Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:52 PM GMT

PDB ID	:	3V9H
Title	:	Crystal structure of human 1-pyrroline-5-carboxylate dehydrogenase mutant S352A
Authors	:	Tanner, J.J.; Singh, RK
Deposited on	:	2011-12-27
Resolution	:	2.40 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 ⓘ symbol.

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

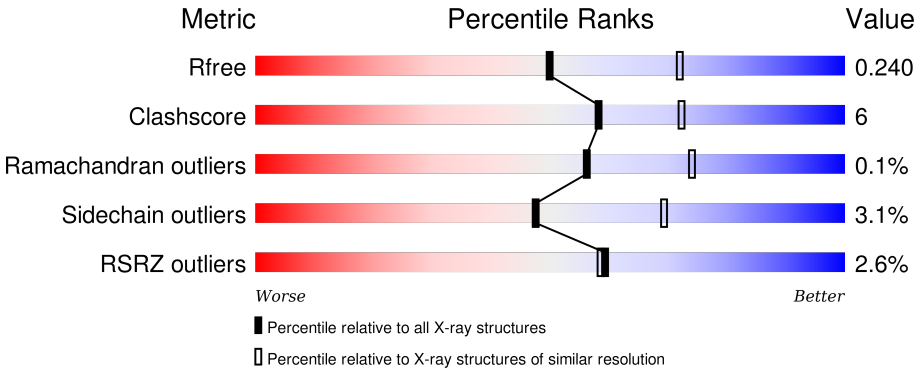
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	566	82% 13%
1	B	566	81% 13%
1	C	566	3% 81% 12% 5%
1	D	566	7% 81% 11% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	565	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15844 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 Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4048	2592	682	759	15			
1	B	541	Total	C	N	O	S	0	0	0
			4025	2581	680	749	15			
1	C	538	Total	C	N	O	S	0	0	0
			3853	2452	660	726	15			
1	D	531	Total	C	N	O	S	0	0	0
			3716	2358	645	699	14			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P30038
A	-1	GLY	-	EXPRESSION TAG	UNP P30038
A	0	SER	-	EXPRESSION TAG	UNP P30038
A	1	SER	-	EXPRESSION TAG	UNP P30038
A	2	HIS	-	EXPRESSION TAG	UNP P30038
A	3	HIS	-	EXPRESSION TAG	UNP P30038
A	4	HIS	-	EXPRESSION TAG	UNP P30038
A	5	HIS	-	EXPRESSION TAG	UNP P30038
A	6	HIS	-	EXPRESSION TAG	UNP P30038
A	7	HIS	-	EXPRESSION TAG	UNP P30038
A	8	SER	-	EXPRESSION TAG	UNP P30038
A	9	SER	-	EXPRESSION TAG	UNP P30038
A	10	GLY	-	EXPRESSION TAG	UNP P30038
A	11	LEU	-	EXPRESSION TAG	UNP P30038
A	12	VAL	-	EXPRESSION TAG	UNP P30038
A	13	PRO	-	EXPRESSION TAG	UNP P30038
A	14	ARG	-	EXPRESSION TAG	UNP P30038
A	15	GLY	-	EXPRESSION TAG	UNP P30038
A	16	SER	-	EXPRESSION TAG	UNP P30038
A	17	HIS	-	EXPRESSION TAG	UNP P30038
A	352	ALA	SER	ENGINEERED MUTATION	UNP P30038

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	EXPRESSION TAG	UNP P30038
B	-1	GLY	-	EXPRESSION TAG	UNP P30038
B	0	SER	-	EXPRESSION TAG	UNP P30038
B	1	SER	-	EXPRESSION TAG	UNP P30038
B	2	HIS	-	EXPRESSION TAG	UNP P30038
B	3	HIS	-	EXPRESSION TAG	UNP P30038
B	4	HIS	-	EXPRESSION TAG	UNP P30038
B	5	HIS	-	EXPRESSION TAG	UNP P30038
B	6	HIS	-	EXPRESSION TAG	UNP P30038
B	7	HIS	-	EXPRESSION TAG	UNP P30038
B	8	SER	-	EXPRESSION TAG	UNP P30038
B	9	SER	-	EXPRESSION TAG	UNP P30038
B	10	GLY	-	EXPRESSION TAG	UNP P30038
B	11	LEU	-	EXPRESSION TAG	UNP P30038
B	12	VAL	-	EXPRESSION TAG	UNP P30038
B	13	PRO	-	EXPRESSION TAG	UNP P30038
B	14	ARG	-	EXPRESSION TAG	UNP P30038
B	15	GLY	-	EXPRESSION TAG	UNP P30038
B	16	SER	-	EXPRESSION TAG	UNP P30038
B	17	HIS	-	EXPRESSION TAG	UNP P30038
B	352	ALA	SER	ENGINEERED MUTATION	UNP P30038
C	-2	MET	-	EXPRESSION TAG	UNP P30038
C	-1	GLY	-	EXPRESSION TAG	UNP P30038
C	0	SER	-	EXPRESSION TAG	UNP P30038
C	1	SER	-	EXPRESSION TAG	UNP P30038
C	2	HIS	-	EXPRESSION TAG	UNP P30038
C	3	HIS	-	EXPRESSION TAG	UNP P30038
C	4	HIS	-	EXPRESSION TAG	UNP P30038
C	5	HIS	-	EXPRESSION TAG	UNP P30038
C	6	HIS	-	EXPRESSION TAG	UNP P30038
C	7	HIS	-	EXPRESSION TAG	UNP P30038
C	8	SER	-	EXPRESSION TAG	UNP P30038
C	9	SER	-	EXPRESSION TAG	UNP P30038
C	10	GLY	-	EXPRESSION TAG	UNP P30038
C	11	LEU	-	EXPRESSION TAG	UNP P30038
C	12	VAL	-	EXPRESSION TAG	UNP P30038
C	13	PRO	-	EXPRESSION TAG	UNP P30038
C	14	ARG	-	EXPRESSION TAG	UNP P30038
C	15	GLY	-	EXPRESSION TAG	UNP P30038
C	16	SER	-	EXPRESSION TAG	UNP P30038
C	17	HIS	-	EXPRESSION TAG	UNP P30038
C	352	ALA	SER	ENGINEERED MUTATION	UNP P30038

