Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2022 – 12:58 PM EDT

PDB ID	:	8EMB
Title	:	X-ray crystal structure of Thermosynechococcus elongatus Si3 domain of RNA polymerase RpoC2 subunit
Authors	:	Murakami, K.S.; Imashimizu, M.; Qayyum, M.Z.; Vishwakarma, R.K.; Yuzenkova, Y.
Deposited on	:	2022-09-27
Resolution	:	3.06 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

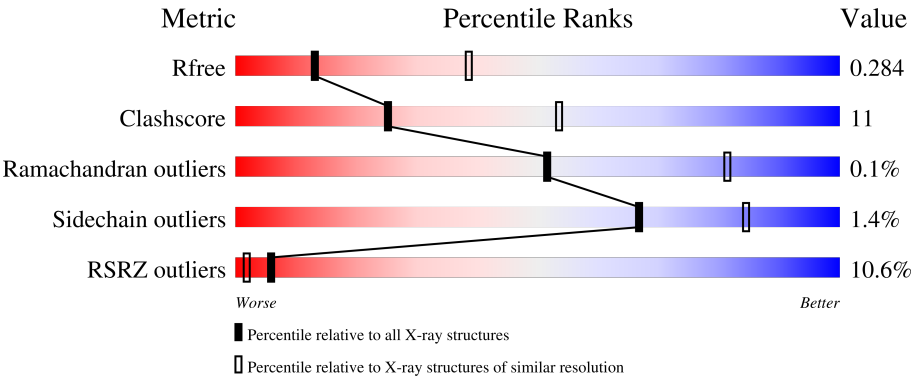
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	553	3% 76% 23%
1	B	553	2% 77% 20%
1	C	553	% 71% 25%
1	D	553	7% 72% 26%
1	E	553	24% 43% 22% 35%

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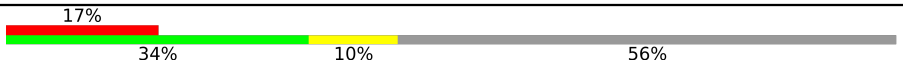
Mol	Chain	Length	Quality of chain
1	F	553	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 21086 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 DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	Se	0	0	0
			4185	2609	736	832	2	6			
1	B	541	Total	C	N	O	S	Se	0	0	0
			4127	2574	726	819	2	6			
1	C	531	Total	C	N	O	S	Se	0	0	0
			4047	2526	711	803	2	5			
1	D	543	Total	C	N	O	S	Se	0	0	0
			4140	2582	728	823	2	5			
1	E	358	Total	C	N	O	S	Se	0	0	0
			2752	1718	476	554	2	2			
1	F	246	Total	C	N	O	Se		0	0	0
			1835	1134	335	363	3				

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	GLY	-	expression tag	UNP Q8DL57
A	432	SER	-	expression tag	UNP Q8DL57
A	433	HIS	-	expression tag	UNP Q8DL57
A	434	MSE	-	expression tag	UNP Q8DL57
A	508	MSE	LEU	engineered mutation	UNP Q8DL57
A	738	MSE	LEU	engineered mutation	UNP Q8DL57
A	922	MSE	LEU	engineered mutation	UNP Q8DL57
B	431	GLY	-	expression tag	UNP Q8DL57
B	432	SER	-	expression tag	UNP Q8DL57
B	433	HIS	-	expression tag	UNP Q8DL57
B	434	MSE	-	expression tag	UNP Q8DL57
B	508	MSE	LEU	engineered mutation	UNP Q8DL57
B	738	MSE	LEU	engineered mutation	UNP Q8DL57
B	922	MSE	LEU	engineered mutation	UNP Q8DL57
C	431	GLY	-	expression tag	UNP Q8DL57
C	432	SER	-	expression tag	UNP Q8DL57
C	433	HIS	-	expression tag	UNP Q8DL57

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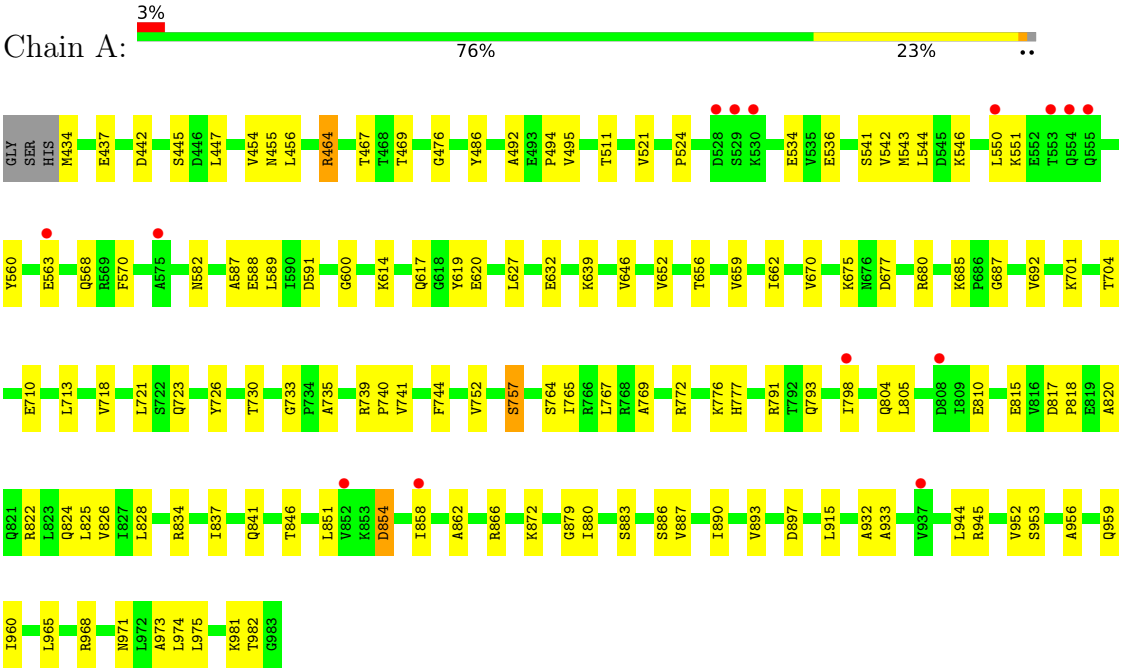
Chain	Residue	Modelled	Actual	Comment	Reference
C	434	MSE	-	expression tag	UNP Q8DL57
C	508	MSE	LEU	engineered mutation	UNP Q8DL57
C	738	MSE	LEU	engineered mutation	UNP Q8DL57
C	922	MSE	LEU	engineered mutation	UNP Q8DL57
D	431	GLY	-	expression tag	UNP Q8DL57
D	432	SER	-	expression tag	UNP Q8DL57
D	433	HIS	-	expression tag	UNP Q8DL57
D	434	MSE	-	expression tag	UNP Q8DL57
D	508	MSE	LEU	engineered mutation	UNP Q8DL57
D	738	MSE	LEU	engineered mutation	UNP Q8DL57
D	922	MSE	LEU	engineered mutation	UNP Q8DL57
E	431	GLY	-	expression tag	UNP Q8DL57
E	432	SER	-	expression tag	UNP Q8DL57
E	433	HIS	-	expression tag	UNP Q8DL57
E	434	MSE	-	expression tag	UNP Q8DL57
E	508	MSE	LEU	engineered mutation	UNP Q8DL57
E	738	MSE	LEU	engineered mutation	UNP Q8DL57
E	922	MSE	LEU	engineered mutation	UNP Q8DL57
F	431	GLY	-	expression tag	UNP Q8DL57
F	432	SER	-	expression tag	UNP Q8DL57
F	433	HIS	-	expression tag	UNP Q8DL57
F	434	MSE	-	expression tag	UNP Q8DL57
F	508	MSE	LEU	engineered mutation	UNP Q8DL57
F	738	MSE	LEU	engineered mutation	UNP Q8DL57
F	922	MSE	LEU	engineered mutation	UNP Q8DL57

