Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 01:49 PM EDT

PDB ID	:	3V9I
Title	:	Crystal structure of human 1-pyrroline-5-carboxylate dehydrogenase mutant S352L
Authors	:	Tanner, J.J.; Singh, R.K.
Deposited on	:	2011-12-27
Resolution	:	2.85 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:

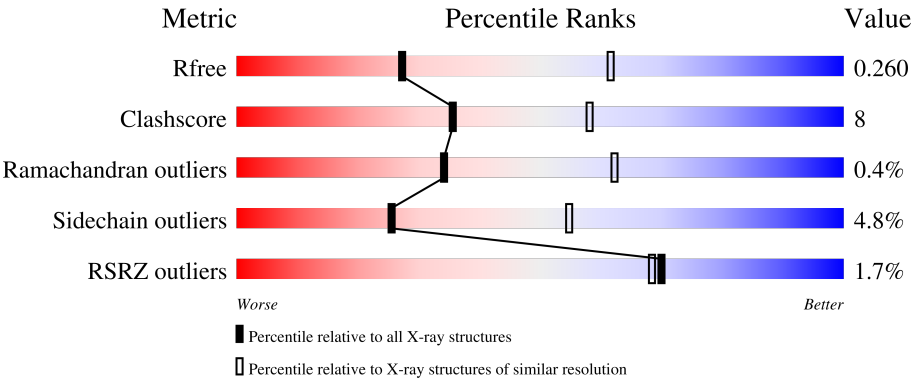
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	566	71% 16% • 11%
1	B	566	72% 15% • 11%
1	C	566	2% 71% 14% • 13%
1	D	566	3% 74% 10% • 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13924 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	506	Total	C	N	O	S	0	0	0
			3738	2414	627	682	15			
1	B	502	Total	C	N	O	S	0	0	0
			3587	2324	599	650	14			
1	C	492	Total	C	N	O	S	0	0	0
			3496	2253	588	642	13			
1	D	482	Total	C	N	O	S	0	0	0
			3103	1974	547	571	11			

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	LEU	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	LEU	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	LEU	SER	engineered mutation	UNP P30038

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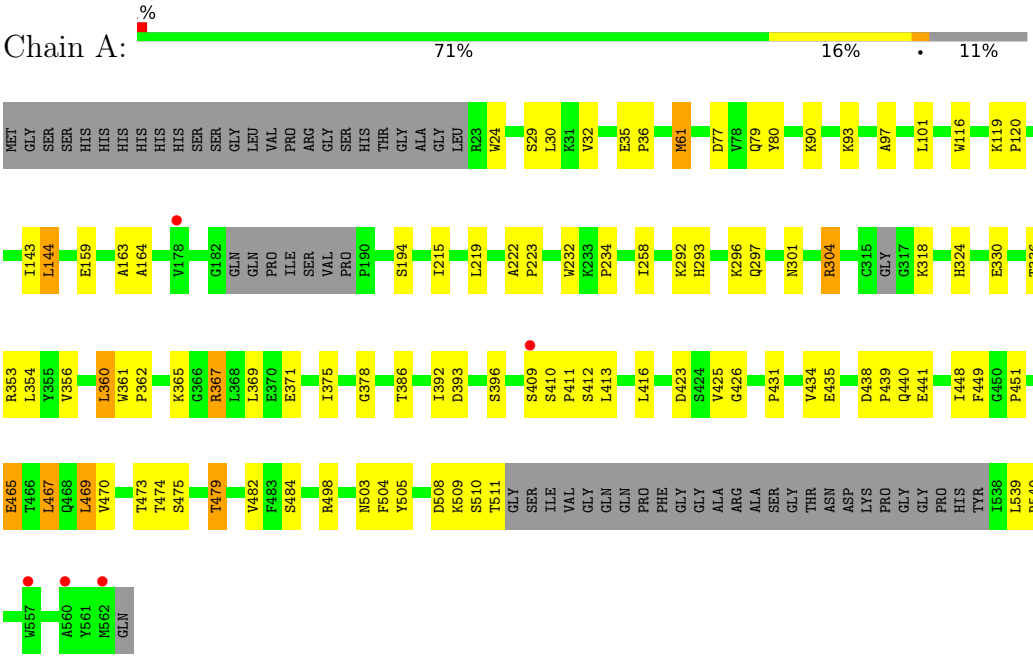
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP P30038
D	-1	GLY	-	expression tag	UNP P30038
D	0	SER	-	expression tag	UNP P30038
D	1	SER	-	expression tag	UNP P30038
D	2	HIS	-	expression tag	UNP P30038
D	3	HIS	-	expression tag	UNP P30038
D	4	HIS	-	expression tag	UNP P30038
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	LEU	SER	engineered mutation	UNP P30038

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.