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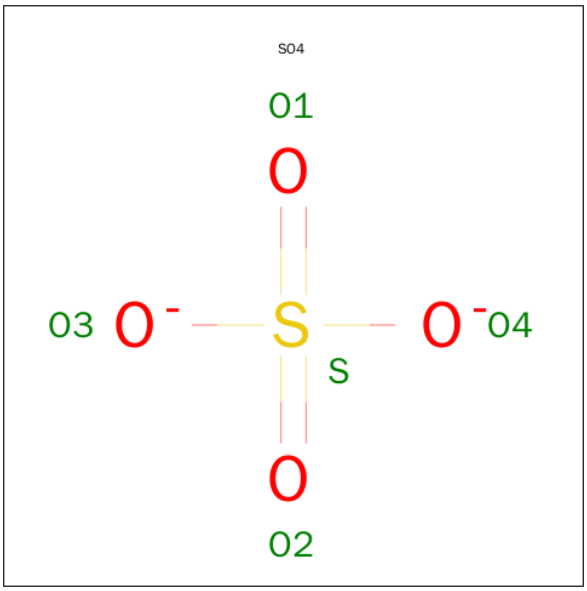
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	EXPRESSION TAG	UNP P30038
D	-1	GLY	-	EXPRESSION TAG	UNP P30038
D	0	SER	-	EXPRESSION TAG	UNP P30038
D	1	SER	-	EXPRESSION TAG	UNP P30038
D	2	HIS	-	EXPRESSION TAG	UNP P30038
D	3	HIS	-	EXPRESSION TAG	UNP P30038
D	4	HIS	-	EXPRESSION TAG	UNP P30038
D	5	HIS	-	EXPRESSION TAG	UNP P30038
D	6	HIS	-	EXPRESSION TAG	UNP P30038
D	7	HIS	-	EXPRESSION TAG	UNP P30038
D	8	SER	-	EXPRESSION TAG	UNP P30038
D	9	SER	-	EXPRESSION TAG	UNP P30038
D	10	GLY	-	EXPRESSION TAG	UNP P30038
D	11	LEU	-	EXPRESSION TAG	UNP P30038
D	12	VAL	-	EXPRESSION TAG	UNP P30038
D	13	PRO	-	EXPRESSION TAG	UNP P30038
D	14	ARG	-	EXPRESSION TAG	UNP P30038
D	15	GLY	-	EXPRESSION TAG	UNP P30038
D	16	SER	-	EXPRESSION TAG	UNP P30038
D	17	HIS	-	EXPRESSION TAG	UNP P30038
D	352	ALA	SER	ENGINEERED MUTATION	UNP P30038

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0

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

- Molecule 3 is water.

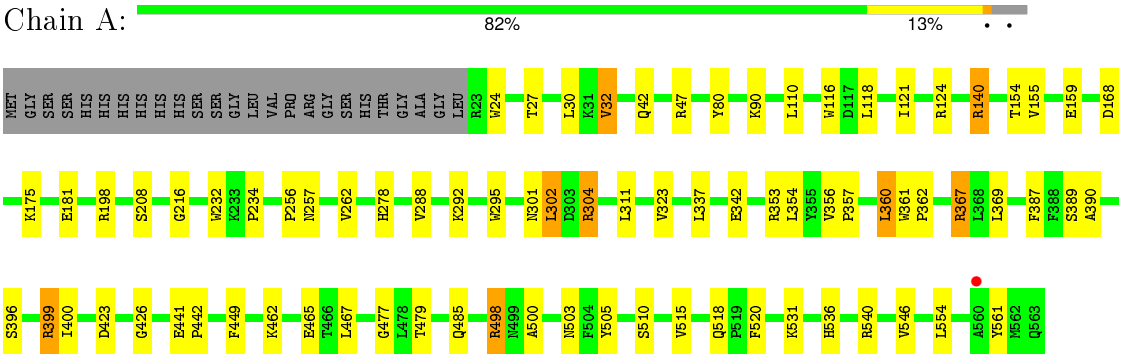
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	61	Total O 61 61	0	0
3	B	74	Total O 74 74	0	0
3	C	17	Total O 17 17	0	0
3	D	15	Total O 15 15	0	0

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.

