Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 12:51 AM EDT

PDB ID	:	5TIG
Title	:	CRYSTAL STRUCTURE OF 4-OXALOCROTONATE TAUTOMERASE INACTIVATED BY BrHPD
Authors	:	Zhang, Y.; Li, W.; Stack, T.
Deposited on	:	2016-10-02
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

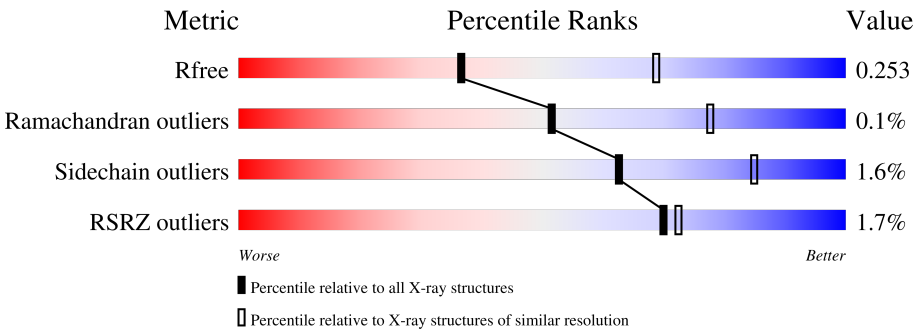
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	62	2%, 94%, 6%
1	B	62	85%, 8%, 6%
1	C	62	87%, 6%, •, 5%
1	D	62	2%, 92%, •, •, •
1	E	62	94%, •, •
1	F	62	3%, 94%, •, •

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Mol	Chain	Length	Quality of chain
1	G	62	2%, 92%
1	H	62	95%
1	I	62	5%, 90%, 5%
1	J	62	2%, 89%, 8%
1	K	62	2%, 90%, 6%
1	L	62	85%, 5%, 6%
1	M	62	3%, 92%, 5%
1	N	62	2%, 90%, 5%
1	O	62	90%, 5%, 5%
1	P	62	84%, 6%, 6%
1	Q	62	3%, 90%, 5%, 5%
1	R	62	2%, 87%, 8%, 5%
1	S	62	6%, 89%, 5%
1	T	62	87%, 5%, 8%
1	U	62	85%, 6%, 8%
1	V	62	87%, 8%
1	W	62	3%, 87%, 6%, 5%
1	X	62	89%, 5%, 5%
1	Y	62	5%, 90%, 5%
1	Z	62	2%, 90%, 5%
1	a	62	89%, 8%
1	b	62	89%, 6%, 5%
1	c	62	5%, 89%, 5%, 5%
1	d	62	3%, 90%, 5%, 5%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	7DH	O	101	-	X	-	-
2	7DH	R	101	-	X	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13661 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 2-hydroxymuconate tautomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	62	477	296	89	91	1	0	0	0
			Total	C	N	O	S			
1	B	58	447	278	81	87	1	0	1	0
			Total	C	N	O	S			
1	C	59	448	279	80	88	1	0	0	0
			Total	C	N	O	S			
1	D	60	455	284	81	89	1	0	0	0
			Total	C	N	O	S			
1	E	60	455	284	81	89	1	0	0	0
			Total	C	N	O	S			
1	F	60	455	284	81	89	1	0	0	0
			Total	C	N	O	S			
1	G	60	455	284	81	89	1	0	0	0
			Total	C	N	O	S			
1	H	60	455	284	81	89	1	0	0	0
			Total	C	N	O	S			
1	I	60	455	284	81	89	1	0	0	0
			Total	C	N	O	S			
1	J	60	455	284	81	89	1	0	0	0
			Total	C	N	O	S			
1	K	60	455	284	81	89	1	0	0	0
			Total	C	N	O	S			
1	L	58	439	273	78	87	1	0	0	0
			Total	C	N	O	S			
1	M	60	455	284	81	89	1	0	0	0
			Total	C	N	O	S			
1	N	59	448	279	80	88	1	0	0	0
			Total	C	N	O	S			
1	O	59	448	279	80	88	1	0	0	0
			Total	C	N	O	S			
1	P	58	439	273	78	87	1	0	0	0

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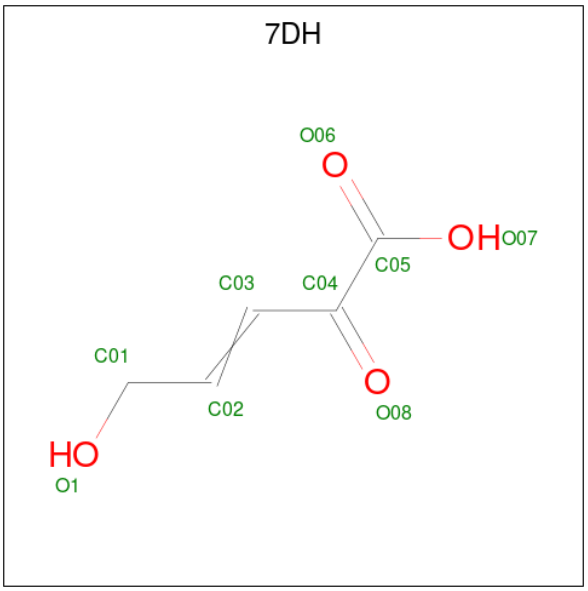
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	59	456	284	83	88	1	0	1	0
			Total	C	N	O	S			
1	R	59	448	279	80	88	1	0	0	0
			Total	C	N	O	S			
1	S	60	455	284	81	89	1	0	0	0
			Total	C	N	O	S			
1	T	57	433	270	77	85	1	0	0	0
			Total	C	N	O	S			
1	U	57	433	270	77	85	1	0	0	0
			Total	C	N	O	S			
1	V	57	433	270	77	85	1	0	0	0
			Total	C	N	O	S			
1	W	59	448	279	80	88	1	0	0	0
			Total	C	N	O	S			
1	X	59	448	279	80	88	1	0	0	0
			Total	C	N	O	S			
1	Y	59	448	279	80	88	1	0	0	0
			Total	C	N	O	S			
1	Z	59	448	279	80	88	1	0	0	0
			Total	C	N	O	S			
1	a	57	433	270	77	85	1	0	0	0
			Total	C	N	O	S			
1	b	59	448	279	80	88	1	0	0	0
			Total	C	N	O	S			
1	c	59	448	279	80	88	1	0	0	0
			Total	C	N	O	S			
1	d	59	448	279	80	88	1	0	0	0