3 Residue-property plots

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.

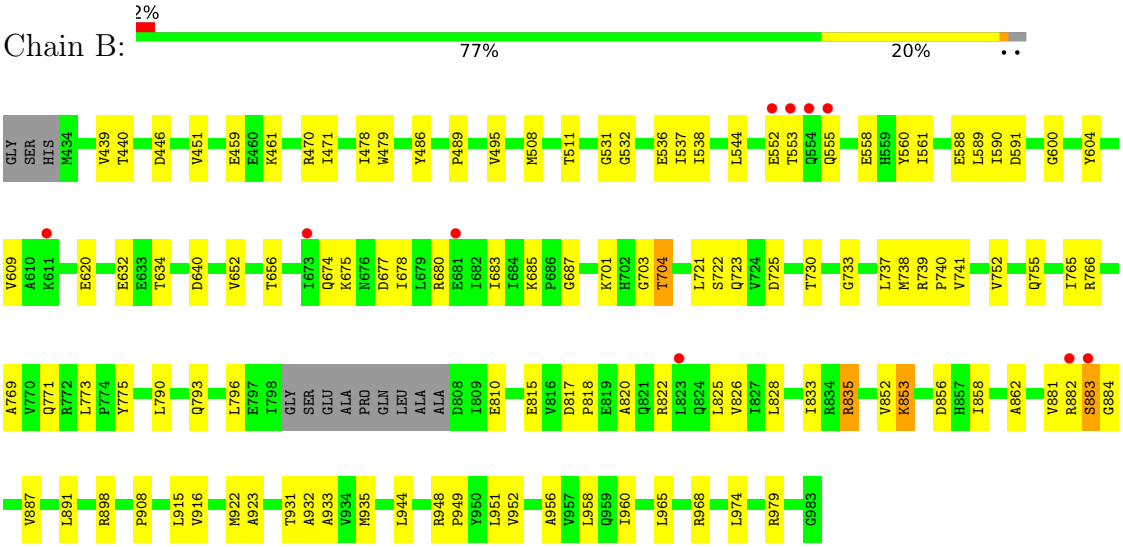
• Molecule 1: DNA-directed RNA polymerase subunit beta'

Chain A:



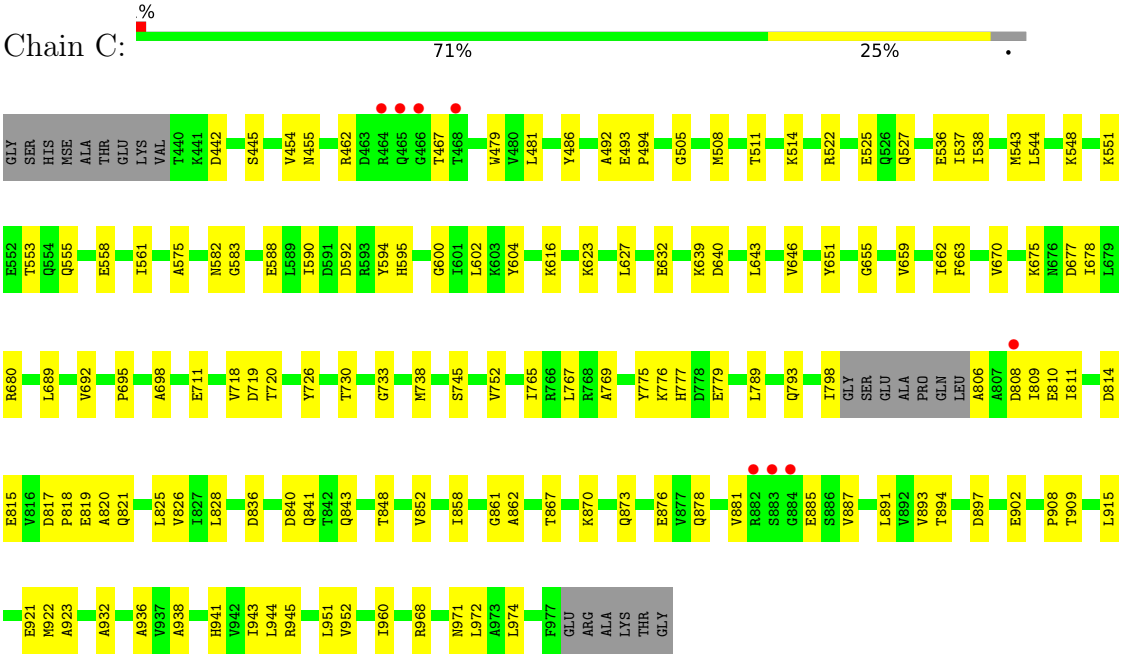
• Molecule 1: DNA-directed RNA polymerase subunit beta'