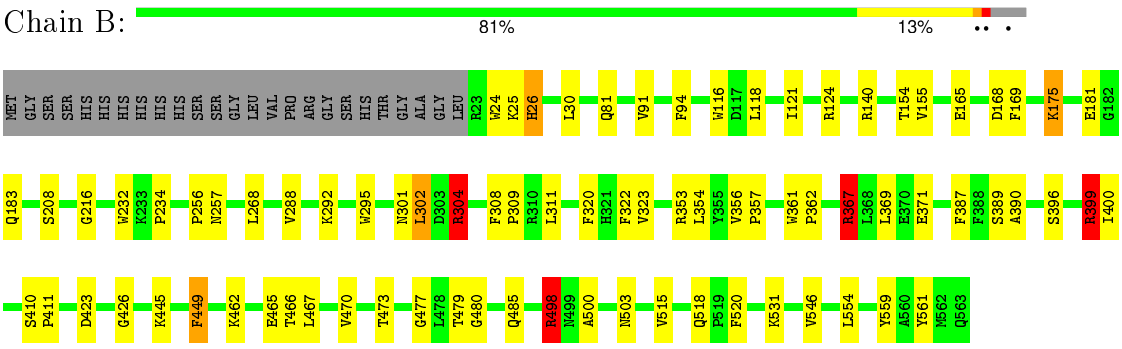
- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

Chain A:



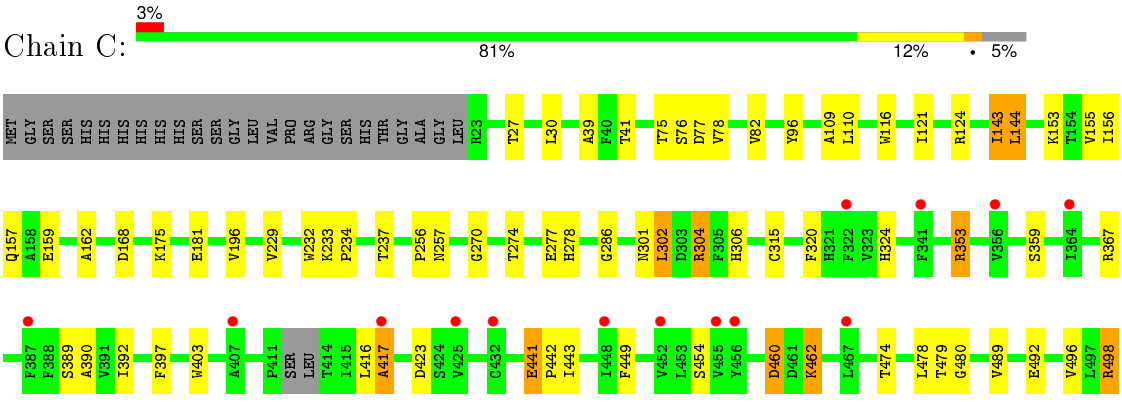
- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

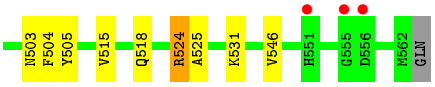
Chain B:



- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

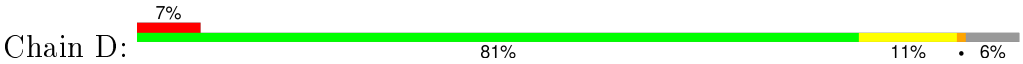
Chain C:

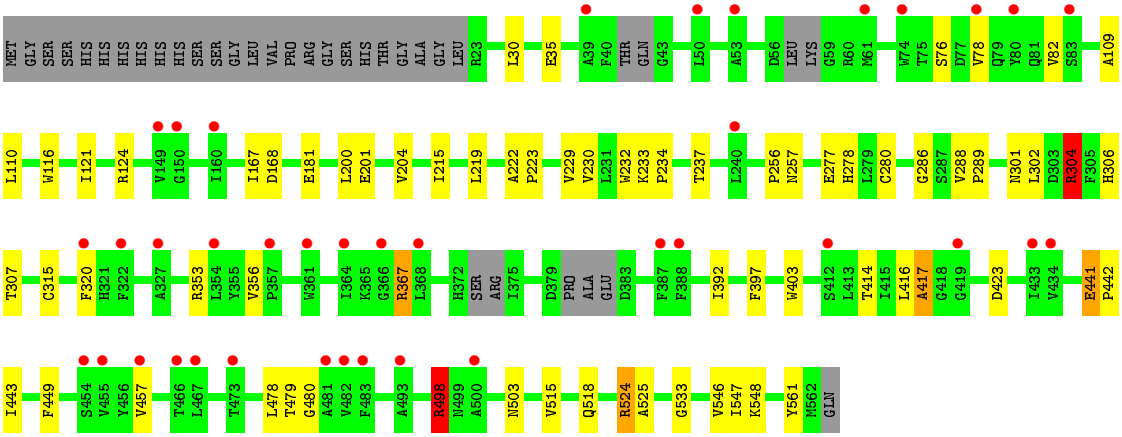




• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	149.13Å 149.13Å 190.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.45 – 2.40 48.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.45-2.40) 99.6 (48.81-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.210 , 0.251 0.195 , 0.240	Depositor DCC
R_{free} test set	2182 reflections (2.34%)	DCC
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.7	EDS
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 93282 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15844	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.49	1/4155 (0.0%)	0.85	17/5672 (0.3%)
1	B	0.48	2/4132 (0.0%)	0.81	18/5642 (0.3%)
1	C	0.37	0/3951	0.71	15/5408 (0.3%)
1	D	0.38	0/3813	0.81	15/5222 (0.3%)
All	All	0.43	3/16051 (0.0%)	0.80	65/21944 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	ARG	CZ-NH2	-8.52	1.22	1.33
1	B	353	ARG	CZ-NH1	-7.74	1.23	1.33
1	B	353	ARG	CZ-NH2	-6.96	1.24	1.33