- Molecule 2 is (3E)-5-hydroxy-2-oxopent-3-enoic acid (three-letter code: 7DH) (formula: $C_5H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	8	5	3	0	0
2	B	1	8	5	3	0	0
2	C	1	8	5	3	0	0
2	F	1	8	5	3	0	0
2	G	1	8	5	3	0	0
2	L	1	8	5	3	0	0
2	O	1	8	5	3	0	0
2	P	1	8	5	3	0	0
2	R	1	8	5	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	7	7	7	0	0
3	B	7	7	7	0	0
3	C	3	3	3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	4	Total O 4 4	0	0
3	E	5	Total O 5 5	0	0
3	F	7	Total O 7 7	0	0
3	G	1	Total O 1 1	0	0
3	H	3	Total O 3 3	0	0
3	I	4	Total O 4 4	0	0
3	J	6	Total O 6 6	0	0
3	K	3	Total O 3 3	0	0
3	L	5	Total O 5 5	0	0
3	M	4	Total O 4 4	0	0
3	N	1	Total O 1 1	0	0
3	O	8	Total O 8 8	0	0
3	P	6	Total O 6 6	0	0
3	Q	2	Total O 2 2	0	0
3	R	5	Total O 5 5	0	0
3	S	2	Total O 2 2	0	0
3	T	2	Total O 2 2	0	0
3	U	4	Total O 4 4	0	0
3	V	1	Total O 1 1	0	0
3	W	4	Total O 4 4	0	0
3	X	4	Total O 4 4	0	0

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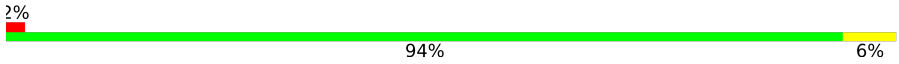
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	Y	1	1	1	0	0
			Total	O		
3	Z	3	3	3	0	0
			Total	O		
3	a	6	6	6	0	0
			Total	O		
3	b	7	7	7	0	0
			Total	O		
3	c	2	2	2	0	0
			Total	O		
3	d	4	4	4	0	0

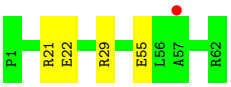
3 Residue-property plots (i)

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: 2-hydroxymuconate tautomerase

Chain A:





• Molecule 1: 2-hydroxymuconate tautomerase

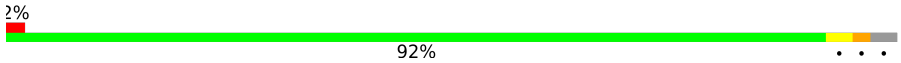
Chain B:

• Molecule 1: 2-hydroxymuconate tautomerase

Chain C:

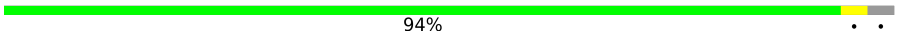
• Molecule 1: 2-hydroxymuconate tautomerase

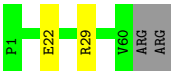
Chain D:



• Molecule 1: 2-hydroxymuconate tautomerase

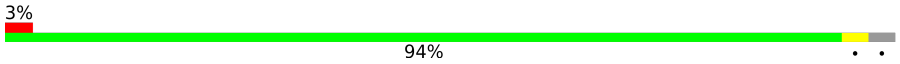
Chain E:

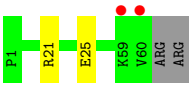




• Molecule 1: 2-hydroxymuconate tautomerase

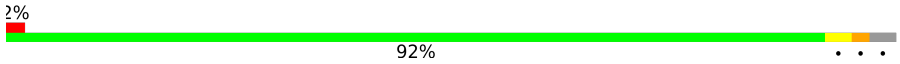
Chain F:

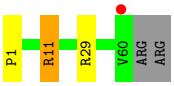




• Molecule 1: 2-hydroxymuconate tautomerase

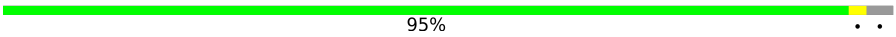
Chain G:

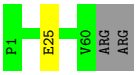




• Molecule 1: 2-hydroxymuconate tautomerase

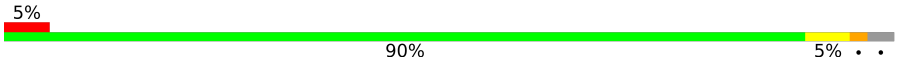
Chain H:





• Molecule 1: 2-hydroxymuconate tautomerase

Chain I:

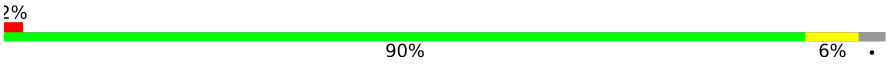


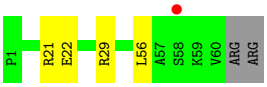
• Molecule 1: 2-hydroxymuconate tautomerase

Chain J:

• Molecule 1: 2-hydroxymuconate tautomerase

Chain K:



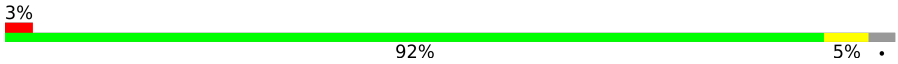


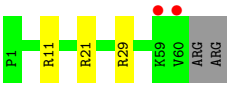
• Molecule 1: 2-hydroxymuconate tautomerase

Chain L:

• Molecule 1: 2-hydroxymuconate tautomerase

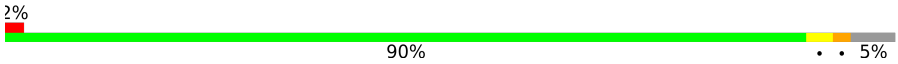
Chain M:

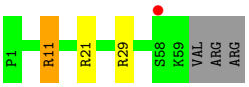




- Molecule 1: 2-hydroxymuconate tautomerase

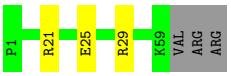
Chain N:





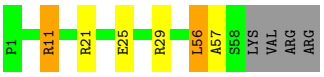
- Molecule 1: 2-hydroxymuconate tautomerase

Chain O:



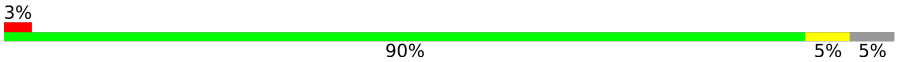
- Molecule 1: 2-hydroxymuconate tautomerase

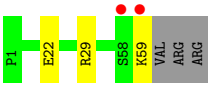
Chain P:



- Molecule 1: 2-hydroxymuconate tautomerase

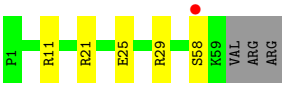
Chain Q:





- Molecule 1: 2-hydroxymuconate tautomerase

Chain R:

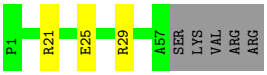


- Molecule 1: 2-hydroxymuconate tautomerase

Chain S:

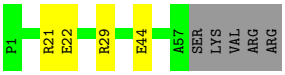
• Molecule 1: 2-hydroxymuconate tautomerase

Chain T:



• Molecule 1: 2-hydroxymuconate tautomerase

Chain U:

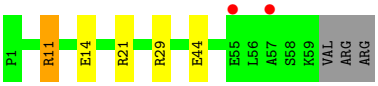


• Molecule 1: 2-hydroxymuconate tautomerase

Chain V:

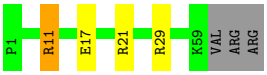
• Molecule 1: 2-hydroxymuconate tautomerase

Chain W:



• Molecule 1: 2-hydroxymuconate tautomerase

Chain X:

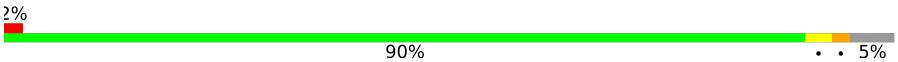


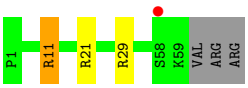
• Molecule 1: 2-hydroxymuconate tautomerase

Chain Y:

• Molecule 1: 2-hydroxymuconate tautomerase

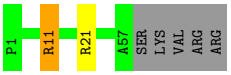
Chain Z:





• Molecule 1: 2-hydroxymuconate tautomerase

Chain a:

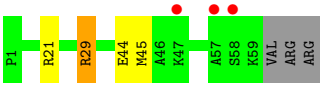


• Molecule 1: 2-hydroxymuconate tautomerase

Chain b:

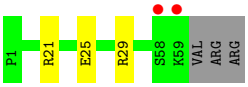
• Molecule 1: 2-hydroxymuconate tautomerase

Chain c:



• Molecule 1: 2-hydroxymuconate tautomerase

Chain d:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.75Å 90.12Å 171.44Å 90.00° 96.85° 90.00°	Depositor
Resolution (Å)	48.06 – 2.70 48.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.06-2.70) 99.8 (48.02-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.254 0.222 , 0.253	Depositor DCC
R_{free} test set	2666 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13661	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: 7DH

