Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 04:12 PM BST

PDB ID	:	6GPG
Title	:	Structure of the RIG-I Singleton-Merten syndrome variant C268F
Authors	:	Laessig, C.; Lammens, K.; Hopfer, K.-P.
Deposited on	:	2018-06-05
Resolution	:	2.89 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 following versions of software and data (see references ①) were used in the production of this report:

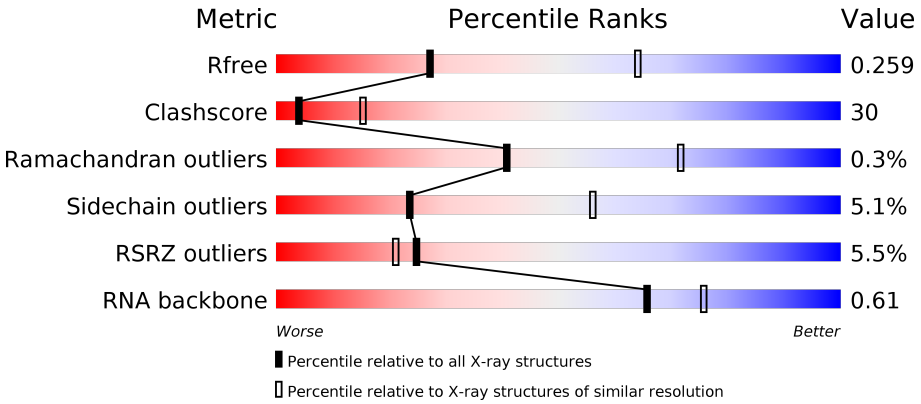
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 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	B	14	29% 57% 7% 7%
1	C	14	21% 43% 29% 7%
2	A	714	5% 51% 37% • • 9%

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
4	MG	A	1002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5812 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 RNA chain called RNA (5'-R(*CP*GP*AP*CP*GP*CP*UP*AP*GP*CP*GP*UP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	13	Total	C	N	O	P	0	0	0
			273	123	49	89	12			
1	C	13	Total	C	N	O	P	0	0	0
			279	124	51	91	13			

- Molecule 2 is a protein called Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	651	Total	C	N	O	S	0	0	0
			5258	3369	893	966	30			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	MET	-	initiating methionine	UNP O95786
A	213	HIS	-	expression tag	UNP O95786
A	214	HIS	-	expression tag	UNP O95786
A	215	HIS	-	expression tag	UNP O95786
A	216	HIS	-	expression tag	UNP O95786
A	217	HIS	-	expression tag	UNP O95786
A	218	HIS	-	expression tag	UNP O95786
A	219	SER	-	expression tag	UNP O95786
A	220	SER	-	expression tag	UNP O95786
A	221	GLY	-	expression tag	UNP O95786
A	222	LEU	-	expression tag	UNP O95786
A	223	GLU	-	expression tag	UNP O95786
A	224	VAL	-	expression tag	UNP O95786
A	225	LEU	-	expression tag	UNP O95786
A	226	PHE	-	expression tag	UNP O95786
A	227	GLN	-	expression tag	UNP O95786
A	228	GLY	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
A	229	PRO	-	expression tag	UNP O95786
A	230	HIS	-	expression tag	UNP O95786
A	231	MET	-	expression tag	UNP O95786
A	268	PHE	CYS	engineered mutation	UNP O95786

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

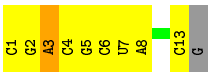
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

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

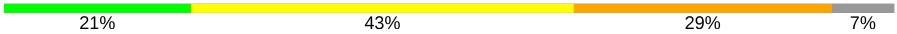
- Molecule 1: RNA (5'-R(*CP*GP*AP*CP*GP*CP*UP*AP*GP*CP*GP*UP*CP*G)-3')

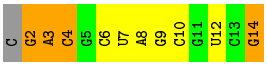
Chain B:



- Molecule 1: RNA (5'-R(*CP*GP*AP*CP*GP*CP*UP*AP*GP*CP*GP*UP*CP*G)-3')

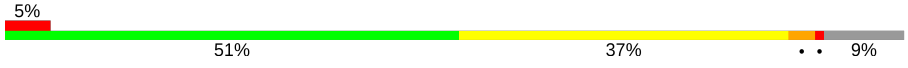
Chain C:

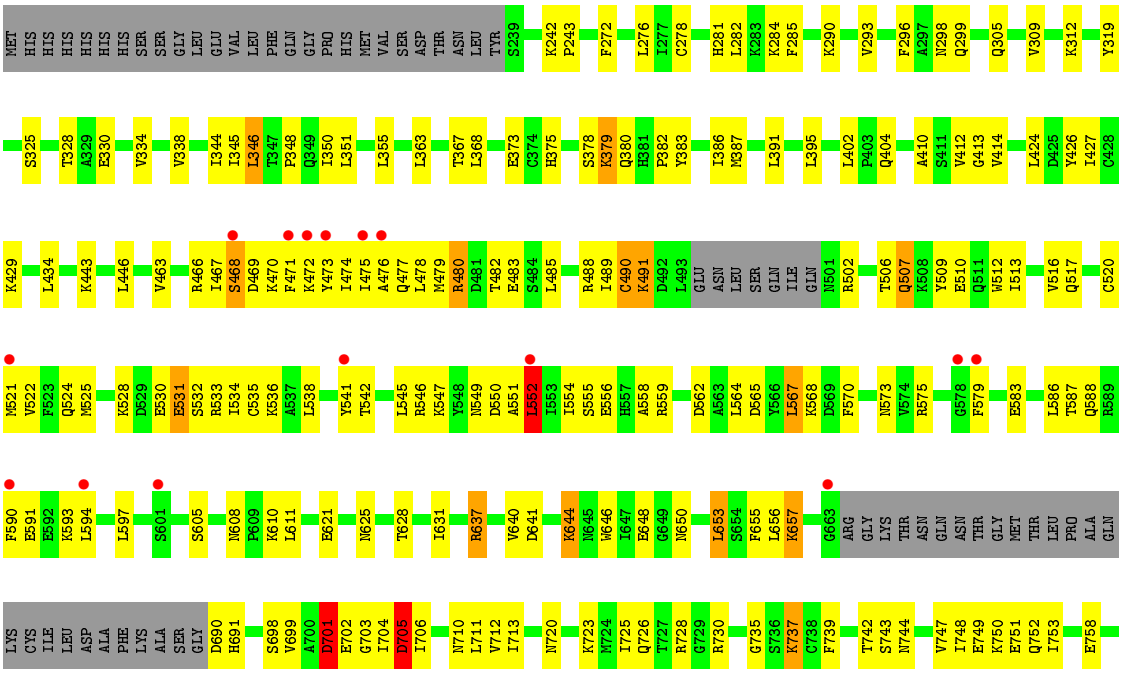


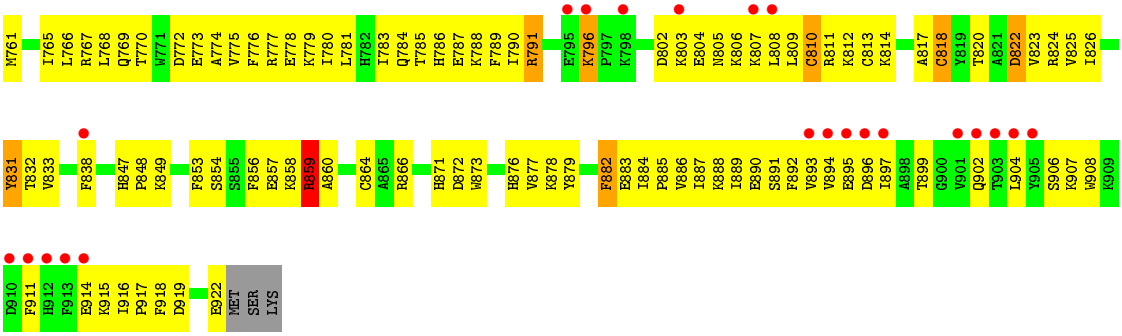


- Molecule 2: Probable ATP-dependent RNA helicase DDX58

Chain A:






M761
I765
L766
R767
L768
Q769
T770
W771
D772
E773
A774
V775
F776
R777
E778
K779
I780
L781
H782
I783
Q784
T785
H786
E787
K788
F789
I790
R791
E795
K796
P797
K798
D802
K803
E804
N805
K806
K807
L808
L809
C810
R811
K812
C813
K814
A817
C818
Y819
T820
A821
D822
V823
R824
V825
I826
Y831
T832
V833
F838
H847
P848
K849
F853
S854
S855
F856
E857
K858
R859
A860
C864
A865
R866
H871
D872
W873
H876
V877
K878
Y879
F882
E883
I884
P885
V886
I887
K888
I889
E890
S891
F892
V893
V894
E895
D896
I897
A898
T899
G900
V901
Q902
T903
L904
Y905
S906
K907
W908
K909
D910
F911
H912
P913
E914
K915
I916
P917
F918
D919
E922
MET
SER
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	175.62Å 175.62Å 109.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.47 – 2.89 46.47 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.47-2.89) 99.7 (46.47-2.89)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.210 , 0.260 0.214 , 0.259	Depositor DCC
R_{free} test set	1110 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	108.1	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 101.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5812	wwPDB-VP
Average B, all atoms (Å^2)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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

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

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	B	0.49	0/304	1.08	0/472
1	C	0.49	0/311	1.09	1/483 (0.2%)
2	A	0.47	0/5368	0.70	5/7237 (0.1%)
All	All	0.47	0/5983	0.75	6/8192 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	859	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	A	567	LEU	CA-CB-CG	6.58	130.44	115.30
2	A	705	ASP	CB-CG-OD1	6.55	124.19	118.30
1	C	4	C	C5-C6-N1	5.60	123.80	121.00
2	A	653	LEU	CA-CB-CG	5.26	127.41	115.30
2	A	552	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	346	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	A	378	SER	Peptide
2	A	507	GLN	Peptide
2	A	701	ASP	Peptide
2	A	853	PHE	Peptide
2	A	879	TYR	Peptide

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	B	273	0	143	16	0
1	C	279	0	142	9	0
2	A	5258	0	5304	331	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
All	All	5812	0	5589	343	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 30.