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	353	ARG	NE-CZ-NH2	-23.52	108.54	120.30
1	D	353	ARG	NE-CZ-NH1	20.17	130.38	120.30
1	A	353	ARG	NE-CZ-NH1	15.69	128.14	120.30
1	A	140	ARG	NE-CZ-NH1	14.71	127.66	120.30
1	A	140	ARG	NE-CZ-NH2	-14.57	113.01	120.30
1	B	498	ARG	NE-CZ-NH2	14.28	127.44	120.30
1	B	399	ARG	NE-CZ-NH1	13.53	127.07	120.30
1	A	399	ARG	NE-CZ-NH1	-13.11	113.74	120.30
1	A	399	ARG	NE-CZ-NH2	13.08	126.84	120.30
1	B	367	ARG	NE-CZ-NH1	-12.96	113.82	120.30
1	A	498	ARG	NE-CZ-NH1	12.78	126.69	120.30
1	D	367	ARG	NE-CZ-NH2	-12.51	114.04	120.30
1	B	399	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	D	498	ARG	NE-CZ-NH2	12.36	126.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	367	ARG	NE-CZ-NH1	12.27	126.43	120.30
1	B	367	ARG	NE-CZ-NH2	12.20	126.40	120.30
1	C	367	ARG	NE-CZ-NH1	-12.12	114.24	120.30
1	A	498	ARG	NE-CZ-NH2	-12.00	114.30	120.30
1	B	498	ARG	NE-CZ-NH1	-12.00	114.30	120.30
1	A	367	ARG	NE-CZ-NH2	-11.69	114.45	120.30
1	C	524	ARG	NE-CZ-NH1	-11.63	114.48	120.30
1	C	524	ARG	NE-CZ-NH2	11.57	126.08	120.30
1	D	367	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	A	304	ARG	NE-CZ-NH2	11.28	125.94	120.30
1	A	304	ARG	NE-CZ-NH1	-11.27	114.66	120.30
1	C	367	ARG	NE-CZ-NH2	11.22	125.91	120.30
1	B	140	ARG	NE-CZ-NH1	-11.20	114.70	120.30
1	C	304	ARG	NE-CZ-NH1	-10.95	114.83	120.30
1	D	498	ARG	NE-CZ-NH1	-10.94	114.83	120.30
1	D	524	ARG	NE-CZ-NH2	-10.67	114.97	120.30
1	B	304	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	D	524	ARG	NE-CZ-NH1	10.31	125.46	120.30
1	B	304	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	C	498	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	C	498	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	D	304	ARG	NE-CZ-NH2	-10.11	115.24	120.30
1	C	353	ARG	NE-CZ-NH1	-10.09	115.25	120.30
1	C	304	ARG	NE-CZ-NH2	10.05	125.32	120.30
1	B	140	ARG	NE-CZ-NH2	10.01	125.31	120.30
1	D	304	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	B	353	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	C	353	ARG	CG-CD-NE	8.85	130.39	111.80
1	B	353	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	353	ARG	NH1-CZ-NH2	-8.39	110.17	119.40
1	D	353	ARG	CD-NE-CZ	8.21	135.10	123.60
1	B	353	ARG	NH1-CZ-NH2	-8.13	110.46	119.40
1	C	353	ARG	NE-CZ-NH2	7.59	124.09	120.30
1	A	498	ARG	CD-NE-CZ	7.36	133.90	123.60
1	A	399	ARG	CD-NE-CZ	7.22	133.71	123.60
1	A	140	ARG	CD-NE-CZ	6.96	133.35	123.60
1	B	498	ARG	CD-NE-CZ	6.70	132.97	123.60
1	D	353	ARG	CG-CD-NE	-6.47	98.21	111.80
1	B	399	ARG	CD-NE-CZ	6.40	132.56	123.60
1	A	367	ARG	CD-NE-CZ	6.38	132.53	123.60
1	B	367	ARG	CD-NE-CZ	6.15	132.21	123.60
1	D	498	ARG	CD-NE-CZ	6.05	132.08	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	353	ARG	CD-NE-CZ	5.99	131.99	123.60
1	C	367	ARG	CD-NE-CZ	5.90	131.85	123.60
1	C	524	ARG	CD-NE-CZ	5.83	131.76	123.60
1	D	367	ARG	CD-NE-CZ	5.80	131.72	123.60
1	A	304	ARG	CD-NE-CZ	5.47	131.26	123.60
1	D	524	ARG	CD-NE-CZ	5.24	130.94	123.60
1	C	498	ARG	CD-NE-CZ	5.18	130.86	123.60
1	B	140	ARG	CD-NE-CZ	5.17	130.84	123.60
1	B	304	ARG	CD-NE-CZ	5.17	130.84	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4048	0	3838	49	0
1	B	4025	0	3805	54	0
1	C	3853	0	3473	53	0
1	D	3716	0	3183	47	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	5	0	0	0	0
3	A	61	0	0	2	0
3	B	74	0	0	1	0
3	C	17	0	0	0	0
3	D	15	0	0	0	0
All	All	15844	0	14299	176	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 6.