Chain B:



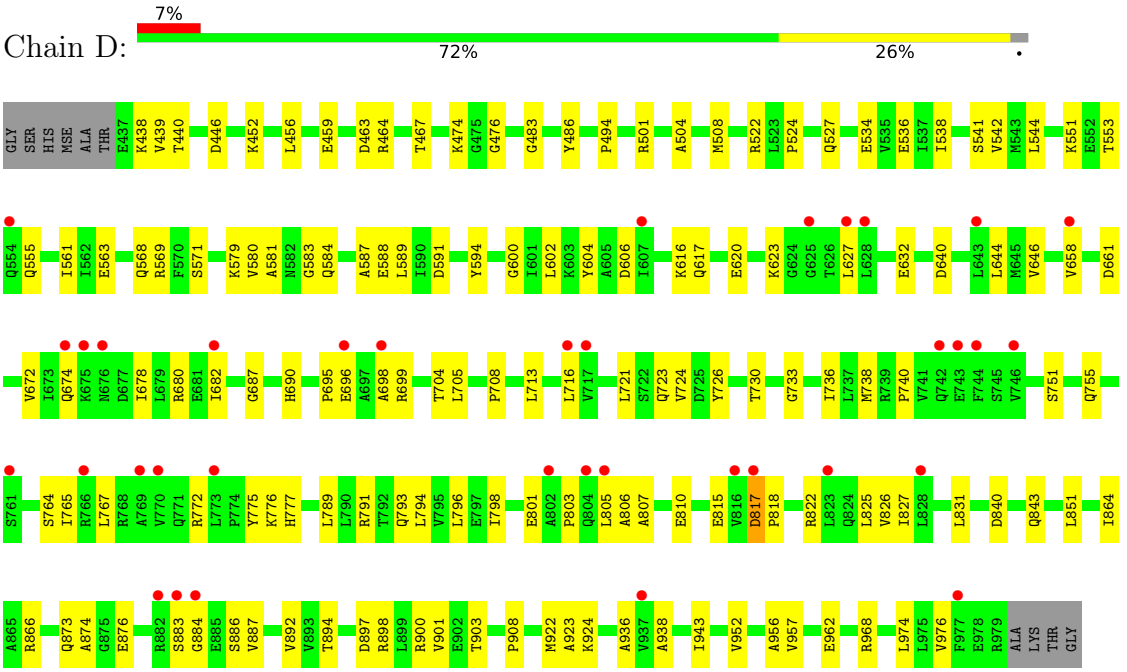
• Molecule 1: DNA-directed RNA polymerase subunit beta'

Chain C:



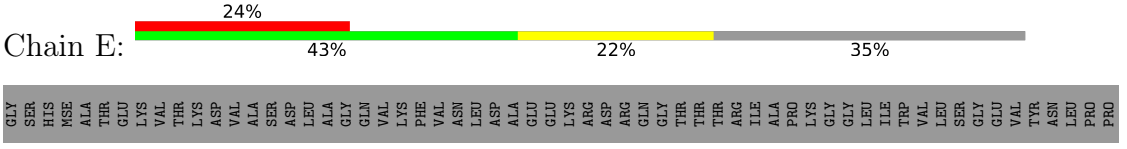
• Molecule 1: DNA-directed RNA polymerase subunit beta'

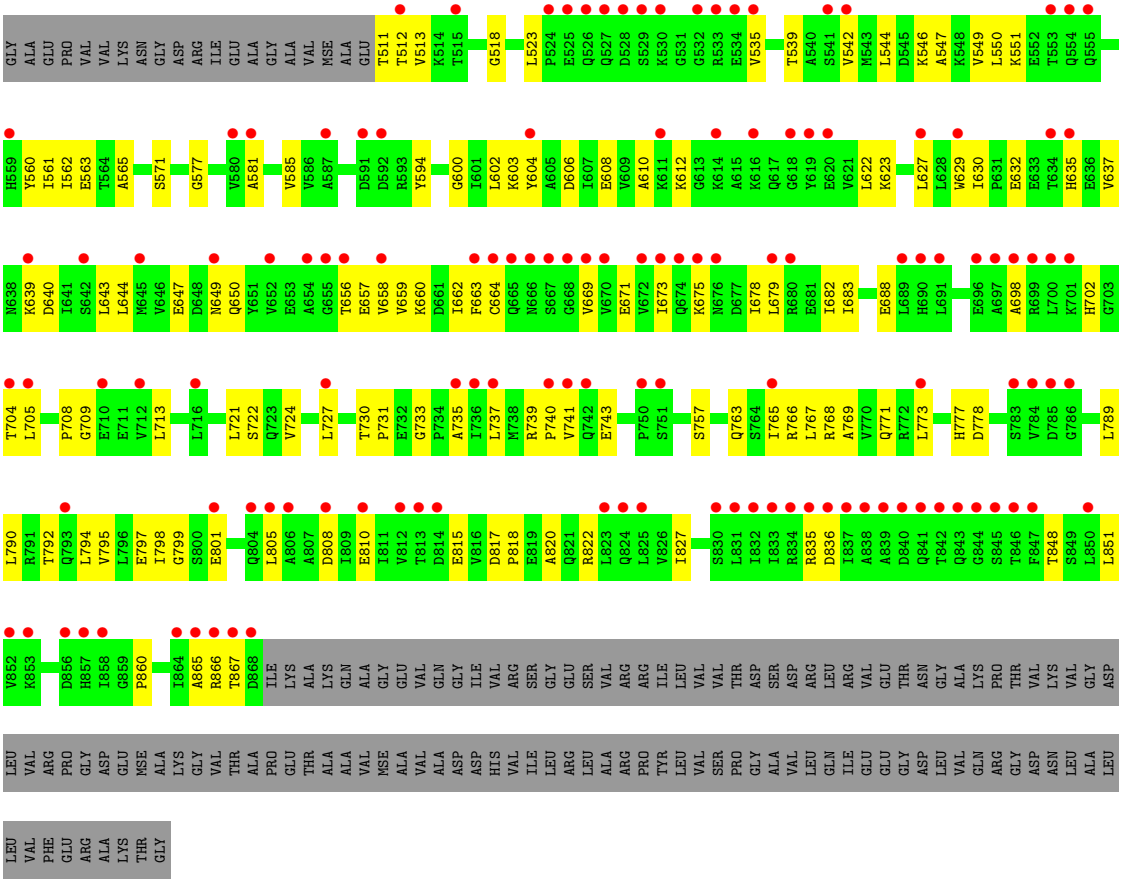
Chain D:



• Molecule 1: DNA-directed RNA polymerase subunit beta'

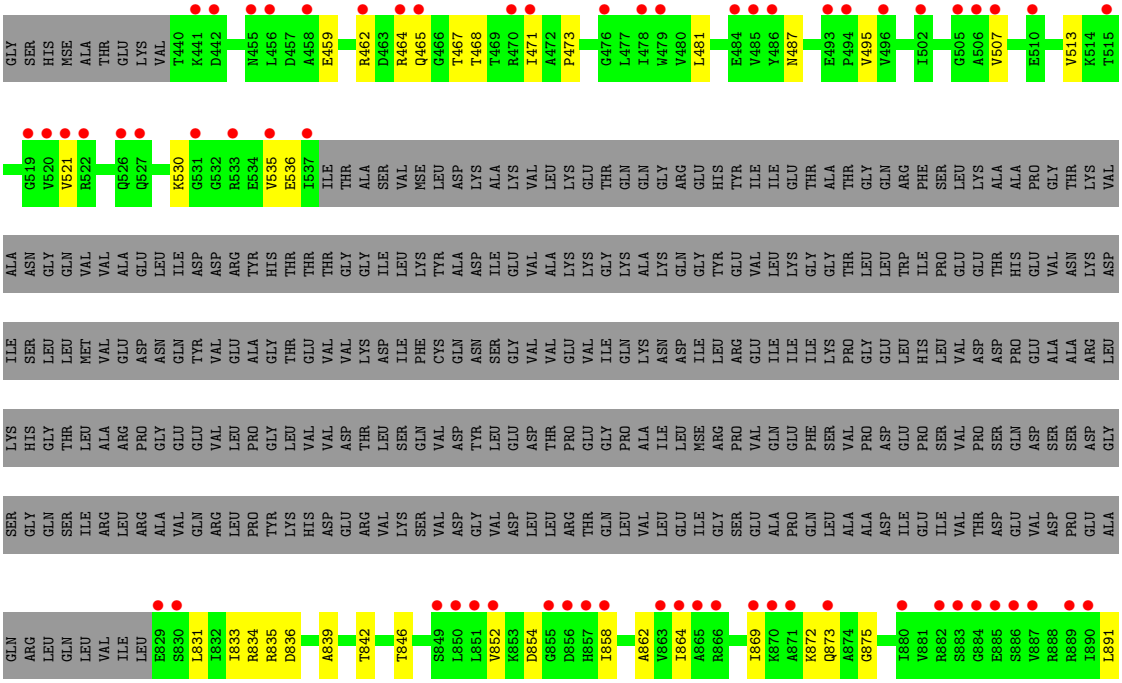
Chain E:

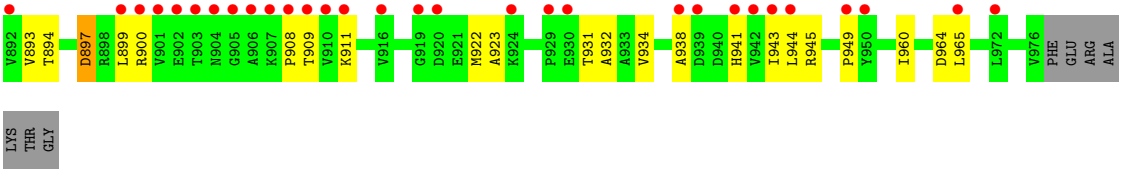




• Molecule 1: DNA-directed RNA polymerase subunit beta'

Chain F:




V892
V893
T894
D897
R898
L899
R900
V901
E902
T903
N904
G905
A906
K907
P908
T909
V910
K911
V916
G919
D920
E921
M922
A923
K924
P929
E930
T931
A932
A933
V934
A938
D939
D940
H941
V942
I943
L944
R945
P949
Y950
I960
D964
L965
L972
V976
PHE
GLU
ARG
ALA
LYS
THR
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	178.66Å 178.66Å 281.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.61 – 3.06 49.61 – 3.06	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.61-3.06) 87.0 (49.61-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.62 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.264 , 0.284 0.263 , 0.284	Depositor DCC
R_{free} test set	1992 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å^2)	73.6	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 64.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	21086	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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	0.27	0/4233	0.58	0/5731
1	B	0.27	0/4173	0.58	0/5647
1	C	0.28	0/4093	0.58	0/5542
1	D	0.27	0/4188	0.59	1/5671 (0.0%)
1	E	0.25	0/2787	0.55	0/3777
1	F	0.25	0/1850	0.56	0/2500
All	All	0.27	0/21324	0.58	1/28868 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	796	LEU	CA-CB-CG	5.34	127.59	115.30

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	4185	0	4263	83	0
1	B	4127	0	4207	70	0
1	C	4047	0	4121	97	0
1	D	4140	0	4214	101	0
1	E	2752	0	2781	80	0
1	F	1835	0	1879	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21086	0	21465	453	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 11.