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	0.83	2/481 (0.4%)	1.44	6/644 (0.9%)
1	B	0.65	1/454 (0.2%)	0.99	6/609 (1.0%)
1	C	0.67	0/452	1.01	6/606 (1.0%)
1	D	0.67	0/459	1.01	6/616 (1.0%)
1	E	0.77	1/459 (0.2%)	0.91	2/616 (0.3%)
1	F	0.71	1/459 (0.2%)	0.96	4/616 (0.6%)
1	G	0.57	0/459	1.00	3/616 (0.5%)
1	H	0.65	0/459	0.75	1/616 (0.2%)
1	I	0.67	0/459	1.27	6/616 (1.0%)
1	J	0.80	1/459 (0.2%)	1.31	8/616 (1.3%)
1	K	0.69	1/459 (0.2%)	1.05	6/616 (1.0%)
1	L	0.85	3/443 (0.7%)	1.13	9/595 (1.5%)
1	M	0.62	0/459	1.10	5/616 (0.8%)
1	N	0.61	0/452	1.28	5/606 (0.8%)
1	O	0.75	1/452 (0.2%)	0.99	4/606 (0.7%)
1	P	0.84	2/443 (0.5%)	1.17	9/595 (1.5%)
1	Q	0.71	1/463 (0.2%)	1.00	4/620 (0.6%)
1	R	0.66	0/452	0.92	5/606 (0.8%)
1	S	0.87	3/459 (0.7%)	1.60	12/616 (1.9%)
1	T	0.83	2/437 (0.5%)	0.93	3/587 (0.5%)
1	U	1.17	4/437 (0.9%)	1.01	4/587 (0.7%)
1	V	0.60	0/437	1.00	4/587 (0.7%)
1	W	0.70	0/452	1.37	7/606 (1.2%)
1	X	0.59	0/452	1.11	8/606 (1.3%)
1	Y	0.64	0/452	2.66	6/606 (1.0%)
1	Z	0.69	0/452	1.05	5/606 (0.8%)
1	a	0.62	0/437	1.30	6/587 (1.0%)
1	b	0.63	1/452 (0.2%)	0.97	5/606 (0.8%)
1	c	0.92	2/452 (0.4%)	1.25	10/606 (1.7%)
1	d	0.63	1/452 (0.2%)	0.91	4/606 (0.7%)
All	All	0.73	27/13594 (0.2%)	1.20	169/18237 (0.9%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	44	GLU	CD-OE1	-14.25	1.09	1.25
1	U	44	GLU	CD-OE2	-12.58	1.11	1.25
1	T	25	GLU	CG-CD	9.89	1.66	1.51
1	P	25	GLU	CD-OE2	-9.19	1.15	1.25
1	c	44	GLU	CD-OE1	-9.03	1.15	1.25
1	S	25	GLU	CD-OE1	-8.98	1.15	1.25
1	A	22	GLU	CD-OE1	8.59	1.35	1.25
1	E	22	GLU	CD-OE1	8.48	1.34	1.25
1	U	22	GLU	CD-OE1	8.45	1.34	1.25
1	T	25	GLU	CD-OE2	8.15	1.34	1.25
1	L	55	GLU	CD-OE1	-7.34	1.17	1.25
1	K	22	GLU	CD-OE2	-5.95	1.19	1.25
1	L	55	GLU	CG-CD	-5.85	1.43	1.51
1	S	25	GLU	CB-CG	5.74	1.63	1.52
1	S	25	GLU	CG-CD	5.74	1.60	1.51
1	Q	22	GLU	CD-OE2	-5.71	1.19	1.25
1	c	44	GLU	CD-OE2	5.67	1.31	1.25
1	J	58	SER	CB-OG	-5.55	1.35	1.42
1	L	25	GLU	CD-OE1	5.40	1.31	1.25
1	U	44	GLU	CG-CD	-5.38	1.43	1.51
1	P	25	GLU	CB-CG	5.25	1.62	1.52
1	d	25	GLU	CD-OE1	5.10	1.31	1.25
1	O	25	GLU	CD-OE1	5.08	1.31	1.25
1	b	25	GLU	CD-OE1	5.06	1.31	1.25
1	B	25	GLU	CD-OE1	5.05	1.31	1.25
1	A	55	GLU	CD-OE2	5.02	1.31	1.25
1	F	25	GLU	CD-OE1	5.02	1.31	1.25