All (176) 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:D:301:ASN:HB3	1:D:304:ARG:HD3	1.22	1.13
1:D:121:ILE:HG21	1:D:181:GLU:HG3	1.51	0.91
1:A:498:ARG:HH11	1:B:118:LEU:HD23	1.36	0.90
1:C:121:ILE:HG21	1:C:181:GLU:HG3	1.53	0.89
1:A:121:ILE:HG21	1:A:181:GLU:HG3	1.55	0.88
1:A:118:LEU:HD23	1:B:498:ARG:HH11	1.39	0.87
1:B:121:ILE:HG21	1:B:181:GLU:HG3	1.59	0.85
1:A:292:LYS:HG2	1:B:302:LEU:HD13	1.56	0.85
1:A:396:SER:HA	1:A:399:ARG:HH11	1.39	0.84
1:A:302:LEU:HD13	1:B:292:LYS:HG2	1.58	0.84
1:C:353:ARG:HH11	1:C:474:THR:CG2	1.99	0.74
1:C:155:VAL:HB	1:D:561:TYR:CE2	2.26	0.71
1:C:301:ASN:O	1:C:304:ARG:HG2	1.90	0.70
1:C:524:ARG:HD2	1:D:201:GLU:OE1	1.90	0.70
1:B:301:ASN:HB3	1:B:304:ARG:HD2	1.73	0.69
1:A:498:ARG:NH1	1:B:118:LEU:HD23	2.07	0.67
1:D:288:VAL:HB	1:D:289:PRO:HD3	1.76	0.67
1:B:396:SER:HA	1:B:399:ARG:NH1	2.10	0.67
1:C:518:GLN:HA	1:D:546:VAL:HG11	1.77	0.67
1:C:353:ARG:HH11	1:C:474:THR:HG23	1.60	0.66
1:B:396:SER:HA	1:B:399:ARG:HH11	1.61	0.66
1:B:322:PHE:CZ	1:B:467:LEU:HD22	2.31	0.65
1:C:196:VAL:HG11	1:D:498:ARG:HH21	1.62	0.65
1:C:277:GLU:HG3	1:C:306:HIS:CD2	2.34	0.62
1:C:196:VAL:CG1	1:D:498:ARG:HH21	2.12	0.61
1:C:353:ARG:NH1	1:C:474:THR:HG23	2.16	0.60
1:B:301:ASN:CG	1:B:304:ARG:HH11	2.06	0.59
1:B:367:ARG:HE	1:B:367:ARG:HA	1.67	0.59
1:A:423:ASP:HA	1:A:426:GLY:O	2.03	0.57
1:A:232:TRP:O	1:A:234:PRO:HD3	2.03	0.57
1:D:301:ASN:CB	1:D:304:ARG:HD3	2.16	0.56
1:D:168:ASP:HB3	1:D:515:VAL:HB	1.87	0.56
1:C:196:VAL:CG1	1:D:498:ARG:NH2	2.69	0.56
1:A:323:VAL:O	1:A:357:PRO:HD3	2.05	0.56
1:D:232:TRP:O	1:D:234:PRO:HD3	2.06	0.56
1:C:144:LEU:HD11	1:C:159:GLU:HA	1.86	0.56
1:A:357:PRO:HG2	1:A:360:LEU:HB2	1.87	0.55
1:A:546:VAL:HG11	1:B:518:GLN:HA	1.87	0.55
1:D:277:GLU:HG3	1:D:306:HIS:CD2	2.41	0.55
1:C:237:THR:HB	1:C:392:ILE:HD11	1.88	0.55
1:C:505:TYR:CD2	1:D:548:LYS:HB3	2.42	0.55
1:C:168:ASP:HB3	1:C:515:VAL:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HG2	1:B:498:ARG:HH21	1.73	0.54
1:D:237:THR:HB	1:D:392:ILE:HD11	1.91	0.53
1:C:546:VAL:HG11	1:D:518:GLN:HA	1.91	0.53
1:B:232:TRP:O	1:B:234:PRO:HD3	2.08	0.53
1:B:423:ASP:HA	1:B:426:GLY:O	2.08	0.53
1:B:323:VAL:O	1:B:357:PRO:HD3	2.09	0.52
1:D:397:PHE:CZ	1:D:423:ASP:HB3	2.45	0.52
1:A:498:ARG:HH11	1:B:118:LEU:CD2	2.15	0.52
1:A:154:THR:HG21	1:A:387:PHE:O	2.10	0.52
1:D:110:LEU:CD1	1:D:278:HIS:HD2	2.23	0.52
1:C:232:TRP:O	1:C:234:PRO:HD3	2.10	0.51
1:B:24:TRP:HZ3	1:B:26:HIS:NE2	2.08	0.51
1:B:479:THR:HG22	1:B:503:ASN:HB2	1.92	0.51
1:C:479:THR:HG22	1:C:503:ASN:HB2	1.92	0.51
1:C:462:LYS:N	1:C:462:LYS:HD2	2.22	0.50
1:B:462:LYS:O	1:B:465:GLU:HG2	2.11	0.50
1:C:492:GLU:O	1:C:496:VAL:HG23	2.11	0.50
1:C:504:PHE:O	1:D:547:ILE:HA	2.11	0.50
1:C:153:LYS:HG2	1:C:157:GLN:HB3	1.94	0.50
1:C:359:SER:HB3	1:C:460:ASP:OD1	2.11	0.50