All (453) 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:828:LEU:HD11	1:E:801:GLU:HG3	1.46	0.96
1:C:588:GLU:HG3	1:C:793:GLN:HG2	1.58	0.86
1:A:815:GLU:HG3	1:A:818:PRO:HD2	1.59	0.84
1:A:589:LEU:HD22	1:A:591:ASP:HB2	1.63	0.80
1:D:587:ALA:HB3	1:D:794:LEU:HD21	1.64	0.79
1:E:704:THR:HG22	1:E:705:LEU:H	1.48	0.78
1:C:600:GLY:HA2	1:C:632:GLU:HG2	1.65	0.77
1:D:589:LEU:HG	1:D:591:ASP:HB2	1.66	0.77
1:C:808:ASP:OD2	1:C:825:LEU:HB3	1.85	0.76
1:C:602:LEU:HD11	1:C:627:LEU:HG	1.68	0.75
1:E:630:ILE:HG12	1:E:741:VAL:HG12	1.69	0.75
1:B:931:THR:HG21	1:B:949:PRO:HD3	1.69	0.74
1:D:600:GLY:HA2	1:D:632:GLU:HG2	1.66	0.74
1:A:600:GLY:HA2	1:A:632:GLU:HG2	1.69	0.73
1:D:494:PRO:HD3	1:D:887:VAL:HG21	1.70	0.72
1:B:898:ARG:HH12	1:B:935:MSE:HB2	1.54	0.72
1:A:893:VAL:HG23	1:A:897:ASP:HB2	1.72	0.71
1:F:931:THR:HG21	1:F:949:PRO:HD3	1.71	0.71
1:C:765:ILE:HG13	1:C:798:ILE:HG22	1.71	0.71
1:F:530:LYS:HB2	1:F:834:ARG:HH22	1.55	0.71
1:B:600:GLY:HA2	1:B:632:GLU:HG2	1.73	0.70
1:A:817:ASP:HB2	1:A:818:PRO:HD3	1.73	0.70
1:B:553:THR:HA	1:B:558:GLU:HB2	1.74	0.70
1:E:671:GLU:HB3	1:E:683:ILE:HB	1.73	0.70
1:A:494:PRO:HD3	1:A:887:VAL:HG21	1.74	0.69
1:B:916:VAL:HG11	1:B:922:MSE:HE3	1.74	0.69
1:D:815:GLU:HG2	1:D:822:ARG:HG3	1.73	0.69
1:B:440:THR:HB	1:B:974:LEU:HD11	1.75	0.69
1:E:600:GLY:HA2	1:E:632:GLU:HG3	1.75	0.69
1:E:765:ILE:HD11	1:E:827:ILE:HD11	1.76	0.68
1:D:900:ARG:HD3	1:D:943:ILE:HG12	1.75	0.68
1:C:765:ILE:HD11	1:C:808:ASP:OD2	1.93	0.68
1:C:481:LEU:HB3	1:C:945:ARG:HE	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:810:GLU:HB3	1:C:825:LEU:HG	1.77	0.67
1:C:680:ARG:NH1	1:E:708:PRO:O	2.28	0.66
1:E:702:HIS:HA	1:E:724:VAL:HG12	1.76	0.66
1:E:768:ARG:HH21	1:E:797:GLU:HB3	1.60	0.66
1:E:602:LEU:HD11	1:E:627:LEU:HG	1.78	0.65
1:B:858:ILE:HG23	1:B:862:ALA:HB3	1.78	0.65
1:B:817:ASP:HB2	1:B:818:PRO:HD3	1.77	0.65
1:E:602:LEU:HD13	1:E:629:TRP:HE3	1.62	0.65
1:B:588:GLU:HG2	1:B:793:GLN:HG2	1.80	0.64
1:A:675:LYS:HE3	1:A:680:ARG:HG3	1.79	0.64
1:B:685:LYS:HG2	1:B:739:ARG:NH2	2.13	0.64
1:D:602:LEU:HD11	1:D:627:LEU:HG	1.80	0.64
1:E:848:THR:HA	1:E:867:THR:HG22	1.79	0.64
1:E:610:ALA:HB2	1:E:622:LEU:HD13	1.80	0.63
1:A:721:LEU:HD22	1:A:741:VAL:CG1	2.29	0.63
1:D:568:GLN:NE2	1:D:751:SER:OG	2.29	0.63
1:B:544:LEU:HD23	1:B:755:GLN:HB3	1.81	0.63
1:F:900:ARG:HH21	1:F:943:ILE:HD11	1.64	0.63
1:E:544:LEU:HD11	1:E:767:LEU:HD12	1.81	0.62
1:A:685:LYS:HG2	1:A:739:ARG:NH2	2.14	0.62
1:C:627:LEU:HD23	1:C:789:LEU:HD13	1.80	0.62
1:A:437:GLU:HB2	1:A:981:LYS:HB2	1.80	0.62
1:D:908:PRO:HA	1:D:923:ALA:HB2	1.81	0.62
1:C:817:ASP:HB2	1:C:818:PRO:HD3	1.80	0.62
1:A:721:LEU:HD22	1:A:741:VAL:HG11	1.81	0.61
1:B:773:LEU:HD23	1:B:790:LEU:HD23	1.82	0.61
1:C:525:GLU:HB2	1:C:527:GLN:NE2	2.16	0.61
1:D:936:ALA:HB3	1:D:943:ILE:HD12	1.82	0.61
1:A:687:GLY:HA2	1:A:740:PRO:HD3	1.81	0.60
1:A:692:VAL:HG12	1:A:735:ALA:HA	1.81	0.60
1:C:841:GLN:OE1	1:C:968:ARG:NH2	2.33	0.60
1:F:932:ALA:HB3	1:F:944:LEU:HD12	1.81	0.60
1:B:852:VAL:HG11	1:B:858:ILE:HD11	1.83	0.60
1:B:853:LYS:HE3	1:B:856:ASP:OD2	2.01	0.60