All (343) 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)
2:A:847:HIS:CG	2:A:858:LYS:HZ1	1.27	1.48
2:A:847:HIS:CG	2:A:858:LYS:NZ	1.98	1.27
2:A:657:LYS:HZ2	2:A:691:HIS:CA	1.51	1.24
2:A:786:HIS:O	2:A:790:ILE:HD12	1.37	1.22
2:A:847:HIS:CD2	2:A:858:LYS:NZ	2.14	1.15
2:A:657:LYS:NZ	2:A:691:HIS:HA	1.64	1.13
2:A:657:LYS:HZ2	2:A:691:HIS:HA	0.99	1.08
2:A:653:LEU:HB2	2:A:656:LEU:CD2	1.85	1.06
2:A:282:LEU:HD13	2:A:319:TYR:CE1	1.91	1.05
2:A:787:GLU:HA	2:A:790:ILE:HD13	1.33	1.05
2:A:653:LEU:HB2	2:A:656:LEU:HD23	1.02	0.99
2:A:608:ASN:HB3	2:A:611:LEU:HD23	1.43	0.97
2:A:588:GLN:HA	2:A:591:GLU:HG2	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:653:LEU:CB	2:A:656:LEU:HD23	1.96	0.96
2:A:657:LYS:HZ2	2:A:691:HIS:N	1.64	0.96
2:A:847:HIS:CD2	2:A:858:LYS:HZ1	1.80	0.93
2:A:742:THR:HG22	2:A:744:ASN:H	1.30	0.93
2:A:282:LEU:CD1	2:A:319:TYR:CZ	2.56	0.89
2:A:847:HIS:CD2	2:A:858:LYS:HZ2	1.87	0.86
2:A:786:HIS:O	2:A:790:ILE:CD1	2.24	0.84
2:A:541:TYR:HE1	2:A:586:LEU:HD11	1.40	0.84
2:A:847:HIS:CB	2:A:858:LYS:NZ	2.41	0.83
2:A:344:ILE:HG22	2:A:346:LEU:CD1	2.10	0.82
2:A:467:ILE:CD1	2:A:468:SER:HB2	2.08	0.82
2:A:778:GLU:N	2:A:778:GLU:OE1	2.13	0.81
2:A:470:LYS:N	2:A:470:LYS:HE2	1.95	0.80
2:A:787:GLU:HA	2:A:790:ILE:CD1	2.12	0.80
2:A:536:LYS:NZ	2:A:811:ARG:O	2.14	0.80
2:A:774:ALA:O	2:A:778:GLU:OE1	1.98	0.80
2:A:810:CYS:SG	2:A:813:CYS:N	2.55	0.80
2:A:477:GLN:HA	2:A:480:ARG:HD3	1.62	0.80
1:B:6:C:P	2:A:379:LYS:HZ1	2.05	0.79
2:A:657:LYS:HZ1	2:A:690:ASP:HB3	1.47	0.78
2:A:871:HIS:HB3	2:A:873:TRP:HE1	1.48	0.78
2:A:520:CYS:SG	2:A:538:LEU:HD11	2.24	0.78
2:A:375:HIS:NE2	2:A:701:ASP:OD2	2.15	0.78
2:A:344:ILE:HG22	2:A:346:LEU:HD11	1.66	0.77
2:A:525:MET:HG3	2:A:531:GLU:HB3	1.66	0.77
2:A:657:LYS:NZ	2:A:690:ASP:C	2.39	0.76
2:A:804:GLU:HB2	2:A:806:LYS:HE3	1.68	0.76
2:A:550:ASP:O	2:A:554:ILE:HD12	1.86	0.75
2:A:285:PHE:HZ	2:A:367:THR:HG21	1.52	0.74
2:A:887:ILE:CD1	2:A:908:TRP:HH2	2.01	0.74
2:A:485:LEU:O	2:A:488:ARG:HG2	1.88	0.73
2:A:657:LYS:HZ2	2:A:690:ASP:C	1.91	0.73
2:A:786:HIS:C	2:A:790:ILE:HD12	2.08	0.73
2:A:657:LYS:NZ	2:A:691:HIS:CA	2.36	0.73
2:A:467:ILE:HD12	2:A:468:SER:HB2	1.69	0.72
2:A:882:PHE:HB2	2:A:884:ILE:HD11	1.71	0.71
2:A:467:ILE:HD12	2:A:468:SER:N	2.05	0.71
2:A:742:THR:HG21	2:A:747:VAL:HB	1.71	0.71
2:A:847:HIS:CB	2:A:858:LYS:HZ3	2.03	0.71
2:A:282:LEU:CD1	2:A:319:TYR:CE1	2.68	0.70
2:A:860:ALA:HB3	2:A:876:HIS:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:847:HIS:HB3	2:A:858:LYS:HZ3	1.56	0.70
2:A:587:THR:HG22	2:A:591:GLU:OE2	1.91	0.69
2:A:786:HIS:C	2:A:790:ILE:CD1	2.61	0.69
1:C:8:A:H2'	1:C:9:G:C8	2.27	0.69
2:A:583:GLU:OE2	2:A:583:GLU:N	2.25	0.69
2:A:812:LYS:O	2:A:812:LYS:HG3	1.92	0.69
2:A:742:THR:CG2	2:A:744:ASN:H	2.06	0.68
2:A:325:SER:H	2:A:328:THR:HG22	1.59	0.68
2:A:474:ILE:HD13	2:A:597:LEU:HD21	1.76	0.68
2:A:282:LEU:HD13	2:A:319:TYR:CZ	2.24	0.68
2:A:509:TYR:HD2	2:A:549:ASN:HD22	1.40	0.68
2:A:558:ALA:HA	2:A:611:LEU:HD21	1.75	0.68
2:A:575:ARG:HG3	2:A:579:PHE:CZ	2.29	0.68
2:A:525:MET:HG3	2:A:531:GLU:CB	2.23	0.67