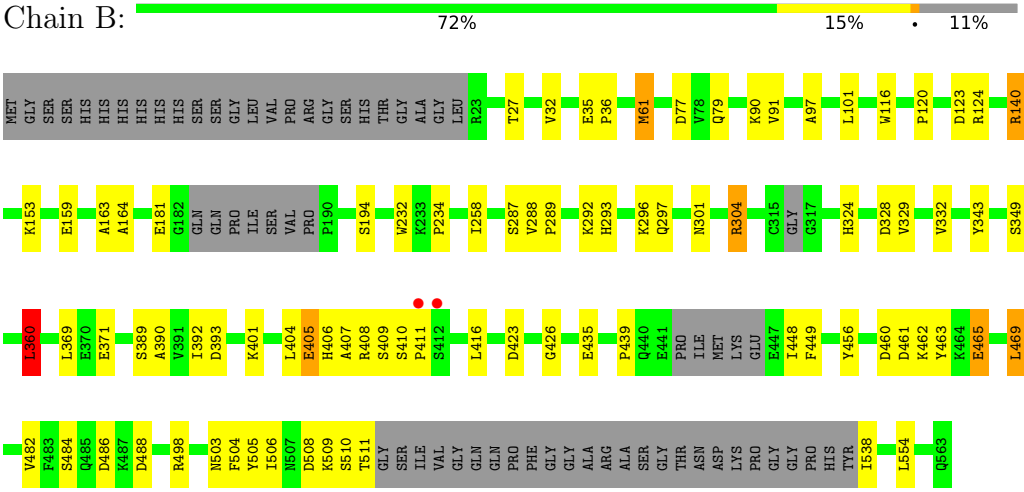
• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

Chain A:



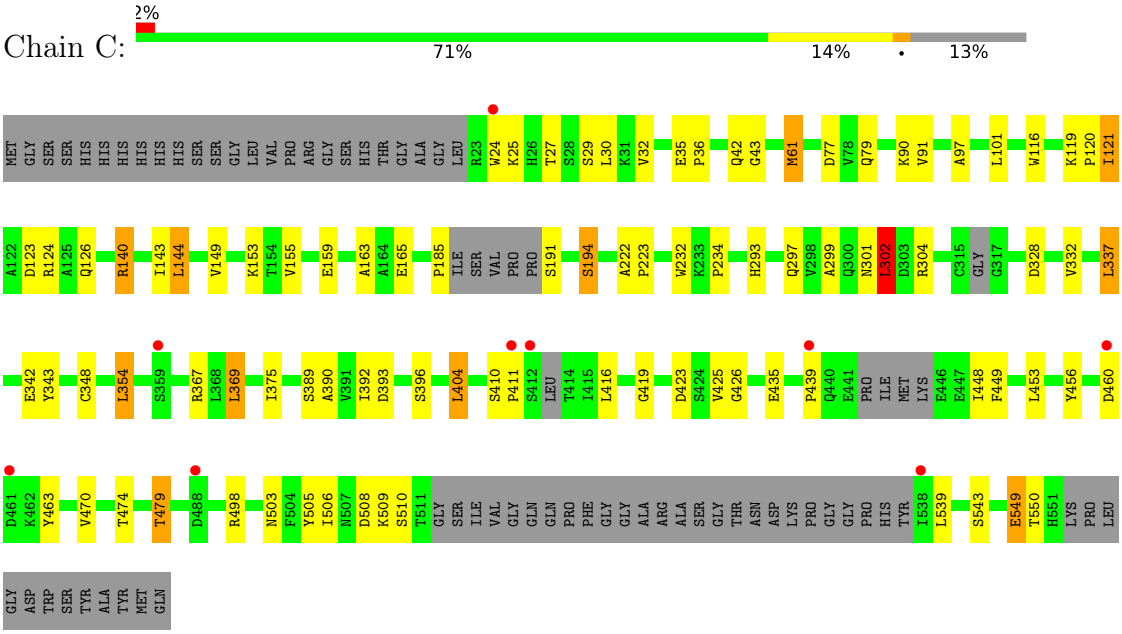
• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

Chain B:



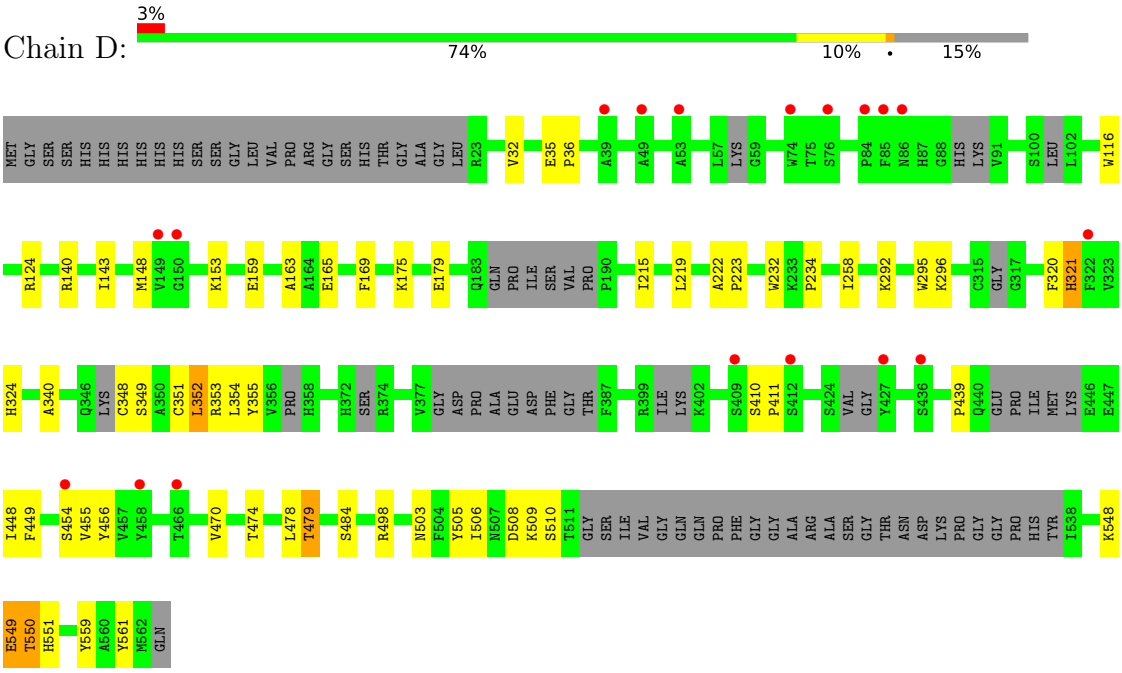
• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

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	150.38Å 150.38Å 192.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.83 – 2.85 45.71 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.83-2.85) 97.1 (45.71-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.209 , 0.264 0.206 , 0.260	Depositor DCC
R_{free} test set	1338 reflections (2.39%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 67.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13924	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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

5.1 Standard geometry

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	0.58	1/3834 (0.0%)	0.82	15/5239 (0.3%)
1	B	0.59	3/3677 (0.1%)	0.73	10/5038 (0.2%)
1	C	0.50	0/3579	0.71	9/4898 (0.2%)
1	D	0.42	0/3164	0.67	6/4343 (0.1%)
All	All	0.53	4/14254 (0.0%)	0.74	40/19518 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	371	GLU	CD-OE1	8.75	1.35	1.25
1	B	371	GLU	CD-OE2	7.46	1.33	1.25
1	B	371	GLU	CG-CD	6.95	1.62	1.51
1	A	425	VAL	CB-CG2	-5.05	1.42	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	ARG	NE-CZ-NH2	-15.99	112.30	120.30
1	A	140	ARG	NE-CZ-NH1	14.29	127.44	120.30
1	B	498	ARG	NE-CZ-NH1	-13.28	113.66	120.30
1	D	140	ARG	NE-CZ-NH1	13.24	126.92	120.30
1	A	304	ARG	NE-CZ-NH1	-12.97	113.81	120.30
1	D	498	ARG	NE-CZ-NH1	-12.77	113.91	120.30
1	B	498	ARG	NE-CZ-NH2	12.62	126.61	120.30
1	D	498	ARG	NE-CZ-NH2	12.59	126.60	120.30
1	A	498	ARG	NE-CZ-NH2	-12.58	114.01	120.30
1	D	140	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	C	498	ARG	NE-CZ-NH2	-12.13	114.23	120.30
1	A	367	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	C	140	ARG	NE-CZ-NH2	11.45	126.02	120.30
1	B	304	ARG	NE-CZ-NH2	-11.13	114.74	120.30
1	C	367	ARG	NE-CZ-NH1	-10.78	114.91	120.30
1	A	498	ARG	NE-CZ-NH1	10.56	125.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	367	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	A	304	ARG	NE-CZ-NH2	10.50	125.55	120.30
1	C	498	ARG	NE-CZ-NH1	10.41	125.51	120.30
1	C	367	ARG	NE-CZ-NH2	9.93	125.27	120.30
1	C	140	ARG	NE-CZ-NH1	-9.91	115.34	120.30
1	B	304	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	B	140	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	B	140	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	A	360	LEU	CB-CG-CD1	7.75	124.17	111.00
1	A	360	LEU	CA-CB-CG	7.29	132.07	115.30
1	A	140	ARG	CD-NE-CZ	6.68	132.95	123.60
1	D	498	ARG	CD-NE-CZ	6.54	132.76	123.60
1	A	360	LEU	CB-CG-CD2	-6.27	100.33	111.00
1	B	498	ARG	CD-NE-CZ	6.24	132.34	123.60
1	D	140	ARG	CD-NE-CZ	6.14	132.20	123.60
1	C	302	LEU	CB-CG-CD2	-6.09	100.64	111.00
1	B	360	LEU	CB-CG-CD1	-6.09	100.65	111.00
1	A	367	ARG	CD-NE-CZ	5.88	131.83	123.60
1	C	367	ARG	CD-NE-CZ	5.76	131.66	123.60
1	C	140	ARG	CD-NE-CZ	5.64	131.50	123.60
1	B	140	ARG	CD-NE-CZ	5.16	130.83	123.60
1	A	467	LEU	CB-CG-CD1	5.14	119.75	111.00
1	A	498	ARG	CD-NE-CZ	5.13	130.79	123.60
1	B	360	LEU	CB-CG-CD2	5.09	119.65	111.00