1:B:652:VAL:HG22	1:B:656:THR:OG1	2.01	0.60
1:B:815:GLU:HG2	1:B:822:ARG:HG2	1.82	0.60
1:D:583:GLY:O	1:D:616:LYS:NZ	2.30	0.60
1:A:454:VAL:HG23	1:A:455:ASN:H	1.67	0.60
1:A:542:VAL:HG23	1:A:765:ILE:HB	1.83	0.60
1:E:610:ALA:HB1	1:E:612:LYS:HD2	1.84	0.60
1:F:846:THR:HG22	1:F:869:ILE:HG13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:GLU:HB3	1:A:825:LEU:HG	1.84	0.59
1:B:765:ILE:O	1:B:766:ARG:HG2	2.01	0.59
1:C:525:GLU:HG3	1:E:539:THR:HG21	1.83	0.59
1:C:675:LYS:HE3	1:C:680:ARG:HG3	1.85	0.59
1:F:893:VAL:HG11	1:F:945:ARG:HD2	1.84	0.59
1:D:765:ILE:HD11	1:D:827:ILE:HG13	1.84	0.59
1:A:536:GLU:HG2	1:A:828:LEU:HD13	1.84	0.59
1:A:883:SER:OG	1:A:886:SER:OG	2.21	0.59
1:C:814:ASP:OD1	1:C:821:GLN:NE2	2.34	0.59
1:D:840:ASP:OD1	1:D:843:GLN:HG2	2.02	0.59
1:E:765:ILE:O	1:E:766:ARG:HG3	2.03	0.59
1:A:815:GLU:OE2	1:A:820:ALA:HB3	2.03	0.58
1:E:649:ASN:HA	1:E:669:VAL:HG13	1.85	0.58
1:A:804:GLN:HA	1:D:569:ARG:HH22	1.69	0.58
1:C:442:ASP:HA	1:C:974:LEU:HA	1.84	0.58
1:A:486:TYR:OH	1:A:872:LYS:HB2	2.04	0.58
1:A:492:ALA:HA	1:A:511:THR:HG22	1.85	0.58
1:C:692:VAL:HG21	1:C:698:ALA:HB2	1.85	0.58
1:C:718:VAL:HG12	1:C:720:THR:O	2.04	0.58
1:D:544:LEU:HD23	1:D:755:GLN:HB3	1.86	0.58
1:C:536:GLU:HB3	1:C:828:LEU:HD12	1.86	0.58
1:B:891:LEU:HB2	1:B:965:LEU:HD13	1.86	0.57
1:D:873:GLN:HG3	1:D:894:THR:HG21	1.86	0.57
1:F:858:ILE:HG23	1:F:862:ALA:HB3	1.84	0.57
1:C:514:LYS:HD3	1:C:861:GLY:O	2.05	0.57
1:A:544:LEU:HD21	1:A:767:LEU:HD12	1.86	0.57
1:B:589:LEU:HG	1:B:591:ASP:HB2	1.86	0.57
1:D:581:ALA:HB1	1:D:805:LEU:HD11	1.87	0.57
1:E:769:ALA:HA	1:E:794:LEU:HA	1.86	0.57
1:F:495:VAL:HG21	1:F:507:VAL:HG12	1.87	0.57
1:C:840:ASP:OD1	1:C:843:GLN:HG2	2.05	0.57
1:C:873:GLN:HG3	1:C:894:THR:HG21	1.87	0.57
1:C:548:LYS:HG2	1:C:820:ALA:HB1	1.86	0.57
1:E:656:THR:HG22	1:E:657:GLU:H	1.68	0.57
1:D:724:VAL:HG13	1:D:736:ILE:HD11	1.87	0.56
1:E:730:THR:OG1	1:E:733:GLY:O	2.24	0.56
1:C:938:ALA:HB3	1:C:941:HIS:HB2	1.87	0.56
1:A:541:SER:HB2	1:A:826:VAL:HG12	1.87	0.56
1:D:524:PRO:HD3	1:D:536:GLU:OE1	2.05	0.56
1:F:934:VAL:HA	1:F:944:LEU:HA	1.88	0.56
1:C:522:ARG:NH2	1:E:801:GLU:HB2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:MSE:SE	1:D:464:ARG:HG3	2.55	0.56
1:D:690:HIS:HB2	1:D:736:ILE:HG23	1.88	0.56
1:E:658:VAL:HG22	1:E:664:CYS:HB2	1.88	0.56
1:A:815:GLU:OE2	1:A:818:PRO:HG2	2.06	0.56
1:E:656:THR:HG22	1:E:657:GLU:N	2.20	0.56
1:C:858:ILE:HG12	1:C:862:ALA:HB3	1.88	0.55
1:C:494:PRO:HG3	1:C:887:VAL:HG21	1.89	0.55
1:A:550:LEU:HD12	1:A:563:GLU:OE2	2.06	0.55
1:D:736:ILE:HG12	1:D:738:MSE:HE3	1.88	0.55
1:C:893:VAL:HG23	1:C:897:ASP:HB2	1.89	0.55
1:E:513:VAL:HB	1:E:865:ALA:HB3	1.88	0.55
1:B:609:VAL:HG11	1:B:773:LEU:HD12	1.89	0.55
1:D:438:LYS:HB2	1:D:976:VAL:HG12	1.88	0.55
1:A:542:VAL:HG22	1:A:757:SER:HB2	1.89	0.54
1:D:588:GLU:HG3	1:D:793:GLN:HG2	1.89	0.54
1:A:588:GLU:HG2	1:A:793:GLN:HG2	1.88	0.54
1:C:640:ASP:HA	1:C:678:ILE:HA	1.88	0.54
1:B:884:GLY:HA3	1:D:884:GLY:HA3	1.89	0.54
1:E:673:ILE:HG22	1:E:675:LYS:HE2	1.89	0.54