1:A:561:TYR:CE2	1:B:155:VAL:HB	2.47	0.50
1:B:256:PRO:O	1:B:257:ASN:HB2	2.12	0.50
1:D:416:LEU:O	1:D:417:ALA:HB2	2.12	0.49
1:C:397:PHE:CZ	1:C:423:ASP:HB3	2.47	0.49
1:B:26:HIS:H	1:B:26:HIS:CD2	2.29	0.49
1:D:76:SER:O	1:D:78:VAL:N	2.44	0.49
1:C:143:ILE:HD13	1:C:162:ALA:HB1	1.94	0.49
1:B:295:TRP:HA	1:B:311:LEU:CD2	2.43	0.49
1:C:76:SER:O	1:C:78:VAL:N	2.46	0.48
1:D:35:GLU:HG2	1:D:167:ILE:HD12	1.96	0.48
1:C:110:LEU:CD1	1:C:278:HIS:HD2	2.27	0.48
1:A:295:TRP:HA	1:A:311:LEU:CD2	2.43	0.48
1:C:324:HIS:CE1	1:C:489:VAL:HG21	2.48	0.48
1:C:389:SER:OG	1:C:390:ALA:N	2.44	0.48
1:A:80:TYR:CD2	1:A:90:LYS:HD3	2.48	0.48
1:A:389:SER:OG	1:A:390:ALA:N	2.47	0.48
1:C:441:GLU:CD	1:C:442:PRO:HD2	2.34	0.48
1:B:399:ARG:NH2	1:B:449:PHE:HB3	2.29	0.48
1:A:140:ARG:NH1	1:A:159:GLU:OE2	2.47	0.48
1:B:154:THR:HG21	1:B:387:PHE:O	2.14	0.47
1:C:39:ALA:HB1	1:C:41:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ARG:HD2	1:A:367:ARG:HA	1.54	0.47
1:A:462:LYS:O	1:A:465:GLU:HG2	2.13	0.47
1:C:256:PRO:O	1:C:257:ASN:HB2	2.14	0.47
1:D:109:ALA:HB1	1:D:229:VAL:HB	1.96	0.47
1:C:416:LEU:O	1:C:417:ALA:HB2	2.15	0.47
1:A:518:GLN:HA	1:B:546:VAL:HG11	1.97	0.47
1:D:441:GLU:CD	1:D:442:PRO:HD2	2.35	0.47
1:D:121:ILE:CG2	1:D:181:GLU:HG3	2.35	0.46
1:A:479:THR:HG22	1:A:503:ASN:HB2	1.97	0.46
1:C:277:GLU:HG3	1:C:306:HIS:NE2	2.30	0.46
1:D:479:THR:HG22	1:D:503:ASN:HB2	1.97	0.46
1:A:24:TRP:CE2	1:C:30:LEU:HD11	2.51	0.46
1:C:524:ARG:HB3	1:C:525:ALA:H	1.65	0.46
1:A:168:ASP:HB3	1:A:515:VAL:HB	1.98	0.45
1:C:75:THR:OG1	1:C:96:TYR:O	2.23	0.45
1:A:396:SER:O	1:A:400:ILE:HG13	2.16	0.45
1:A:540:ARG:HD2	3:A:609:HOH:O	2.16	0.45
1:A:208:SER:HB3	1:A:216:GLY:HA2	1.98	0.45
1:A:554:LEU:HD23	1:A:554:LEU:HA	1.72	0.45
1:B:208:SER:HB3	1:B:216:GLY:HA2	1.98	0.45
1:B:367:ARG:NH1	1:B:371:GLU:OE2	2.50	0.45
1:B:554:LEU:HD23	1:B:554:LEU:HA	1.77	0.45
1:A:301:ASN:CG	1:A:304:ARG:HH11	2.20	0.45
1:B:354:LEU:HG	1:B:356:VAL:HG23	1.98	0.45
1:D:35:GLU:HG2	1:D:167:ILE:CD1	2.47	0.45
1:B:81:GLN:O	1:B:91:VAL:N	2.49	0.45
1:D:110:LEU:HD13	1:D:278:HIS:CD2	2.51	0.44
1:A:262:VAL:O	1:A:262:VAL:HG23	2.17	0.44
1:D:116:TRP:CZ2	1:D:124:ARG:HD2	2.52	0.44
1:C:153:LYS:HG2	1:C:157:GLN:CB	2.47	0.44
1:B:389:SER:OG	1:B:390:ALA:N	2.51	0.44
1:A:30:LEU:HG	1:A:32:VAL:CG1	2.48	0.44
1:C:116:TRP:CZ2	1:C:124:ARG:HD2	2.52	0.44
1:D:256:PRO:O	1:D:257:ASN:HB2	2.18	0.44
1:C:531:LYS:HE3	1:D:546:VAL:HG23	2.00	0.44
1:B:361:TRP:HB3	1:B:362:PRO:HD3	2.00	0.44
1:D:320:PHE:CZ	1:D:480:GLY:HA3	2.53	0.44
1:A:396:SER:HA	1:A:399:ARG:NH1	2.20	0.43
1:C:441:GLU:OE1	1:C:442:PRO:HD2	2.17	0.43
1:D:524:ARG:HB3	1:D:525:ALA:H	1.66	0.43
1:A:342:GLU:HB2	3:A:570:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ALA:HB3	1:D:223:PRO:HD3	1.98	0.43
1:C:121:ILE:CG2	1:C:181:GLU:HG3	2.36	0.43
1:B:30:LEU:O	1:B:175:LYS:HG3	2.18	0.43