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	3738	0	3492	67	0
1	B	3587	0	3236	60	0
1	C	3496	0	3151	58	0
1	D	3103	0	2428	42	0
All	All	13924	0	12307	212	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 8.

All (212) 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:506:ILE:HB	1:D:549:GLU:HG3	1.52	0.91
1:B:439:PRO:HB3	1:B:469:LEU:HD11	1.58	0.86
1:D:354:LEU:HD22	1:D:455:VAL:HG13	1.59	0.82
1:C:299:ALA:HA	1:C:302:LEU:HD12	1.62	0.82
1:C:470:VAL:O	1:C:474:THR:HG23	1.82	0.79
1:A:470:VAL:O	1:A:474:THR:HG23	1.83	0.79
1:C:42:GLN:CB	1:C:43:GLY:HA3	2.12	0.79
1:A:439:PRO:HB3	1:A:469:LEU:HD11	1.66	0.78
1:D:470:VAL:O	1:D:474:THR:HG23	1.84	0.77
1:B:301:ASN:HB3	1:B:304:ARG:CD	2.15	0.76
1:B:470:VAL:O	1:B:474:THR:HG23	1.84	0.76
1:A:318:LYS:HE2	1:A:475:SER:H	1.54	0.72
1:D:352:LEU:HG	1:D:352:LEU:O	1.90	0.70
1:A:413:LEU:HD22	1:A:434:VAL:CG1	2.21	0.70
1:A:29:SER:O	1:C:25:LYS:N	2.22	0.68
1:B:301:ASN:HB3	1:B:304:ARG:HD3	1.75	0.67
1:B:301:ASN:HB3	1:B:304:ARG:HD2	1.77	0.66
1:C:506:ILE:HB	1:D:549:GLU:CG	2.25	0.66
1:B:416:LEU:HD11	1:B:435:GLU:HB2	1.79	0.65
1:C:416:LEU:HD11	1:C:435:GLU:HB2	1.79	0.64
1:D:351:CYS:O	1:D:353:ARG:N	2.31	0.64
1:B:329:VAL:CG2	1:B:360:LEU:HD23	2.28	0.64
1:C:423:ASP:HA	1:C:426:GLY:O	1.98	0.64
1:C:42:GLN:CB	1:C:43:GLY:CA	2.75	0.64
1:B:423:ASP:HA	1:B:426:GLY:O	1.98	0.64
1:C:404:LEU:O	1:C:404:LEU:HD23	1.99	0.63
1:A:549:GLU:HB2	1:B:506:ILE:HB	1.81	0.62
1:C:506:ILE:CB	1:D:549:GLU:HG3	2.30	0.61
1:A:423:ASP:HA	1:A:426:GLY:O	1.99	0.61
1:C:155:VAL:HB	1:D:561:TYR:CE2	2.37	0.60
1:A:351:CYS:HB3	1:A:448:ILE:HD13	1.84	0.59
1:C:479:THR:HG22	1:C:503:ASN:HB2	1.83	0.59
1:A:301:ASN:O	1:A:304:ARG:HG2	2.02	0.59
1:B:354:LEU:HG	1:B:356:VAL:HG23	1.84	0.59
1:A:416:LEU:HD11	1:A:435:GLU:HB2	1.85	0.59
1:A:482:VAL:HG23	1:A:504:PHE:CZ	2.37	0.59
1:A:140:ARG:HG2	1:A:144:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:LEU:C	1:D:354:LEU:HD23	2.24	0.58
1:D:340:ALA:HB2	1:D:352:LEU:HD23	1.86	0.58
1:D:479:THR:HG22	1:D:503:ASN:HB2	1.86	0.58
1:A:80:TYR:CD2	1:A:90:LYS:HD3	2.38	0.58
1:A:412:SER:HB2	1:A:441:GLU:OE2	2.05	0.57
1:A:413:LEU:HD22	1:A:434:VAL:HG11	1.86	0.57
1:B:482:VAL:HG23	1:B:504:PHE:CZ	2.40	0.56
1:B:405:GLU:O	1:B:407:ALA:N	2.38	0.56
1:B:479:THR:HG22	1:B:503:ASN:HB2	1.88	0.56
1:D:549:GLU:OE1	1:D:551:HIS:CE1	2.58	0.56
1:B:61:MET:HB2	1:B:90:LYS:O	2.06	0.56
1:A:479:THR:HG22	1:A:503:ASN:HB2	1.88	0.56
1:B:405:GLU:C	1:B:407:ALA:H	2.07	0.55