1:B:721:LEU:HD22	1:B:741:VAL:CG1	2.38	0.54
1:D:463:ASP:OD2	1:D:467:THR:HB	2.08	0.54
1:B:687:GLY:HA2	1:B:740:PRO:HD3	1.89	0.54
1:D:620:GLU:HG3	1:D:772:ARG:NH1	2.23	0.54
1:E:817:ASP:HB2	1:E:818:PRO:HD3	1.89	0.54
1:D:696:GLU:HA	1:D:699:ARG:HG2	1.90	0.54
1:D:924:LYS:HE3	1:F:911:LYS:HD2	1.89	0.54
1:E:767:LEU:HD22	1:E:794:LEU:HD12	1.90	0.54
1:C:932:ALA:CB	1:C:944:LEU:HD13	2.38	0.53
1:E:546:LYS:HB3	1:E:565:ALA:HB2	1.90	0.53
1:F:835:ARG:HG2	1:F:836:ASP:OD2	2.07	0.53
1:A:841:GLN:OE1	1:A:968:ARG:NH2	2.31	0.53
1:D:738:MSE:HE2	1:D:738:MSE:HA	1.89	0.53
1:F:487:ASN:HD22	1:F:842:THR:HB	1.73	0.53
1:A:815:GLU:HG3	1:A:818:PRO:CD	2.35	0.53
1:B:620:GLU:OE1	1:B:620:GLU:N	2.41	0.53
1:B:952:VAL:HG13	1:B:956:ALA:HB3	1.90	0.53
1:C:908:PRO:HA	1:C:923:ALA:HB2	1.91	0.53
1:D:508:MSE:HE2	1:D:892:VAL:HG21	1.91	0.53
1:A:701:LYS:HE3	1:A:726:TYR:HE2	1.73	0.53
1:D:708:PRO:HD3	1:D:721:LEU:HG	1.90	0.52
1:E:815:GLU:OE1	1:E:822:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:464:ARG:HG3	1:F:465:GLN:N	2.24	0.52
1:C:454:VAL:HG23	1:C:455:ASN:H	1.74	0.52
1:F:459:GLU:HB2	1:F:471:ILE:HG22	1.90	0.52
1:D:486:TYR:CE1	1:D:508:MSE:HE1	2.45	0.52
1:E:640:ASP:HA	1:E:678:ILE:HG22	1.91	0.52
1:B:531:GLY:O	1:B:835:ARG:HG3	2.10	0.52
1:B:915:LEU:HD23	1:B:933:ALA:HB2	1.91	0.52
1:D:541:SER:HB2	1:D:826:VAL:HG12	1.92	0.52
1:E:549:VAL:HG22	1:E:562:ILE:HG12	1.91	0.52
1:A:543:MSE:HB2	1:A:824:GLN:HG3	1.92	0.52
1:A:915:LEU:HD23	1:A:933:ALA:HB2	1.91	0.52
1:B:703:GLY:O	1:B:723:GLN:HG3	2.10	0.52
1:A:551:LYS:HE2	1:A:560:TYR:CZ	2.45	0.52
1:B:771:GLN:HB3	1:B:790:LEU:HD21	1.91	0.52
1:A:521:VAL:HB	1:A:858:ILE:HD12	1.92	0.52
1:A:692:VAL:CG2	1:A:713:LEU:HD11	2.40	0.52
1:C:798:ILE:HD11	1:C:806:ALA:HB1	1.92	0.51
1:E:561:ILE:HD13	1:E:571:SER:HA	1.92	0.51
1:B:459:GLU:HA	1:D:459:GLU:HA	1.92	0.51
1:C:881:VAL:HB	1:C:887:VAL:HA	1.92	0.51
1:C:893:VAL:HB	1:C:945:ARG:NH1	2.25	0.51
1:D:698:ALA:HB2	1:D:713:LEU:HD11	1.92	0.51
1:E:542:VAL:HG12	1:E:757:SER:HB3	1.93	0.51
1:F:873:GLN:HB2	1:F:894:THR:HG21	1.91	0.51
1:C:659:VAL:HB	1:C:662:ILE:HB	1.91	0.51
1:C:752:VAL:HG22	1:C:769:ALA:HB3	1.93	0.51
1:D:705:LEU:HD22	1:D:723:GLN:HB2	1.92	0.51
1:D:696:GLU:HG2	1:D:699:ARG:HH11	1.75	0.51
1:E:815:GLU:OE2	1:E:820:ALA:HB3	2.11	0.51
1:F:938:ALA:HB3	1:F:941:HIS:HB2	1.92	0.51
1:C:553:THR:HG22	1:C:558:GLU:HG2	1.93	0.51
1:D:776:LYS:HG2	1:D:777:HIS:H	1.76	0.51
1:C:538:ILE:HG23	1:C:826:VAL:HB	1.93	0.51
1:B:532:GLY:HA2	1:B:833:ILE:O	2.11	0.51
1:C:643:LEU:O	1:C:659:VAL:HG13	2.11	0.51
1:D:658:VAL:HG21	1:D:682:ILE:HD12	1.93	0.51
1:E:644:LEU:HD13	1:E:679:LEU:HD11	1.92	0.51
1:B:725:ASP:HB3	1:B:737:LEU:HB3	1.94	0.50
1:A:524:PRO:HD2	1:A:534:GLU:O	2.11	0.50
1:F:481:LEU:HB3	1:F:945:ARG:HH21	1.76	0.50
1:C:815:GLU:OE1	1:C:817:ASP:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:815:GLU:HB3	1:C:818:PRO:HD2	1.94	0.50
1:E:657:GLU:OE2	1:E:660:LYS:HD3	2.11	0.50
1:E:765:ILE:HG23	1:E:798:ILE:HG22	1.93	0.50
1:E:727:LEU:HD11	1:E:737:LEU:HB2	1.93	0.50
1:B:588:GLU:OE2	1:B:793:GLN:NE2	2.28	0.50