2:A:725:ILE:HD11	2:A:758:GLU:HG3	1.74	0.67
2:A:657:LYS:CE	2:A:691:HIS:HA	2.24	0.67
2:A:887:ILE:HD11	2:A:908:TRP:HH2	1.60	0.67
2:A:541:TYR:CE1	2:A:586:LEU:HD11	2.29	0.66
2:A:610:LYS:HE2	2:A:743:SER:HB3	1.78	0.66
2:A:806:LYS:HB2	2:A:820:THR:HG23	1.78	0.66
2:A:657:LYS:NZ	2:A:691:HIS:N	2.42	0.65
2:A:814:LYS:NZ	2:A:902:GLN:HE21	1.93	0.65
2:A:895:GLU:HG3	2:A:902:GLN:HB3	1.78	0.65
2:A:522:VAL:HG12	2:A:902:GLN:HG2	1.78	0.64
2:A:887:ILE:CD1	2:A:908:TRP:CH2	2.81	0.64
2:A:480:ARG:HA	2:A:483:GLU:HG2	1.80	0.64
2:A:476:ALA:O	2:A:480:ARG:HD2	1.98	0.64
2:A:575:ARG:HG3	2:A:579:PHE:HZ	1.62	0.64
2:A:847:HIS:HD2	2:A:849:LYS:H	1.44	0.64
2:A:796:LYS:HD3	2:A:796:LYS:H	1.63	0.63
2:A:810:CYS:SG	2:A:811:ARG:N	2.71	0.63
2:A:477:GLN:HA	2:A:480:ARG:CD	2.29	0.63
1:B:1:C:H5"	2:A:888:LYS:HG2	1.81	0.62
1:C:10:C:OP1	2:A:637:ARG:HG2	1.99	0.62
2:A:876:HIS:NE2	2:A:883:GLU:OE1	2.32	0.62
2:A:787:GLU:CA	2:A:790:ILE:HD13	2.20	0.62
2:A:535:CYS:O	2:A:536:LYS:HE2	1.99	0.62
2:A:346:LEU:HG	2:A:350:ILE:HD11	1.82	0.62
2:A:805:ASN:C	2:A:806:LYS:HE2	2.20	0.62
2:A:824:ARG:HH21	2:A:916:ILE:HD13	1.65	0.62
2:A:506:THR:HG22	2:A:507:GLN:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:467:ILE:HD13	2:A:468:SER:HB2	1.81	0.61
2:A:528:LYS:HA	2:A:531:GLU:HG2	1.83	0.61
2:A:810:CYS:SG	2:A:812:LYS:N	2.73	0.61
1:B:4:C:H5"	2:A:380:GLN:HB3	1.82	0.61
2:A:742:THR:HG22	2:A:744:ASN:N	2.10	0.60
2:A:521:MET:SD	2:A:904:LEU:HD11	2.41	0.60
2:A:424:LEU:CD2	2:A:768:LEU:HD22	2.31	0.59
2:A:657:LYS:NZ	2:A:690:ASP:HB3	2.17	0.59
2:A:774:ALA:O	2:A:778:GLU:CD	2.39	0.59
2:A:625:ASN:HB3	2:A:628:THR:HG23	1.84	0.59
2:A:765:ILE:O	2:A:769:GLN:HG3	2.03	0.59
2:A:847:HIS:CD2	2:A:849:LYS:H	2.20	0.59
1:B:1:C:H5"	2:A:888:LYS:CG	2.33	0.59
2:A:807:LYS:NZ	2:A:897:ILE:HA	2.18	0.59
2:A:412:VAL:HG23	2:A:413:GLY:O	2.03	0.58
2:A:325:SER:H	2:A:328:THR:CG2	2.17	0.58
2:A:463:VAL:O	2:A:743:SER:HA	2.04	0.58
1:C:8:A:H2'	1:C:9:G:H8	1.66	0.58
2:A:502:ARG:HD2	2:A:509:TYR:CE1	2.38	0.57
2:A:530:GLU:O	2:A:534:ILE:HG23	2.04	0.57
2:A:424:LEU:HD21	2:A:768:LEU:HD22	1.85	0.57
2:A:467:ILE:HD12	2:A:468:SER:CB	2.33	0.57
2:A:699:VAL:HG11	2:A:730:ARG:HH21	1.68	0.57
2:A:806:LYS:HE2	2:A:806:LYS:N	2.19	0.57
2:A:871:HIS:HD1	2:A:873:TRP:HD1	1.49	0.57
2:A:412:VAL:HG21	2:A:427:ILE:HG12	1.87	0.57
1:C:14:G:O2'	2:A:854:SER:HB3	2.05	0.57
2:A:644:LYS:NZ	2:A:648:GLU:OE2	2.37	0.56
2:A:856:PHE:HB3	2:A:877:VAL:CG2	2.36	0.56
2:A:856:PHE:HB3	2:A:877:VAL:HG21	1.87	0.56
2:A:806:LYS:HB2	2:A:820:THR:CG2	2.36	0.56
2:A:536:LYS:HD3	2:A:812:LYS:HA	1.87	0.56
2:A:473:TYR:O	2:A:477:GLN:NE2	2.38	0.56
2:A:559:ARG:HD3	2:A:646:TRP:HD1	1.70	0.56
2:A:474:ILE:HD11	2:A:597:LEU:HD11	1.88	0.56
2:A:482:THR:HB	2:A:545:LEU:HD21	1.88	0.56
2:A:859:ARG:NH1	2:A:878:LYS:HE3	2.20	0.55
2:A:889:ILE:HD11	2:A:908:TRP:CZ2	2.40	0.55
2:A:502:ARG:HD2	2:A:509:TYR:HE1	1.71	0.55
2:A:628:THR:HA	2:A:710:ASN:HD21	1.72	0.55
2:A:894:VAL:HG21	2:A:911:PHE:HE2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:305:GLN:O	2:A:309:VAL:HG12	2.06	0.55