1:A:354:LEU:HG	1:A:356:VAL:HG23	1.89	0.55
1:B:292:LYS:O	1:B:296:LYS:HG3	2.07	0.55
1:A:30:LEU:HD13	1:C:24:TRP:CD2	2.42	0.55
1:D:321:HIS:CD2	1:D:352:LEU:HD11	2.41	0.55
1:D:354:LEU:HD23	1:D:355:TYR:N	2.22	0.55
1:A:448:ILE:O	1:A:449:PHE:HB2	2.07	0.54
1:C:448:ILE:O	1:C:449:PHE:HB2	2.07	0.54
1:D:165:GLU:O	1:D:169:PHE:CD2	2.61	0.54
1:A:293:HIS:O	1:A:297:GLN:HG3	2.08	0.54
1:C:29:SER:OG	1:C:30:LEU:N	2.40	0.54
1:A:409:SER:OG	1:A:410:SER:N	2.40	0.54
1:A:549:GLU:HG3	1:A:549:GLU:O	2.06	0.53
1:A:539:LEU:O	1:A:542:THR:HG22	2.08	0.53
1:C:337:LEU:HD22	1:C:375:ILE:HD11	1.90	0.53
1:D:175:LYS:HZ2	1:D:179:GLU:CD	2.11	0.53
1:C:77:ASP:OD1	1:C:79:GLN:NE2	2.42	0.53
1:D:448:ILE:O	1:D:449:PHE:HB2	2.08	0.53
1:A:413:LEU:HD22	1:A:434:VAL:HG12	1.89	0.52
1:B:349:SER:HA	1:B:449:PHE:CZ	2.44	0.52
1:B:407:ALA:C	1:B:409:SER:H	2.12	0.52
1:A:292:LYS:O	1:A:296:LYS:HG3	2.09	0.52
1:A:336:THR:HG21	1:A:354:LEU:HD22	1.90	0.52
1:C:404:LEU:HD21	1:C:419:GLY:O	2.10	0.52
1:B:77:ASP:OD1	1:B:79:GLN:NE2	2.41	0.52
1:D:159:GLU:O	1:D:163:ALA:HB3	2.10	0.52
1:D:349:SER:HB3	1:D:449:PHE:CE2	2.45	0.51
1:A:330:GLU:OE2	1:A:367:ARG:HD3	2.10	0.51
1:C:116:TRP:CZ2	1:C:124:ARG:HD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ARG:HG2	1:C:144:LEU:HD22	1.92	0.51
1:B:97:ALA:CB	1:B:101:LEU:HD23	2.41	0.51
1:D:232:TRP:O	1:D:234:PRO:HD3	2.11	0.51
1:A:352:LEU:HD12	1:A:353:ARG:N	2.26	0.50
1:A:509:LYS:HD2	1:A:511:THR:OG1	2.11	0.50
1:A:116:TRP:CZ2	1:A:124:ARG:HD2	2.47	0.50
1:D:175:LYS:O	1:D:179:GLU:HG3	2.10	0.50
1:A:508:ASP:HA	1:B:554:LEU:HD11	1.92	0.50
1:B:120:PRO:O	1:B:123:ASP:HB2	2.12	0.50
1:B:448:ILE:O	1:B:449:PHE:HB2	2.11	0.49
1:A:508:ASP:OD1	1:A:509:LYS:N	2.45	0.49
1:D:508:ASP:OD1	1:D:509:LYS:N	2.45	0.49
1:C:293:HIS:O	1:C:297:GLN:HG3	2.13	0.49
1:B:357:PRO:HG2	1:B:360:LEU:HB2	1.95	0.49
1:A:61:MET:HB2	1:A:90:LYS:O	2.13	0.48
1:C:549:GLU:HG3	1:C:550:THR:N	2.27	0.48
1:A:337:LEU:HD22	1:A:375:ILE:HD11	1.95	0.48
1:D:116:TRP:CZ2	1:D:124:ARG:HD2	2.49	0.48
1:B:116:TRP:CZ2	1:B:124:ARG:HD2	2.49	0.48
1:C:302:LEU:HD11	1:D:295:TRP:CD1	2.49	0.48
1:C:121:ILE:HD12	1:C:124:ARG:HH21	1.79	0.48
1:A:97:ALA:CB	1:A:101:LEU:HD23	2.44	0.48
1:B:509:LYS:HD2	1:B:511:THR:OG1	2.14	0.47
1:D:439:PRO:HG3	1:D:456:TYR:CZ	2.49	0.47
1:A:324:HIS:HB3	1:A:484:SER:HB2	1.96	0.47
1:B:293:HIS:O	1:B:297:GLN:HG3	2.14	0.47
1:B:479:THR:HB	1:B:510:SER:HB2	1.96	0.47
1:A:24:TRP:HZ2	1:C:126:GLN:OE1	1.98	0.47
1:A:361:TRP:CZ2	1:A:365:LYS:HD2	2.48	0.47
