR	3.9
1	C	962	ASP	3.8
1	D	676	LEU	3.7
1	C	963	ALA	3.7
1	B	895	MET	3.7
1	C	933	TRP	3.7
1	D	525	LEU	3.6
1	D	875	PHE	3.6
1	C	937	LEU	3.6
1	B	1067	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	922	LEU	3.4
1	C	941	ALA	3.4
1	B	750	ASP	3.4
1	B	905	VAL	3.4
1	C	897	SER	3.4
1	D	1001	TYR	3.4
1	D	631	TYR	3.3
1	D	512	ASN	3.2
1	B	891	MET	3.2
1	D	961	LEU	3.1
1	C	934	PRO	3.1
1	C	912	VAL	3.1
1	C	913	SER	3.1
1	C	875	PHE	3.0
1	C	942	LEU	3.0
1	D	1014	TYR	3.0
1	C	922	LEU	3.0
1	D	1052	PHE	3.0
1	B	485	VAL	2.9
1	C	508	TYR	2.9
1	B	684	THR	2.8
1	D	479	TYR	2.8
1	B	896	VAL	2.8
1	C	553	SER	2.8
1	B	864	VAL	2.8
1	C	893	LEU	2.8
1	A	1029	GLY	2.7
1	C	780	ASN	2.7
1	B	892	ALA	2.7
1	B	1041	ALA	2.7
1	B	963	ALA	2.7
1	D	481	ALA	2.7
1	B	872	ASN	2.7
1	D	981	PHE	2.7
1	A	513	GLY	2.7
1	D	738	GLU	2.6
1	A	778	SER	2.6
1	D	972	LEU	2.6
1	D	1003	PRO	2.6
1	C	936	ALA	2.5
1	C	509	ALA	2.5
1	B	753	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	695	TYR	2.5
1	B	751	THR	2.5
1	D	976	VAL	2.5
1	B	830	GLY	2.5
1	D	521	LEU	2.5
1	D	742	LEU	2.5
1	B	944	GLY	2.5
1	D	527	PRO	2.5
1	D	934	PRO	2.5
1	C	874	MET	2.5
1	A	512	ASN	2.4
1	D	1013	PHE	2.4
1	B	992	THR	2.4
1	D	526	GLY	2.4
1	B	934	PRO	2.4
1	C	947	PRO	2.4
1	D	909	ASP	2.3
1	D	737	ARG	2.3
1	C	659	TRP	2.3
1	C	864	VAL	2.3
1	C	894	MET	2.3
1	D	965	ARG	2.3
1	B	887	VAL	2.3
1	B	904	ASP	2.3
1	D	513	GLY	2.3
1	D	921	MET	2.3
1	D	937	LEU	2.2
1	B	936	ALA	2.2
1	C	753	GLY	2.2
1	B	871	ALA	2.2
1	D	959	ALA	2.2
1	B	1066	ARG	2.2
1	C	639	PHE	2.2
1	D	1036	ASN	2.2
1	B	933	TRP	2.2
1	D	960	ASP	2.2
1	B	755	ALA	2.2
1	D	524	THR	2.1
1	A	1050	VAL	2.1
1	C	781	THR	2.1
1	D	975	GLU	2.1
1	A	514	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	779	GLY	2.1
1	D	914	PHE	2.1
1	C	964	GLU	2.1
1	D	1051	PHE	2.1
1	D	945	GLU	2.1
1	C	552	GLN	2.1
1	D	1037	GLN	2.1
1	B	782	SER	2.0
1	B	1040	SER	2.0
1	C	748	THR	2.0
1	C	891	MET	2.0
1	D	840	MET	2.0
1	A	477	LEU	2.0
1	D	1047	MET	2.0
1	B	938	GLN	2.0
1	C	981	PHE	2.0
1	C	557	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
1	KCX	D	718	12/13	0.93	0.31	93,96,98,99	0
1	KCX	C	718	12/13	0.95	0.26	72,75,85,86	0
1	KCX	A	718	12/13	0.96	0.25	51,54,60,66	0
1	KCX	B	718	12/13	0.96	0.23	78,81,91,93	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	CL	A	1102	1/1	0.93	0.10	77,77,77,77	0
3	CL	C	1102	1/1	0.96	0.06	86,86,86,86	0
2	ZN	B	1101	1/1	0.98	0.17	77,77,77,77	0
2	ZN	D	1101	1/1	0.99	0.21	94,94,94,94	0
2	ZN	A	1101	1/1	0.99	0.21	58,58,58,58	0
2	ZN	C	1101	1/1	0.99	0.25	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.