2:A:509:TYR:HB3	2:A:549:ASN:ND2	2.20	0.55
2:A:787:GLU:O	2:A:791:ARG:HG2	2.07	0.55
2:A:876:HIS:HE1	2:A:883:GLU:HB2	1.72	0.55
2:A:296:PHE:HZ	2:A:351:LEU:HD23	1.72	0.54
2:A:535:CYS:C	2:A:536:LYS:HE2	2.28	0.54
2:A:608:ASN:HB3	2:A:611:LEU:CD2	2.27	0.54
2:A:894:VAL:HG21	2:A:911:PHE:CE2	2.42	0.54
2:A:424:LEU:HD22	2:A:768:LEU:CD2	2.37	0.54
2:A:550:ASP:O	2:A:554:ILE:CD1	2.55	0.54
2:A:831:TYR:HB2	2:A:908:TRP:CH2	2.43	0.54
2:A:475:ILE:O	2:A:479:MET:HG2	2.08	0.53
2:A:532:SER:O	2:A:536:LYS:HG2	2.08	0.53
2:A:919:ASP:OD1	2:A:922:GLU:N	2.40	0.53
2:A:808:LEU:O	2:A:808:LEU:HD12	2.08	0.53
2:A:344:ILE:CG2	2:A:346:LEU:HD11	2.38	0.53
2:A:650:ASN:HB3	2:A:653:LEU:HD21	1.89	0.53
2:A:334:VAL:O	2:A:338:VAL:HG23	2.09	0.53
2:A:781:LEU:O	2:A:785:THR:HG23	2.08	0.53
2:A:330:GLU:HG3	2:A:854:SER:O	2.09	0.52
2:A:772:ASP:HB3	2:A:775:VAL:HG12	1.91	0.52
2:A:896:ASP:HB3	2:A:899:THR:OG1	2.10	0.52
2:A:887:ILE:O	2:A:908:TRP:HZ3	1.93	0.52
2:A:469:ASP:HB2	2:A:472:LYS:HB3	1.92	0.52
2:A:809:LEU:HD23	2:A:814:LYS:O	2.09	0.52
2:A:556:GLU:O	2:A:608:ASN:ND2	2.39	0.51
2:A:871:HIS:CB	2:A:873:TRP:HE1	2.22	0.51
2:A:786:HIS:CG	2:A:790:ILE:HD11	2.45	0.51
2:A:282:LEU:HD12	2:A:319:TYR:CZ	2.43	0.51
2:A:768:LEU:HD12	2:A:776:PHE:CE1	2.45	0.51
2:A:535:CYS:SG	2:A:536:LYS:HE3	2.50	0.51
2:A:517:GLN:O	2:A:521:MET:HG3	2.10	0.51
2:A:513:ILE:O	2:A:516:VAL:HG22	2.10	0.51
2:A:713:ILE:HG23	2:A:739:PHE:HB2	1.93	0.51
2:A:872:ASP:C	2:A:873:TRP:HD1	2.14	0.51
2:A:590:PHE:CZ	2:A:594:LEU:HD12	2.46	0.50
2:A:641:ASP:HA	2:A:644:LYS:HG2	1.93	0.50
2:A:348:PRO:HB2	2:A:382:PRO:HB2	1.93	0.50
2:A:559:ARG:HD3	2:A:646:TRP:CD1	2.46	0.50
2:A:488:ARG:HG2	2:A:489:ILE:HD12	1.94	0.50
2:A:373:GLU:HG3	2:A:701:ASP:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:889:ILE:HG12	2:A:908:TRP:CE3	2.47	0.50
2:A:699:VAL:HG11	2:A:730:ARG:NH2	2.27	0.50
1:B:8:A:H5"	2:A:750:LYS:HE2	1.93	0.50
2:A:859:ARG:HH21	2:A:878:LYS:N	2.10	0.50
2:A:807:LYS:HZ1	2:A:897:ILE:HA	1.77	0.50
2:A:355:LEU:HD11	2:A:363:LEU:HD11	1.93	0.50
2:A:887:ILE:HD12	2:A:887:ILE:O	2.12	0.50
2:A:657:LYS:HE3	2:A:690:ASP:O	2.12	0.49
2:A:490:CYS:C	2:A:491:LYS:HD3	2.33	0.49
2:A:509:TYR:HD2	2:A:549:ASN:ND2	2.09	0.49
2:A:528:LYS:O	2:A:531:GLU:HG3	2.11	0.49
2:A:780:ILE:O	2:A:784:GLN:HB3	2.12	0.49
1:C:3:A:H2'	1:C:4:C:C6	2.46	0.49
2:A:298:ASN:N	2:A:298:ASN:OD1	2.45	0.49
2:A:893:VAL:HG22	2:A:904:LEU:HD21	1.93	0.49
2:A:890:GLU:HB3	2:A:906:SER:O	2.12	0.49
2:A:894:VAL:HG11	2:A:911:PHE:HZ	1.77	0.49
1:B:1:C:H2'	1:B:2:G:O4'	2.12	0.49
2:A:657:LYS:HD2	2:A:657:LYS:O	2.13	0.49
2:A:728:ARG:NH2	2:A:758:GLU:OE1	2.44	0.49
1:B:5:G:P	2:A:380:GLN:HB2	2.53	0.49
2:A:467:ILE:HD12	2:A:468:SER:H	1.78	0.49
2:A:502:ARG:HG2	2:A:502:ARG:HH21	1.78	0.49
1:B:7:U:H2'	1:B:8:A:C8	2.48	0.49
2:A:772:ASP:OD1	2:A:773:GLU:N	2.46	0.49
2:A:476:ALA:HA	2:A:479:MET:HG2	1.95	0.48
2:A:564:LEU:O	2:A:568:LYS:HG3	2.12	0.48
2:A:831:TYR:HB2	2:A:908:TRP:CZ2	2.48	0.48
2:A:873:TRP:N	2:A:873:TRP:CD1	2.80	0.48
2:A:282:LEU:HD13	2:A:319:TYR:CD1	2.47	0.48