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	29	ARG	NE-CZ-NH1	-43.11	98.75	120.30
1	Y	29	ARG	NE-CZ-NH2	41.00	140.80	120.30
1	S	29	ARG	NE-CZ-NH1	-19.90	110.35	120.30
1	A	29	ARG	NE-CZ-NH2	18.65	129.62	120.30
1	A	29	ARG	NE-CZ-NH1	-18.00	111.30	120.30
1	W	11	ARG	NE-CZ-NH1	17.98	129.29	120.30
1	N	11	ARG	NE-CZ-NH2	17.92	129.26	120.30
1	I	11	ARG	NE-CZ-NH1	17.48	129.04	120.30
1	N	11	ARG	NE-CZ-NH1	-16.69	111.95	120.30
1	a	11	ARG	NE-CZ-NH1	16.62	128.61	120.30
1	Y	29	ARG	CD-NE-CZ	13.59	142.63	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	25	GLU	OE1-CD-OE2	-12.67	108.09	123.30
1	J	11	ARG	NE-CZ-NH1	-12.50	114.05	120.30
1	S	56	LEU	CB-CG-CD2	12.32	131.95	111.00
1	J	11	ARG	NE-CZ-NH2	12.26	126.43	120.30
1	M	29	ARG	NE-CZ-NH1	12.17	126.39	120.30
1	D	11	ARG	NE-CZ-NH1	12.05	126.33	120.30
1	S	29	ARG	NE-CZ-NH2	11.95	126.27	120.30
1	G	11	ARG	NE-CZ-NH1	11.81	126.20	120.30
1	Y	21	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	T	25	GLU	OE1-CD-OE2	-11.37	109.66	123.30
1	Z	11	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	X	11	ARG	NE-CZ-NH1	11.25	125.92	120.30
1	W	11	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	V	11	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	I	11	ARG	NE-CZ-NH2	-11.07	114.76	120.30
1	c	44	GLU	CG-CD-OE1	-10.43	97.43	118.30
1	a	11	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	O	21	ARG	NE-CZ-NH1	-10.22	115.19	120.30
1	A	29	ARG	CD-NE-CZ	9.85	137.39	123.60
1	P	56	LEU	N-CA-C	9.78	137.41	111.00
1	U	44	GLU	OE1-CD-OE2	-9.73	111.63	123.30
1	K	22	GLU	OE1-CD-OE2	-9.71	111.65	123.30
1	d	21	ARG	NE-CZ-NH1	-9.63	115.48	120.30
1	a	11	ARG	CD-NE-CZ	9.54	136.95	123.60
1	Q	22	GLU	OE1-CD-OE2	-9.51	111.89	123.30
1	J	21	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	C	21	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	W	21	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	b	21	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	S	21	ARG	NE-CZ-NH1	9.29	124.95	120.30
1	W	21	ARG	NE-CZ-NH2	-9.27	115.66	120.30
1	I	11	ARG	CD-NE-CZ	9.20	136.48	123.60
1	a	21	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	L	55	GLU	CG-CD-OE1	-9.10	100.11	118.30
1	a	21	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	S	21	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	C	21	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	M	11	ARG	CG-CD-NE	-8.96	92.98	111.80
1	A	21	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	P	11	ARG	NE-CZ-NH1	-8.85	115.88	120.30
1	Y	21	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	c	44	GLU	CG-CD-OE2	8.80	135.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	21	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	K	21	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	W	11	ARG	CD-NE-CZ	8.77	135.88	123.60
1	c	21	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	F	21	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	K	56	LEU	CB-CG-CD1	-8.72	96.18	111.00
1	F	21	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	b	21	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	J	21	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	B	21	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	c	21	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	X	21	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	I	21	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	D	11	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	L	21	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	X	21	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	J	11	ARG	CD-NE-CZ	8.38	135.33	123.60
1	G	11	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	P	25	GLU	CG-CD-OE1	8.37	135.03	118.30
1	L	21	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	V	11	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	R	11	ARG	CA-CB-CG	-8.30	95.13	113.40
1	X	11	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	Z	11	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	P	25	GLU	OE1-CD-OE2	-7.87	113.86	123.30
1	A	21	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	P	11	ARG	NE-CZ-NH2	7.47	124.04	120.30
1	M	21	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	E	22	GLU	CG-CD-OE2	-7.21	103.88	118.30
1	A	22	GLU	CG-CD-OE2	-7.13	104.05	118.30
1	K	21	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	O	21	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	U	22	GLU	CG-CD-OE2	-6.99	104.33	118.30
1	B	21	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	D	11	ARG	CD-NE-CZ	6.88	133.24	123.60
1	X	11	ARG	CD-NE-CZ	6.86	133.21	123.60
1	T	25	GLU	CG-CD-OE2	6.82	131.94	118.30
1	I	21	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	V	21	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	R	11	ARG	CG-CD-NE	-6.78	97.56	111.80
1	T	21	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	R	21	ARG	NE-CZ-NH1	-6.76	116.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	21	ARG	NE-CZ-NH1	-6.75	116.92	120.30
1	N	21	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	S	45	MET	CA-CB-CG	-6.72	101.88	113.30
1	P	11	ARG	CG-CD-NE	-6.67	97.80	111.80
1	U	21	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	Z	21	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	c	45	MET	CA-CB-CG	-6.48	102.28	113.30
1	N	11	ARG	CD-NE-CZ	6.42	132.58	123.60
1	Z	11	ARG	CD-NE-CZ	6.39	132.54	123.60
1	c	44	GLU	N-CA-CB	-6.38	99.11	110.60
1	S	45	MET	CG-SD-CE	-6.31	90.11	100.20
1	E	29	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	G	11	ARG	CD-NE-CZ	6.27	132.38	123.60
1	B	11[A]	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	B	11[B]	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	S	25	GLU	CG-CD-OE2	6.25	130.81	118.30
1	V	11	ARG	CD-NE-CZ	6.25	132.35	123.60
1	L	11	ARG	CA-CB-CG	-6.19	99.78	113.40
1	d	21	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	P	56	LEU	CB-CA-C	-5.85	99.08	110.20
1	d	29	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	P	57	ALA	N-CA-CB	5.85	118.28	110.10
1	Y	36	THR	CA-CB-OG1	5.78	121.14	109.00
1	M	11	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	D	25	GLU	CG-CD-OE1	5.71	129.72	118.30
1	K	29	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	L	55	GLU	CG-CD-OE2	5.69	129.69	118.30
1	c	29	ARG	N-CA-CB	-5.67	100.40	110.60
1	L	55	GLU	OE1-CD-OE2	5.66	130.09	123.30
1	b	25	GLU	CG-CD-OE1	5.64	129.59	118.30
1	O	25	GLU	CG-CD-OE1	5.64	129.59	118.30
1	c	45	MET	CG-SD-CE	-5.61	91.23	100.20
1	S	25	GLU	CA-CB-CG	5.57	125.65	113.40
1	L	25	GLU	CG-CD-OE1	5.56	129.42	118.30
1	R	25	GLU	CG-CD-OE1	5.53	129.36	118.30
1	S	45	MET	CB-CA-C	5.52	121.44	110.40
1	B	29	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	29	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	H	25	GLU	CG-CD-OE1	5.50	129.30	118.30
1	a	21	ARG	CD-NE-CZ	5.49	131.28	123.60
1	W	29	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	11	ARG	CG-CD-NE	-5.47	100.31	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	25	GLU	CG-CD-OE1	5.47	129.24	118.30
1	d	25	GLU	CG-CD-OE1	5.46	129.23	118.30
1	B	25	GLU	CG-CD-OE1	5.45	129.21	118.30
1	L	21	ARG	CD-NE-CZ	5.45	131.22	123.60
1	S	21	ARG	CD-NE-CZ	5.42	131.18	123.60
1	F	25	GLU	CG-CD-OE1	5.41	129.11	118.30
1	O	29	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	J	25	GLU	CG-CD-OE1	5.38	129.06	118.30
1	U	29	ARG	N-CA-CB	-5.37	100.94	110.60
1	Q	22	GLU	CG-CD-OE1	5.32	128.94	118.30
1	N	29	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	K	22	GLU	CG-CD-OE1	5.27	128.84	118.30
1	L	29	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	X	17	GLU	N-CA-CB	5.25	120.05	110.60
1	b	21	ARG	CD-NE-CZ	5.25	130.95	123.60
1	I	29	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	Q	29	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	c	21	ARG	CD-NE-CZ	5.22	130.90	123.60
1	D	29	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	Z	29	ARG	N-CA-CB	-5.21	101.23	110.60
1	W	21	ARG	CD-NE-CZ	5.20	130.87	123.60
1	c	45	MET	CB-CA-C	5.19	120.79	110.40
1	X	21	ARG	CD-NE-CZ	5.18	130.85	123.60
1	b	29	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	21	ARG	CD-NE-CZ	5.14	130.80	123.60
1	J	21	ARG	CD-NE-CZ	5.14	130.80	123.60
1	D	25	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	X	29	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	Q	59	LYS	N-CA-C	-5.09	97.25	111.00
1	R	29	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	21	ARG	CD-NE-CZ	5.05	130.67	123.60
1	J	11	ARG	CG-CD-NE	-5.04	101.20	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
1	B	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	C	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	D	58/62 (94%)	56 (97%)	2 (3%)	0	100	100
1	E	58/62 (94%)	58 (100%)	0	0	100	100
1	F	58/62 (94%)	57 (98%)	1 (2%)	0	100	100
1	G	58/62 (94%)	57 (98%)	1 (2%)	0	100	100
1	H	58/62 (94%)	58 (100%)	0	0	100	100
1	I	58/62 (94%)	57 (98%)	1 (2%)	0	100	100
1	J	58/62 (94%)	58 (100%)	0	0	100	100
1	K	58/62 (94%)	57 (98%)	1 (2%)	0	100	100
1	L	56/62 (90%)	55 (98%)	1 (2%)	0	100	100
1	M	58/62 (94%)	57 (98%)	1 (2%)	0	100	100
1	N	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	O	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	P	56/62 (90%)	54 (96%)	1 (2%)	1 (2%)	8	21
1	Q	58/62 (94%)	57 (98%)	1 (2%)	0	100	100
1	R	57/62 (92%)	56 (98%)	0	1 (2%)	8	21
1	S	58/62 (94%)	58 (100%)	0	0	100	100
1	T	55/62 (89%)	55 (100%)	0	0	100	100
1	U	55/62 (89%)	55 (100%)	0	0	100	100
1	V	55/62 (89%)	55 (100%)	0	0	100	100
1	W	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	X	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	Y	57/62 (92%)	56 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	a	55/62 (89%)	55 (100%)	0	0	100	100
1	b	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	c	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	d	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
All	All	1714/1860 (92%)	1690 (99%)	22 (1%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	56	LEU
1	R	58	SER