1:A:505:TYR:CD1	1:A:510:SER:HA	2.50	0.47
1:A:352:LEU:HD12	1:A:353:ARG:H	1.78	0.47
1:A:367:ARG:NH2	1:A:371:GLU:OE2	2.30	0.47
1:B:401:LYS:O	1:B:404:LEU:HB2	2.15	0.47
1:B:439:PRO:HG3	1:B:456:TYR:CZ	2.49	0.47
1:C:301:ASN:O	1:C:304:ARG:HG2	2.14	0.47
1:D:222:ALA:HB3	1:D:223:PRO:HD3	1.96	0.47
1:D:215:ILE:O	1:D:219:LEU:HG	2.14	0.47
1:C:508:ASP:OD1	1:C:509:LYS:N	2.47	0.47
1:B:329:VAL:CG2	1:B:360:LEU:CD2	2.92	0.46
1:D:320:PHE:HA	1:D:353:ARG:O	2.16	0.46
1:A:438:ASP:HB3	1:A:441:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:GLU:OE2	1:A:465:GLU:N	2.47	0.46
1:B:324:HIS:HB3	1:B:484:SER:HB2	1.97	0.46
1:B:486:ASP:OD1	1:B:486:ASP:C	2.55	0.45
1:B:486:ASP:OD1	1:B:488:ASP:N	2.49	0.45
1:C:91:VAL:HG11	1:C:149:VAL:HG12	1.97	0.45
1:C:549:GLU:HB2	1:D:506:ILE:HB	1.97	0.45
1:B:116:TRP:CG	1:B:258:ILE:HD12	2.51	0.45
1:B:479:THR:CG2	1:B:503:ASN:HB2	2.46	0.45
1:C:232:TRP:O	1:C:234:PRO:HD3	2.16	0.45
1:C:508:ASP:HB2	1:D:550:THR:OG1	2.16	0.45
1:A:393:ASP:OD1	1:A:396:SER:CB	2.64	0.45
1:B:91:VAL:HG11	1:B:149:VAL:HG12	1.98	0.45
1:C:159:GLU:O	1:C:163:ALA:HB3	2.17	0.45
1:A:159:GLU:O	1:A:163:ALA:HB3	2.17	0.45
1:B:407:ALA:O	1:B:409:SER:N	2.50	0.45
1:D:505:TYR:CD1	1:D:510:SER:HA	2.51	0.45
1:C:222:ALA:HB3	1:C:223:PRO:HD3	1.99	0.45
1:A:215:ILE:O	1:A:219:LEU:HG	2.17	0.44
1:A:482:VAL:CG2	1:A:504:PHE:HZ	2.29	0.44
1:B:140:ARG:HG2	1:B:144:LEU:HD22	1.98	0.44
1:C:61:MET:HB2	1:C:90:LYS:O	2.17	0.44
1:A:232:TRP:O	1:A:234:PRO:HD3	2.17	0.44
1:A:392:ILE:HG23	1:A:393:ASP:N	2.30	0.44
1:B:505:TYR:CD1	1:B:510:SER:HA	2.51	0.44
1:C:35:GLU:CD	1:C:36:PRO:HD2	2.37	0.44
1:C:342:GLU:OE2	1:D:559:TYR:HE2	2.01	0.44
1:C:439:PRO:HG3	1:C:456:TYR:CZ	2.53	0.44
1:B:329:VAL:HG22	1:B:360:LEU:HD23	1.96	0.44
1:B:328:ASP:O	1:B:332:VAL:HG23	2.18	0.44
1:B:389:SER:OG	1:B:390:ALA:N	2.51	0.44
1:A:410:SER:HA	1:A:411:PRO:HD3	1.68	0.44
1:B:349:SER:HA	1:B:449:PHE:CE2	2.53	0.44
1:C:369:LEU:HD12	1:C:369:LEU:HA	1.74	0.44
1:C:389:SER:OG	1:C:390:ALA:N	2.50	0.44
1:B:508:ASP:OD1	1:B:509:LYS:N	2.50	0.43
1:C:392:ILE:HG23	1:C:393:ASP:N	2.33	0.43
1:D:324:HIS:HB3	1:D:484:SER:HB2	2.00	0.43
1:A:482:VAL:CG2	1:A:504:PHE:CZ	3.01	0.43
1:B:287:SER:HB2	1:B:289:PRO:HD2	2.01	0.43
1:C:479:THR:CG2	1:C:503:ASN:HB2	2.48	0.43
1:A:222:ALA:HB3	1:A:223:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:HD11	1:D:295:TRP:CE2	2.54	0.43
1:D:348:CYS:HB3	1:D:478:LEU:HD23	2.00	0.43
1:D:410:SER:HA	1:D:411:PRO:HD3	1.72	0.43
1:B:97:ALA:HB1	1:B:101:LEU:HD23	2.01	0.43