2:A:859:ARG:HH21	2:A:877:VAL:C	2.17	0.48
2:A:565:ASP:HA	2:A:568:LYS:HE2	1.95	0.48
2:A:803:LYS:HG3	2:A:914:GLU:HG3	1.95	0.48
2:A:631:ILE:HG22	2:A:712:VAL:HG12	1.95	0.48
2:A:831:TYR:O	2:A:886:VAL:HG23	2.14	0.48
2:A:272:PHE:HE1	2:A:276:LEU:HD22	1.79	0.48
2:A:720:ASN:ND2	2:A:723:LYS:HD2	2.29	0.48
2:A:243:PRO:HB3	2:A:272:PHE:CE1	2.48	0.48
2:A:887:ILE:HD12	2:A:887:ILE:C	2.34	0.48
2:A:814:LYS:HZ1	2:A:902:GLN:HE21	1.59	0.48
2:A:637:ARG:HA	2:A:640:VAL:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:859:ARG:HH11	2:A:859:ARG:HG2	1.78	0.47
2:A:826:ILE:HD11	2:A:832:THR:HG23	1.96	0.47
2:A:876:HIS:CE1	2:A:883:GLU:HB2	2.50	0.47
2:A:653:LEU:HA	2:A:655:PHE:CE1	2.49	0.47
1:B:4:C:O3'	2:A:380:GLN:HB2	2.14	0.47
2:A:536:LYS:HA	2:A:536:LYS:HE2	1.96	0.47
2:A:808:LEU:HD11	2:A:818:CYS:SG	2.53	0.47
2:A:814:LYS:HZ3	2:A:902:GLN:HE21	1.62	0.47
1:B:6:C:P	2:A:379:LYS:NZ	2.83	0.47
2:A:281:HIS:CE1	2:A:368:LEU:HB2	2.49	0.47
2:A:414:VAL:HA	2:A:426:TYR:CD2	2.50	0.47
2:A:387:MET:HE2	2:A:434:LEU:HA	1.95	0.47
2:A:410:ALA:HB2	2:A:702:GLU:OE2	2.15	0.47
2:A:701:ASP:O	2:A:703:GLY:N	2.47	0.47
2:A:521:MET:HE2	2:A:811:ARG:HG2	1.96	0.47
1:B:3:A:P	2:A:907:LYS:HE2	2.55	0.47
2:A:391:LEU:O	2:A:395:LEU:HG	2.14	0.47
2:A:469:ASP:O	2:A:469:ASP:OD1	2.33	0.47
2:A:528:LYS:HA	2:A:531:GLU:CG	2.44	0.47
2:A:706:ILE:HG12	2:A:730:ARG:NH1	2.30	0.47
2:A:242:LYS:HG3	2:A:242:LYS:O	2.15	0.46
2:A:552:LEU:HA	2:A:555:SER:HB3	1.98	0.46
2:A:787:GLU:CA	2:A:790:ILE:CD1	2.87	0.46
2:A:507:GLN:HA	2:A:510:GLU:HG2	1.98	0.46
2:A:474:ILE:HD12	2:A:475:ILE:N	2.31	0.46
2:A:520:CYS:CB	2:A:538:LEU:HD11	2.45	0.46
2:A:424:LEU:CD2	2:A:768:LEU:CD2	2.93	0.46
2:A:825:VAL:HG11	2:A:915:LYS:HG3	1.97	0.46
2:A:811:ARG:HG3	2:A:892:PHE:HA	1.98	0.46
2:A:806:LYS:HE2	2:A:806:LYS:CA	2.46	0.46
2:A:547:LYS:HA	2:A:550:ASP:OD2	2.16	0.45
2:A:808:LEU:CD1	2:A:817:ALA:HB3	2.47	0.45
2:A:859:ARG:CZ	2:A:878:LYS:HG3	2.46	0.45
1:C:12:U:H5"	2:A:299:GLN:HE21	1.82	0.45
2:A:766:LEU:O	2:A:770:THR:HG23	2.17	0.45
2:A:808:LEU:HD12	2:A:818:CYS:H	1.82	0.45
2:A:857:GLU:O	2:A:877:VAL:HG23	2.17	0.45
2:A:780:ILE:HG13	2:A:781:LEU:N	2.32	0.45
2:A:802:ASP:HB2	2:A:804:GLU:OE1	2.17	0.45
2:A:825:VAL:HG12	2:A:917:PRO:HA	1.98	0.45
2:A:513:ILE:HA	2:A:513:ILE:HD13	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:426:TYR:O	2:A:429:LYS:HG2	2.17	0.44
2:A:779:LYS:O	2:A:783:ILE:HD12	2.18	0.44
2:A:884:ILE:HG22	2:A:885:PRO:O	2.17	0.44
1:B:4:C:H2'	1:B:5:G:H8	1.82	0.44
2:A:474:ILE:O	2:A:478:LEU:HD23	2.18	0.44
2:A:761:MET:O	2:A:765:ILE:HG13	2.17	0.44
1:B:5:G:OP1	2:A:380:GLN:HB2	2.17	0.44
2:A:702:GLU:HG2	2:A:726:GLN:HG2	2.00	0.44
2:A:777:ARG:HA	2:A:780:ILE:HG12	1.99	0.44
2:A:383:TYR:HA	2:A:386:ILE:HD12	1.98	0.44
2:A:859:ARG:CZ	2:A:859:ARG:HB2	2.48	0.44
2:A:864:CYS:SG	2:A:866:ARG:HB3	2.58	0.44
1:C:3:A:H2'	1:C:4:C:H6	1.82	0.44
2:A:545:LEU:HA	2:A:545:LEU:HD23	1.77	0.44
2:A:748:ILE:O	2:A:752:GLN:HG3	2.18	0.44
2:A:368:LEU:HD12	2:A:404:GLN:O	2.17	0.43
2:A:587:THR:O	2:A:590:PHE:HB3	2.18	0.43
2:A:284:LYS:O	2:A:284:LYS:HD2	2.18	0.43