1:B:168:ASP:HB3	1:B:515:VAL:HB	2.01	0.43
1:B:320:PHE:CZ	1:B:480:GLY:HA3	2.53	0.43
1:A:116:TRP:CZ2	1:A:124:ARG:HD2	2.53	0.43
1:B:308:PHE:HA	1:B:309:PRO:HD3	1.91	0.43
1:D:286:GLY:O	1:D:315:CYS:HA	2.18	0.43
1:A:155:VAL:HB	1:B:561:TYR:CE2	2.54	0.43
1:C:110:LEU:HD13	1:C:278:HIS:CD2	2.53	0.43
1:A:42:GLN:HA	1:A:47:ARG:HD3	2.01	0.43
1:B:94:PHE:HB2	3:B:615:HOH:O	2.18	0.42
1:C:403:TRP:CZ3	1:C:443:ILE:HA	2.54	0.42
1:C:320:PHE:CZ	1:C:480:GLY:HA3	2.53	0.42
1:A:354:LEU:HG	1:A:356:VAL:HG23	2.00	0.42
1:B:445:LYS:HD2	1:B:473:THR:O	2.19	0.42
1:D:277:GLU:HB2	1:D:304:ARG:O	2.20	0.42
1:A:536:HIS:NE2	1:B:183:GLN:OE1	2.43	0.42
1:B:477:GLY:HA2	1:B:500:ALA:O	2.19	0.42
1:B:410:SER:HA	1:B:411:PRO:HD3	1.77	0.42
1:A:505:TYR:CD1	1:A:510:SER:HA	2.54	0.42
1:A:520:PHE:O	1:A:531:LYS:HA	2.20	0.42
1:B:165:GLU:HG2	1:B:169:PHE:CE2	2.54	0.42
1:B:25:LYS:O	1:D:30:LEU:HD12	2.20	0.42
1:D:204:VAL:O	1:D:230:VAL:HA	2.20	0.42
1:D:215:ILE:O	1:D:219:LEU:HG	2.20	0.42
1:A:361:TRP:HB3	1:A:362:PRO:HD3	2.01	0.41
1:C:524:ARG:HA	1:D:307:THR:HB	2.01	0.41
1:D:110:LEU:CD1	1:D:278:HIS:CD2	3.03	0.41
1:C:443:ILE:HG12	1:C:454:SER:OG	2.20	0.41
1:C:270:GLY:O	1:C:274:THR:HG23	2.19	0.41
1:D:515:VAL:HG13	1:D:533:GLY:HA2	2.02	0.41
1:A:256:PRO:O	1:A:257:ASN:HB2	2.20	0.41
1:A:531:LYS:HE3	1:B:546:VAL:HG23	2.03	0.41
1:A:477:GLY:HA2	1:A:500:ALA:O	2.21	0.41
1:C:109:ALA:HB1	1:C:229:VAL:HB	2.01	0.41
1:D:403:TRP:CZ3	1:D:443:ILE:HA	2.55	0.41
1:D:356:VAL:O	1:D:457:VAL:HA	2.20	0.41
1:D:200:LEU:HB2	1:D:280:CYS:SG	2.60	0.41
1:A:441:GLU:CD	1:A:442:PRO:HD2	2.41	0.41
1:B:399:ARG:NH2	1:B:449:PHE:CB	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:HD23	1:C:302:LEU:HA	1.88	0.41
1:B:520:PHE:O	1:B:531:LYS:HA	2.21	0.41
1:A:110:LEU:HD11	1:A:278:HIS:CG	2.56	0.41
1:C:156:ILE:HA	1:C:156:ILE:HD12	1.96	0.41
1:B:116:TRP:CZ2	1:B:124:ARG:HD2	2.56	0.40
1:D:76:SER:O	1:D:78:VAL:HG23	2.20	0.40
1:B:466:THR:O	1:B:470:VAL:HG23	2.21	0.40
1:C:286:GLY:O	1:C:315:CYS:HA	2.20	0.40
1:B:396:SER:O	1:B:400:ILE:HG13	2.21	0.40
1:A:342:GLU:OE2	1:B:559:TYR:OH	2.27	0.40
1:D:441:GLU:OE1	1:D:442:PRO:HD2	2.22	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	539/566 (95%)	525 (97%)	14 (3%)	0	100	100
1	B	539/566 (95%)	522 (97%)	17 (3%)	0	100	100
1	C	534/566 (94%)	505 (95%)	27 (5%)	2 (0%)	39	56
1	D	521/566 (92%)	490 (94%)	30 (6%)	1 (0%)	52	69
All	All	2133/2264 (94%)	2042 (96%)	88 (4%)	3 (0%)	56	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	417	ALA
1	C	77	ASP
1	C	417	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	407/463 (88%)	396 (97%)	11 (3%)	52 73
1	B	399/463 (86%)	387 (97%)	12 (3%)	48 70
1	C	355/463 (77%)	342 (96%)	13 (4%)	41 62
1	D	314/463 (68%)	304 (97%)	10 (3%)	46 68
All	All	1475/1852 (80%)	1429 (97%)	46 (3%)	47 69