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	52/52 (100%)	52 (100%)	0	100	100
1	B	49/52 (94%)	48 (98%)	1 (2%)	55	81
1	C	49/52 (94%)	48 (98%)	1 (2%)	55	81
1	D	50/52 (96%)	49 (98%)	1 (2%)	55	81
1	E	50/52 (96%)	50 (100%)	0	100	100
1	F	50/52 (96%)	50 (100%)	0	100	100
1	G	50/52 (96%)	47 (94%)	3 (6%)	19	42
1	H	50/52 (96%)	50 (100%)	0	100	100
1	I	50/52 (96%)	50 (100%)	0	100	100
1	J	50/52 (96%)	49 (98%)	1 (2%)	55	81
1	K	50/52 (96%)	50 (100%)	0	100	100
1	L	48/52 (92%)	46 (96%)	2 (4%)	30	58
1	M	50/52 (96%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	49/52 (94%)	48 (98%)	1 (2%)	55	81
1	O	49/52 (94%)	49 (100%)	0	100	100
1	P	48/52 (92%)	46 (96%)	2 (4%)	30	58
1	Q	50/52 (96%)	50 (100%)	0	100	100
1	R	49/52 (94%)	49 (100%)	0	100	100
1	S	50/52 (96%)	48 (96%)	2 (4%)	31	60
1	T	47/52 (90%)	46 (98%)	1 (2%)	53	80
1	U	47/52 (90%)	47 (100%)	0	100	100
1	V	47/52 (90%)	45 (96%)	2 (4%)	29	57
1	W	49/52 (94%)	48 (98%)	1 (2%)	55	81
1	X	49/52 (94%)	48 (98%)	1 (2%)	55	81
1	Y	49/52 (94%)	48 (98%)	1 (2%)	55	81
1	Z	49/52 (94%)	48 (98%)	1 (2%)	55	81
1	a	47/52 (90%)	47 (100%)	0	100	100
1	b	49/52 (94%)	48 (98%)	1 (2%)	55	81
1	c	49/52 (94%)	48 (98%)	1 (2%)	55	81
1	d	49/52 (94%)	49 (100%)	0	100	100
All	All	1474/1560 (94%)	1451 (98%)	23 (2%)	62	85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	PRO
1	C	11	ARG
1	D	11	ARG
1	G	1	PRO
1	G	11	ARG
1	G	29	ARG
1	J	55	GLU
1	L	11	ARG
1	L	55	GLU
1	N	11	ARG
1	P	11	ARG
1	P	29	ARG
1	S	29	ARG
1	S	56	LEU