1:B:410:SER:HA	1:B:411:PRO:HD3	1.71	0.43
1:A:120:PRO:O	1:A:123:ASP:HB2	2.18	0.43
1:B:153:LYS:HG2	1:B:343:TYR:CE1	2.54	0.43
1:A:318:LYS:CE	1:A:475:SER:H	2.28	0.42
1:D:116:TRP:CG	1:D:258:ILE:HD12	2.55	0.42
1:A:413:LEU:HA	1:A:413:LEU:HD23	1.84	0.42
1:D:292:LYS:O	1:D:296:LYS:HG3	2.18	0.42
1:D:479:THR:HB	1:D:510:SER:HB2	2.02	0.42
1:C:144:LEU:HD12	1:C:144:LEU:HA	1.87	0.42
1:C:348:CYS:O	1:C:449:PHE:CD1	2.73	0.42
1:C:505:TYR:HA	1:D:548:LYS:O	2.20	0.42
1:B:159:GLU:O	1:B:163:ALA:HB3	2.18	0.42
1:C:119:LYS:HA	1:C:120:PRO:HD3	1.94	0.42
1:A:378:GLY:H	1:A:386:THR:HG23	1.83	0.42
1:B:407:ALA:C	1:B:409:SER:N	2.73	0.42
1:B:392:ILE:HG23	1:B:393:ASP:N	2.35	0.41
1:B:482:VAL:CG2	1:B:504:PHE:HZ	2.33	0.41
1:B:482:VAL:CG2	1:B:504:PHE:CZ	3.02	0.41
1:C:97:ALA:CB	1:C:101:LEU:HD23	2.51	0.41
1:C:185:PRO:HD2	1:C:194:SER:HA	2.01	0.41
1:A:80:TYR:CE2	1:A:93:LYS:HG3	2.55	0.41
1:A:119:LYS:HA	1:A:120:PRO:HD3	1.97	0.41
1:B:461:ASP:OD2	1:B:462:LYS:HG3	2.20	0.41
1:C:153:LYS:HG2	1:C:343:TYR:CE1	2.56	0.41
1:B:232:TRP:O	1:B:234:PRO:HD3	2.21	0.41
1:C:505:TYR:CD1	1:C:510:SER:HA	2.55	0.41
1:B:405:GLU:C	1:B:407:ALA:N	2.72	0.41
1:B:462:LYS:O	1:B:465:GLU:HG2	2.20	0.41
1:A:163:ALA:O	1:A:164:ALA:C	2.58	0.41
1:C:328:ASP:O	1:C:332:VAL:HG23	2.21	0.41
1:A:479:THR:HB	1:A:510:SER:HB2	2.02	0.41
1:B:288:VAL:HB	1:B:289:PRO:HD3	2.03	0.41
1:C:120:PRO:O	1:C:123:ASP:HB2	2.21	0.41
1:C:410:SER:HA	1:C:411:PRO:HD3	1.70	0.41
1:A:116:TRP:CG	1:A:258:ILE:HD12	2.55	0.41
1:C:354:LEU:HB2	1:C:453:LEU:HD11	2.02	0.41
1:D:35:GLU:CD	1:D:36:PRO:HD2	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:MET:HG2	1:D:153:LYS:O	2.21	0.40
1:A:35:GLU:CD	1:A:36:PRO:HD2	2.41	0.40
1:C:191:SER:HA	1:C:549:GLU:O	2.21	0.40
1:A:61:MET:O	1:A:61:MET:CG	2.68	0.40
1:A:77:ASP:OD1	1:A:79:GLN:NE2	2.54	0.40
1:C:337:LEU:CD2	1:C:375:ILE:HD11	2.51	0.40
1:C:393:ASP:OD1	1:C:396:SER:CB	2.70	0.40
1:A:361:TRP:HB3	1:A:362:PRO:HD3	2.04	0.40
1:A:375:ILE:HG21	1:A:375:ILE:HD13	1.81	0.40
1:A:431:PRO:HA	1:A:451:PRO:HB2	2.04	0.40
1:B:35:GLU:CD	1:B:36:PRO:HD2	2.42	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	498/566 (88%)	477 (96%)	20 (4%)	1 (0%)	47	75
1	B	492/566 (87%)	462 (94%)	25 (5%)	5 (1%)	15	40
1	C	480/566 (85%)	459 (96%)	20 (4%)	1 (0%)	47	75
1	D	454/566 (80%)	431 (95%)	22 (5%)	1 (0%)	47	75
All	All	1924/2264 (85%)	1829 (95%)	87 (4%)	8 (0%)	34	62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	406	HIS
1	D	352	LEU
1	B	408	ARG
1	B	405	GLU