2:A:346:LEU:HD23	2:A:351:LEU:HB2	2.00	0.43
2:A:296:PHE:CZ	2:A:351:LEU:HD23	2.53	0.43
2:A:538:LEU:O	2:A:542:THR:HG23	2.19	0.43
2:A:312:LYS:HB2	2:A:312:LYS:HE2	1.73	0.43
2:A:766:LEU:HD12	2:A:766:LEU:O	2.18	0.43
2:A:889:ILE:C	2:A:891:SER:H	2.22	0.43
2:A:469:ASP:OD2	2:A:472:LYS:HE2	2.19	0.43
2:A:650:ASN:HB3	2:A:653:LEU:CD2	2.48	0.43
2:A:749:GLU:O	2:A:752:GLN:HB2	2.18	0.43
2:A:278:CYS:SG	2:A:293:VAL:HG11	2.58	0.43
2:A:825:VAL:HG23	2:A:831:TYR:CD1	2.54	0.43
2:A:847:HIS:CG	2:A:848:PRO:HD2	2.54	0.43
2:A:637:ARG:H	2:A:637:ARG:HG2	1.71	0.43
1:B:3:A:H2'	1:B:4:C:H6	1.84	0.43
2:A:883:GLU:O	2:A:884:ILE:HG13	2.19	0.42
2:A:657:LYS:HZ1	2:A:690:ASP:CB	2.23	0.42
2:A:750:LYS:O	2:A:753:ILE:HG13	2.19	0.42
2:A:276:LEU:HD12	2:A:276:LEU:HA	1.90	0.42
2:A:720:ASN:HD22	2:A:723:LYS:HD2	1.84	0.42
2:A:704:ILE:HG12	2:A:705:ASP:N	2.35	0.42
2:A:345:ILE:C	2:A:346:LEU:HD12	2.40	0.42
2:A:485:LEU:HD22	2:A:488:ARG:HE	1.85	0.42
2:A:826:ILE:CD1	2:A:832:THR:HG23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:593:LYS:O	2:A:597:LEU:HD23	2.19	0.42
2:A:804:GLU:CB	2:A:806:LYS:HE3	2.45	0.42
1:B:4:C:H2'	1:B:5:G:C8	2.55	0.42
2:A:896:ASP:OD1	2:A:897:ILE:N	2.52	0.42
2:A:826:ILE:HG13	2:A:918:PHE:HB2	2.02	0.42
2:A:446:LEU:HD23	2:A:446:LEU:HA	1.85	0.42
2:A:525:MET:HG3	2:A:531:GLU:HB2	2.01	0.42
2:A:547:LYS:HE3	2:A:547:LYS:HB3	1.75	0.42
2:A:608:ASN:CB	2:A:611:LEU:HD23	2.29	0.42
2:A:902:GLN:OE1	2:A:902:GLN:N	2.52	0.42
2:A:621:GLU:HG3	2:A:711:LEU:HD22	2.01	0.41
2:A:810:CYS:HB2	2:A:873:TRP:CH2	2.55	0.41
2:A:811:ARG:HG3	2:A:892:PHE:CA	2.50	0.41
1:C:6:C:H2'	1:C:7:U:C6	2.55	0.41
2:A:524:GLN:OE1	2:A:524:GLN:N	2.49	0.41
2:A:559:ARG:HH21	2:A:562:ASP:CG	2.24	0.41
2:A:567:LEU:HA	2:A:570:PHE:HB3	2.03	0.41
2:A:653:LEU:HD12	2:A:656:LEU:HG	2.02	0.41
2:A:809:LEU:N	2:A:809:LEU:HD12	2.35	0.41
2:A:570:PHE:O	2:A:573:ASN:HB3	2.20	0.41
2:A:656:LEU:N	2:A:656:LEU:HD22	2.36	0.41
2:A:832:THR:CG2	2:A:884:ILE:HG21	2.50	0.41
2:A:655:PHE:CD2	2:A:656:LEU:HD22	2.56	0.41
2:A:550:ASP:OD1	2:A:551:ALA:N	2.53	0.41
2:A:808:LEU:HD12	2:A:817:ALA:HB3	2.03	0.41
2:A:469:ASP:C	2:A:470:LYS:HE2	2.41	0.41
2:A:644:LYS:HE2	2:A:644:LYS:HB2	1.72	0.41
2:A:786:HIS:CD2	2:A:790:ILE:HD11	2.56	0.41
2:A:402:LEU:HA	2:A:402:LEU:HD23	1.71	0.41
2:A:466:ARG:NH1	2:A:555:SER:O	2.54	0.41
2:A:823:VAL:HG12	2:A:833:VAL:HG22	2.02	0.41
2:A:471:PHE:CE1	2:A:475:ILE:HG13	2.56	0.41
2:A:565:ASP:OD1	2:A:568:LYS:NZ	2.29	0.41
2:A:783:ILE:O	2:A:786:HIS:HB3	2.21	0.40
2:A:822:ASP:OD1	2:A:822:ASP:N	2.54	0.40
1:B:3:A:H2'	1:B:4:C:C6	2.56	0.40
1:C:2:G:O2'	1:C:3:A:OP1	2.37	0.40
2:A:470:LYS:HA	2:A:473:TYR:CD2	2.56	0.40
2:A:735:GLY:O	2:A:737:LYS:HD2	2.22	0.40
2:A:889:ILE:HD11	2:A:908:TRP:CE2	2.57	0.40
2:A:512:TRP:O	2:A:516:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:535:CYS:O	2:A:538:LEU:HG	2.22	0.40
2:A:768:LEU:CD1	2:A:776:PHE:CE1	3.04	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
2	A	645/714 (90%)	598 (93%)	45 (7%)	2 (0%)	41 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	379	LYS
2	A	705	ASP