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Mol	Chain	Res	Type
1	T	29	ARG
1	V	11	ARG
1	V	29	ARG
1	W	44	GLU
1	X	11	ARG
1	Y	36	THR
1	Z	11	ARG
1	b	11	ARG
1	c	29	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	49	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	7DH	B	101	1	7,7,8	1.85	2 (28%)	8,8,9	1.81	3 (37%)
2	7DH	F	101	1	7,7,8	1.80	2 (28%)	8,8,9	1.78	2 (25%)
2	7DH	G	101	1	7,7,8	1.74	2 (28%)	8,8,9	1.50	2 (25%)
2	7DH	A	101	1	7,7,8	1.90	2 (28%)	8,8,9	1.18	1 (12%)
2	7DH	P	101	1	7,7,8	1.78	2 (28%)	8,8,9	1.55	1 (12%)
2	7DH	C	101	1	7,7,8	1.50	1 (14%)	8,8,9	2.80	5 (62%)
2	7DH	L	101	1	7,7,8	1.33	0	8,8,9	3.07	4 (50%)
2	7DH	O	101	1	7,7,8	1.73	2 (28%)	8,8,9	2.43	5 (62%)
2	7DH	R	101	1	7,7,8	1.46	1 (14%)	8,8,9	3.63	7 (87%)

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	7DH	B	101	1	-	1/7/7/8	-
2	7DH	F	101	1	-	3/7/7/8	-
2	7DH	G	101	1	-	0/7/7/8	-
2	7DH	A	101	1	-	5/7/7/8	-
2	7DH	P	101	1	-	5/7/7/8	-
2	7DH	C	101	1	-	2/7/7/8	-
2	7DH	L	101	1	-	2/7/7/8	-
2	7DH	O	101	1	-	2/7/7/8	-
2	7DH	R	101	1	-	3/7/7/8	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	101	7DH	C03-C04	3.60	1.53	1.47
2	A	101	7DH	C03-C04	3.49	1.52	1.47
2	O	101	7DH	C03-C04	3.29	1.52	1.47
2	F	101	7DH	C03-C04	3.26	1.52	1.47
2	B	101	7DH	C05-C04	-3.14	1.50	1.54
2	B	101	7DH	C03-C04	2.98	1.52	1.47
2	G	101	7DH	C03-C04	2.96	1.52	1.47
2	R	101	7DH	C03-C04	2.68	1.51	1.47
2	A	101	7DH	C05-C04	-2.54	1.51	1.54
2	O	101	7DH	O06-C05	2.46	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	101	7DH	C03-C04	2.37	1.51	1.47
2	F	101	7DH	C05-C04	-2.31	1.51	1.54
2	P	101	7DH	O06-C05	2.15	1.28	1.22
2	G	101	7DH	C05-C04	-2.10	1.51	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	101	7DH	C01-C02-C03	-5.38	114.72	125.34
2	C	101	7DH	C02-C03-C04	-5.18	115.45	123.00
2	L	101	7DH	C01-C02-C03	-5.16	115.16	125.34
2	L	101	7DH	C02-C03-C04	-4.97	115.76	123.00
2	O	101	7DH	C02-C03-C04	-4.31	116.72	123.00
2	R	101	7DH	O08-C04-C03	-4.30	113.64	121.77
2	R	101	7DH	O07-C05-O06	-4.12	114.18	123.61
2	B	101	7DH	C01-C02-C03	-3.81	117.82	125.34
2	R	101	7DH	C02-C03-C04	-3.71	117.60	123.00
2	F	101	7DH	C01-C02-C03	-3.56	118.32	125.34
2	R	101	7DH	O07-C05-C04	3.50	122.62	113.19
2	C	101	7DH	O07-C05-C04	3.42	122.39	113.19
2	P	101	7DH	C01-C02-C03	-3.29	118.85	125.34
2	L	101	7DH	O07-C05-C04	3.20	121.81	113.19
2	L	101	7DH	O08-C04-C05	3.13	125.07	117.69
2	O	101	7DH	C03-C04-C05	3.04	123.17	116.31
2	G	101	7DH	C01-C02-C03	-3.01	119.41	125.34
2	R	101	7DH	C03-C04-C05	3.00	123.07	116.31
2	C	101	7DH	C03-C04-C05	2.80	122.63	116.31
2	C	101	7DH	C01-C02-C03	-2.77	119.87	125.34
2	F	101	7DH	C02-C03-C04	-2.51	119.35	123.00
2	O	101	7DH	O08-C04-C03	-2.43	117.18	121.77
2	R	101	7DH	O08-C04-C05	2.38	123.29	117.69
2	O	101	7DH	C01-C02-C03	-2.32	120.76	125.34
2	A	101	7DH	O07-C05-C04	2.29	119.35	113.19
2	O	101	7DH	O07-C05-C04	2.18	119.07	113.19
2	B	101	7DH	O07-C05-C04	2.14	118.95	113.19
2	G	101	7DH	O07-C05-C04	2.12	118.90	113.19
2	C	101	7DH	O08-C04-C03	-2.09	117.81	121.77
2	B	101	7DH	C02-C03-C04	-2.03	120.05	123.00