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Mol	Chain	Res	Type
1	B	164	ALA
1	B	181	GLU
1	C	404	LEU
1	A	540	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/464 (77%)	340 (95%)	17 (5%)	25	55
1	B	315/464 (68%)	301 (96%)	14 (4%)	28	58
1	C	311/464 (67%)	292 (94%)	19 (6%)	18	43
1	D	201/464 (43%)	194 (96%)	7 (4%)	36	67
All	All	1184/1856 (64%)	1127 (95%)	57 (5%)	25	55

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	61	MET
1	A	143	ILE
1	A	144	LEU
1	A	194	SER
1	A	337	LEU
1	A	360	LEU
1	A	369	LEU
1	A	440	GLN
1	A	460	ASP
1	A	463	TYR
1	A	465	GLU
1	A	467	LEU
1	A	469	LEU
1	A	473	THR
1	A	479	THR
1	A	549	GLU

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Mol	Chain	Res	Type
1	B	27	THR
1	B	32	VAL
1	B	61	MET
1	B	143	ILE
1	B	144	LEU
1	B	194	SER
1	B	360	LEU
1	B	369	LEU
1	B	460	ASP
1	B	463	TYR
1	B	465	GLU
1	B	469	LEU
1	B	479	THR
1	B	538	ILE
1	C	27	THR
1	C	32	VAL
1	C	61	MET
1	C	121	ILE
1	C	143	ILE
1	C	144	LEU
1	C	165	GLU
1	C	194	SER
1	C	302	LEU
1	C	337	LEU
1	C	354	LEU
1	C	369	LEU
1	C	425	VAL
1	C	460	ASP
1	C	463	TYR
1	C	479	THR
1	C	539	LEU
1	C	543	SER
1	C	549	GLU
1	D	32	VAL
1	D	143	ILE
1	D	321	HIS
1	D	454	SER
1	D	479	THR
1	D	549	GLU
1	D	550	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	506/566 (89%)	-0.07	5 (0%)	82	81	26, 47, 77, 115	0
1	B	502/566 (88%)	-0.12	2 (0%)	92	92	25, 52, 81, 117	0
1	C	492/566 (86%)	-0.12	9 (1%)	68	66	28, 56, 82, 113	0
1	D	482/566 (85%)	0.11	18 (3%)	41	36	24, 67, 104, 136	0
All	All	1982/2264 (87%)	-0.05	34 (1%)	70	68	24, 55, 90, 136	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	560	ALA	4.8
1	D	409	SER	4.3
1	D	149	VAL	4.3
1	D	427	TYR	3.9
1	D	84	PRO	3.4
1	B	412	SER	3.2
1	C	461	ASP	3.1
1	B	411	PRO	3.1
1	C	460	ASP	3.0
1	D	76	SER	2.9
1	D	466	THR	2.8
1	A	178	VAL	2.8
1	C	488	ASP	2.7
1	C	439	PRO	2.7
1	A	557	TRP	2.6
1	D	150	GLY	2.6
1	D	74	TRP	2.6
1	D	412	SER	2.6
1	A	562	MET	2.6
1	D	85	PHE	2.4
1	D	39	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	458	TYR	2.4
1	D	322	PHE	2.2
1	D	53	ALA	2.2
1	A	409	SER	2.2
1	C	359	SER	2.2
1	D	86	ASN	2.2
1	C	412	SER	2.1
1	C	411	PRO	2.1
1	D	436	SER	2.1
1	C	24	TRP	2.1
1	D	454	SER	2.1
1	C	538	ILE	2.1
1	D	49	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.