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	32	VAL
1	A	175	LYS
1	A	288	VAL
1	A	302	LEU
1	A	337	LEU
1	A	360	LEU
1	A	369	LEU
1	A	449	PHE
1	A	467	LEU
1	A	485	GLN
1	B	26	HIS
1	B	175	LYS
1	B	268	LEU
1	B	288	VAL
1	B	302	LEU
1	B	304	ARG
1	B	367	ARG
1	B	369	LEU
1	B	399	ARG
1	B	449	PHE
1	B	485	GLN
1	B	498	ARG
1	C	27	THR

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Mol	Chain	Res	Type
1	C	82	VAL
1	C	143	ILE
1	C	144	LEU
1	C	175	LYS
1	C	233	LYS
1	C	302	LEU
1	C	441	GLU
1	C	449	PHE
1	C	460	ASP
1	C	462	LYS
1	C	478	LEU
1	C	498	ARG
1	D	82	VAL
1	D	233	LYS
1	D	302	LEU
1	D	304	ARG
1	D	367	ARG
1	D	414	THR
1	D	441	GLU
1	D	449	PHE
1	D	478	LEU
1	D	498	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	278	HIS
1	D	306	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

7 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	SO4	A	564	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	A	565	-	4,4,4	0.27	0	6,6,6	0.35	0
2	SO4	B	564	-	4,4,4	0.20	0	6,6,6	0.28	0
2	SO4	B	565	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	C	564	-	4,4,4	0.22	0	6,6,6	0.33	0
2	SO4	C	565	-	4,4,4	0.16	0	6,6,6	0.24	0
2	SO4	D	564	-	4,4,4	0.12	0	6,6,6	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	564	-	-	0/0/0/0	0/0/0/0
2	SO4	A	565	-	-	0/0/0/0	0/0/0/0
2	SO4	B	564	-	-	0/0/0/0	0/0/0/0
2	SO4	B	565	-	-	0/0/0/0	0/0/0/0
2	SO4	C	564	-	-	0/0/0/0	0/0/0/0
2	SO4	C	565	-	-	0/0/0/0	0/0/0/0
2	SO4	D	564	-	-	0/0/0/0	0/0/0/0

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	541/566 (95%)	-0.25	1 (0%) 95 95	20, 33, 50, 68	0
1	B	541/566 (95%)	-0.30	0 100 100	19, 36, 54, 92	0
1	C	538/566 (95%)	0.09	17 (3%) 51 51	30, 59, 86, 110	0
1	D	531/566 (93%)	0.40	38 (7%) 18 18	38, 65, 92, 110	0
All	All	2151/2264 (95%)	-0.02	56 (2%) 59 58	19, 46, 86, 110	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	387	PHE	5.1
1	C	341	PHE	4.7
1	D	322	PHE	4.5
1	C	356	VAL	4.4
1	C	551	HIS	4.4
1	D	368	LEU	4.1
1	D	61	MET	4.0
1	D	455	VAL	4.0
1	D	412	SER	3.9
1	C	467	LEU	3.8
1	D	39	ALA	3.7
1	C	322	PHE	3.6
1	C	425	VAL	3.5
1	C	455	VAL	3.4
1	D	434	VAL	3.3
1	C	387	PHE	3.3
1	A	560	ALA	3.2
1	D	53	ALA	3.2
1	D	454	SER	3.1
1	D	240	LEU	3.0
1	D	482	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	364	ILE	2.9
1	D	457	VAL	2.9
1	D	50	LEU	2.9
1	D	80	TYR	2.9
1	D	467	LEU	2.9
1	D	357	PRO	2.9
1	D	466	THR	2.8
1	D	500	ALA	2.8
1	D	327	ALA	2.8
1	D	493	ALA	2.8
1	C	432	CYS	2.7
1	D	483	PHE	2.7
1	D	433	ILE	2.7
1	D	149	VAL	2.5
1	C	448	ILE	2.5
1	C	555	GLY	2.5
1	C	456	TYR	2.5
1	D	78	VAL	2.5
1	D	354	LEU	2.4
1	C	556	ASP	2.4
1	D	481	ALA	2.4
1	D	150	GLY	2.4
1	D	473	THR	2.4
1	D	419	GLY	2.3
1	D	83	SER	2.3
1	C	452	VAL	2.3
1	D	320	PHE	2.2
1	D	361	TRP	2.2
1	D	388	PHE	2.2
1	D	160	ILE	2.1
1	C	364	ILE	2.1
1	D	366	GLY	2.1
1	C	417	ALA	2.1
1	D	74	TRP	2.0
1	C	407	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	565	5/5	0.99	0.16	2.18	39,41,53,60	0
2	SO4	B	564	5/5	0.98	0.13	-0.06	50,51,60,71	0
2	SO4	A	564	5/5	0.93	0.13	-0.68	37,63,97,101	0
2	SO4	C	564	5/5	0.98	0.11	-1.75	48,55,61,63	0
2	SO4	D	564	5/5	0.97	0.11	-2.04	37,53,73,87	0
2	SO4	C	565	5/5	0.92	0.10	-	76,78,94,96	0
2	SO4	B	565	5/5	0.91	0.13	-	98,100,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.