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	7DH	C01-C02-C03-C04
2	A	101	7DH	C03-C04-C05-O06
2	A	101	7DH	C03-C04-C05-O07
2	C	101	7DH	C01-C02-C03-C04
2	F	101	7DH	C01-C02-C03-C04
2	F	101	7DH	C03-C04-C05-O06
2	L	101	7DH	C01-C02-C03-C04
2	P	101	7DH	C02-C03-C04-C05
2	P	101	7DH	C03-C04-C05-O06
2	P	101	7DH	O08-C04-C05-O07
2	R	101	7DH	C01-C02-C03-C04
2	R	101	7DH	C02-C03-C04-C05
2	R	101	7DH	C02-C03-C04-O08
2	P	101	7DH	C02-C03-C04-O08
2	B	101	7DH	C01-C02-C03-C04
2	O	101	7DH	C01-C02-C03-C04
2	A	101	7DH	C02-C03-C04-O08
2	A	101	7DH	C02-C03-C04-C05
2	F	101	7DH	O08-C04-C05-O07
2	O	101	7DH	O08-C04-C05-O07
2	P	101	7DH	C03-C04-C05-O07
2	C	101	7DH	C03-C04-C05-O06
2	L	101	7DH	C02-C03-C04-C05

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	62/62 (100%)	0.08	1 (1%)	72	74	33, 49, 69, 75	0
1	B	58/62 (93%)	-0.04	0	100	100	27, 42, 67, 102	0
1	C	59/62 (95%)	-0.02	0	100	100	33, 47, 75, 104	0
1	D	60/62 (96%)	-0.05	1 (1%)	70	72	27, 42, 73, 122	0
1	E	60/62 (96%)	0.10	0	100	100	31, 47, 82, 90	0
1	F	60/62 (96%)	-0.01	2 (3%)	46	46	24, 39, 85, 119	0
1	G	60/62 (96%)	0.29	1 (1%)	70	72	41, 61, 100, 122	0
1	H	60/62 (96%)	0.08	0	100	100	32, 52, 85, 101	0
1	I	60/62 (96%)	0.13	3 (5%)	28	27	32, 53, 109, 123	0
1	J	60/62 (96%)	-0.06	1 (1%)	70	72	25, 43, 73, 114	0
1	K	60/62 (96%)	0.10	1 (1%)	70	72	31, 49, 96, 115	0
1	L	58/62 (93%)	-0.19	0	100	100	25, 38, 68, 97	0
1	M	60/62 (96%)	0.20	2 (3%)	46	46	31, 52, 87, 109	0
1	N	59/62 (95%)	0.14	1 (1%)	70	72	33, 56, 80, 115	0
1	O	59/62 (95%)	-0.12	0	100	100	25, 41, 83, 113	0
1	P	58/62 (93%)	-0.17	0	100	100	26, 41, 73, 88	0
1	Q	59/62 (95%)	0.05	2 (3%)	45	45	32, 48, 80, 107	0
1	R	59/62 (95%)	0.19	1 (1%)	70	72	34, 55, 90, 143	0
1	S	60/62 (96%)	0.43	4 (6%)	17	16	39, 69, 114, 138	0
1	T	57/62 (91%)	-0.04	0	100	100	37, 56, 88, 110	0
1	U	57/62 (91%)	0.26	0	100	100	47, 73, 94, 105	0
1	V	57/62 (91%)	0.03	0	100	100	37, 59, 83, 92	0
1	W	59/62 (95%)	0.42	2 (3%)	45	45	43, 61, 96, 113	0
1	X	59/62 (95%)	0.16	0	100	100	36, 59, 90, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	Y	59/62 (95%)	0.62	3 (5%)	28	26	51, 80, 108, 116	0
1	Z	59/62 (95%)	0.34	1 (1%)	70	72	42, 69, 103, 120	0
1	a	57/62 (91%)	0.14	0	100	100	35, 57, 95, 111	0
1	b	59/62 (95%)	-0.10	0	100	100	31, 47, 74, 104	0
1	c	59/62 (95%)	0.54	3 (5%)	28	26	45, 66, 98, 117	0
1	d	59/62 (95%)	0.29	2 (3%)	45	45	38, 58, 101, 130	0
All	All	1772/1860 (95%)	0.13	31 (1%)	70	72	24, 54, 94, 143	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	58	SER	6.6
1	Z	58	SER	6.0
1	S	60	VAL	5.1
1	d	58	SER	4.9
1	c	58	SER	4.8
1	I	60	VAL	3.7
1	D	60	VAL	3.5
1	c	47	LYS	3.3
1	N	58	SER	3.2
1	K	58	SER	3.2
1	c	57	ALA	3.0
1	W	57	ALA	3.0
1	F	60	VAL	2.8
1	Y	58	SER	2.8
1	F	59	LYS	2.7
1	M	60	VAL	2.6
1	S	14	GLU	2.6
1	J	60	VAL	2.6
1	A	57	ALA	2.5
1	Q	58	SER	2.4
1	I	55	GLU	2.4
1	Q	59	LYS	2.4
1	S	57	ALA	2.3
1	Y	59	LYS	2.3
1	I	59	LYS	2.3
1	M	59	LYS	2.2
1	W	55	GLU	2.1
1	d	59	LYS	2.1
1	Y	27	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	S	58	SER	2.0
1	G	60	VAL	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	7DH	P	101	8/9	0.75	0.29	57,77,90,102	0
2	7DH	A	101	8/9	0.81	0.41	85,99,103,108	0
2	7DH	C	101	8/9	0.82	0.36	58,75,95,101	0
2	7DH	G	101	8/9	0.83	0.39	79,89,92,104	0
2	7DH	F	101	8/9	0.83	0.29	65,81,92,92	0
2	7DH	R	101	8/9	0.86	0.21	68,77,89,97	0
2	7DH	O	101	8/9	0.88	0.24	55,70,77,79	0
2	7DH	B	101	8/9	0.88	0.29	61,78,83,93	0
2	7DH	L	101	8/9	0.88	0.23	59,70,77,78	0

6.5 Other polymers (i)

There are no such residues in this entry.