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
2	A	585/640 (91%)	555 (95%)	30 (5%)	24 56

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	290	LYS
2	A	443	LYS
2	A	468	SER
2	A	480	ARG
2	A	490	CYS
2	A	491	LYS
2	A	531	GLU
2	A	533	ARG
2	A	546	ARG
2	A	552	LEU
2	A	605	SER
2	A	637	ARG
2	A	644	LYS
2	A	657	LYS
2	A	698	SER
2	A	701	ASP
2	A	737	LYS
2	A	751	GLU
2	A	767	ARG
2	A	788	LYS
2	A	789	PHE
2	A	791	ARG
2	A	796	LYS
2	A	810	CYS
2	A	818	CYS
2	A	822	ASP
2	A	831	TYR
2	A	838	PHE
2	A	859	ARG
2	A	882	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	299	GLN
2	A	353	ASN
2	A	692	ASN
2	A	847	HIS
2	A	902	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	12/14 (85%)	2 (16%)	0
1	C	13/14 (92%)	2 (15%)	1 (7%)
All	All	25/28 (89%)	4 (16%)	1 (4%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	3	A
1	B	13	C
1	C	3	A
1	C	14	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	2	G

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	B	13/14 (92%)	-0.03	0 100 100	104, 123, 186, 196	0
1	C	13/14 (92%)	0.27	0 100 100	95, 117, 197, 205	0
2	A	651/714 (91%)	0.24	37 (5%) 23 19	68, 130, 220, 259	0
All	All	677/742 (91%)	0.23	37 (5%) 25 21	68, 130, 219, 259	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	894	VAL	5.7
2	A	521	MET	5.5
2	A	895	GLU	4.5
2	A	471	PHE	4.2
2	A	796	LYS	4.2
2	A	905	TYR	4.1
2	A	897	ILE	4.0
2	A	910	ASP	3.9
2	A	911	PHE	3.8
2	A	903	THR	3.5
2	A	472	LYS	3.4
2	A	838	PHE	3.3
2	A	578	GLY	3.2
2	A	798	LYS	3.1
2	A	473	TYR	3.0
2	A	475	ILE	2.9
2	A	663	GLY	2.9
2	A	601	SER	2.8
2	A	552	LEU	2.8
2	A	902	GLN	2.8
2	A	795	GLU	2.7
2	A	893	VAL	2.5
2	A	904	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	807	LYS	2.4
2	A	594	LEU	2.3
2	A	912	HIS	2.3
2	A	476	ALA	2.3
2	A	913	PHE	2.2
2	A	541	TYR	2.2
2	A	579	PHE	2.2
2	A	896	ASP	2.2
2	A	803	LYS	2.2
2	A	901	VAL	2.1
2	A	590	PHE	2.1
2	A	808	LEU	2.1
2	A	468	SER	2.0
2	A	914	GLU	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	1002	1/1	0.69	0.78	83,83,83,83	0
3	ZN	A	1001	1/1	0.97	0.15	160,160,160,160	0

6.5 Other polymers (i)

There are no such residues in this entry.