1:C:936:ALA:HB3	1:C:943:ILE:HB	1.93	0.50
1:C:575:ALA:O	1:C:810:GLU:OE2	2.29	0.49
1:C:809:ILE:HG21	1:E:801:GLU:HG2	1.94	0.49
1:C:815:GLU:OE1	1:C:818:PRO:HD2	2.12	0.49
1:C:819:GLU:O	1:C:819:GLU:OE2	2.30	0.49
1:D:644:LEU:HD11	1:D:672:VAL:HG11	1.94	0.49
1:D:704:THR:HG22	1:D:705:LEU:H	1.77	0.49
1:E:627:LEU:HD23	1:E:789:LEU:HD13	1.94	0.49
1:F:471:ILE:HG23	1:F:473:PRO:HD3	1.94	0.49
1:A:454:VAL:HG11	1:A:915:LEU:HD11	1.94	0.49
1:A:568:GLN:HE21	1:A:589:LEU:HD11	1.78	0.49
1:D:661:ASP:OD1	1:D:661:ASP:N	2.35	0.49
1:D:527:GLN:O	1:D:534:GLU:OE2	2.30	0.49
1:D:801:GLU:OE2	1:D:803:PRO:HB3	2.12	0.49
1:D:483:GLY:HA2	1:D:897:ASP:OD2	2.13	0.49
1:C:639:LYS:HE2	1:C:639:LYS:N	2.28	0.49
1:D:617:GLN:HB3	1:D:791:ARG:HH22	1.78	0.49
1:E:721:LEU:HD22	1:E:741:VAL:HG21	1.95	0.49
1:C:551:LYS:NZ	1:E:757:SER:O	2.35	0.48
1:C:583:GLY:O	1:C:616:LYS:NZ	2.42	0.48
1:D:561:ILE:HD13	1:D:571:SER:HA	1.94	0.48
1:D:957:VAL:HB	1:D:974:LEU:HG	1.96	0.48
1:A:456:LEU:HD13	1:A:476:GLY:HA3	1.94	0.48
1:D:616:LYS:HB2	1:D:772:ARG:HH21	1.77	0.48
1:E:550:LEU:HD23	1:E:551:LYS:H	1.78	0.48
1:C:493:GLU:OE2	1:C:885:GLU:HG2	2.13	0.48
1:D:620:GLU:HG3	1:D:772:ARG:CZ	2.42	0.48
1:E:512:THR:OG1	1:E:865:ALA:O	2.21	0.48
1:F:464:ARG:HG3	1:F:465:GLN:H	1.77	0.48
1:D:704:THR:HG22	1:D:705:LEU:N	2.28	0.48
1:E:550:LEU:HD23	1:E:551:LYS:N	2.28	0.48
1:D:522:ARG:HD3	1:D:538:ILE:HD11	1.95	0.48
1:D:456:LEU:HD13	1:D:476:GLY:HA3	1.96	0.48
1:D:887:VAL:HG23	1:D:887:VAL:O	2.14	0.47
1:E:603:LYS:HA	1:E:777:HIS:O	2.14	0.47
1:E:637:VAL:HG12	1:E:662:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:PHE:HB3	1:A:587:ALA:HB1	1.96	0.47
1:B:730:THR:OG1	1:B:733:GLY:O	2.29	0.47
1:E:763:GLN:HA	1:E:799:GLY:O	2.14	0.47
1:D:687:GLY:HA2	1:D:740:PRO:HD3	1.96	0.47
1:A:752:VAL:HG22	1:A:769:ALA:HB3	1.96	0.47
1:B:815:GLU:HB3	1:B:818:PRO:HD2	1.96	0.47
1:C:462:ARG:HA	1:C:467:THR:O	2.15	0.47
1:D:542:VAL:HG23	1:D:765:ILE:HB	1.95	0.47
1:D:794:LEU:HD23	1:D:794:LEU:H	1.80	0.47
1:A:617:GLN:HB3	1:A:791:ARG:NH2	2.30	0.47
1:D:644:LEU:HD22	1:D:646:VAL:HG12	1.95	0.47
1:D:901:VAL:HG11	1:D:922:MSE:HE2	1.97	0.47
1:E:581:ALA:HB1	1:E:805:LEU:HD22	1.95	0.47
1:E:632:GLU:HB3	1:E:739:ARG:NH2	2.28	0.47
1:B:634:THR:HG23	1:B:683:ILE:HG12	1.97	0.47
1:B:722:SER:HB2	1:B:738:MSE:HE3	1.97	0.47
1:C:492:ALA:HA	1:C:511:THR:HG22	1.97	0.47
1:C:852:VAL:HG11	1:C:858:ILE:HD12	1.96	0.47
1:B:479:TRP:CE2	1:B:915:LEU:HD13	2.50	0.47
1:F:462:ARG:HA	1:F:467:THR:O	2.15	0.47
1:F:513:VAL:HG11	1:F:833:ILE:HD12	1.97	0.47
1:A:620:GLU:N	1:A:620:GLU:OE1	2.47	0.47
1:A:701:LYS:HE3	1:A:726:TYR:CE2	2.50	0.47
1:E:594:TYR:CE2	1:E:790:LEU:HD12	2.50	0.47
1:F:875:GLY:HA3	1:F:893:VAL:O	2.16	0.47
1:A:704:THR:HB	1:A:723:GLN:HG3	1.97	0.46
1:A:851:LEU:HD21	1:A:866:ARG:HH12	1.80	0.46
1:B:810:GLU:HB3	1:B:825:LEU:HG	1.97	0.46
1:F:909:THR:N	1:F:922:MSE:O	2.40	0.46
1:F:891:LEU:HB2	1:F:965:LEU:HD11	1.97	0.46
1:E:644:LEU:HD12	1:E:659:VAL:HG22	1.95	0.46
1:F:535:VAL:O	1:F:831:LEU:HB2	2.15	0.46
1:C:442:ASP:HB2	1:C:971:ASN:OD1	2.15	0.46
1:E:577:GLY:N	1:E:810:GLU:O	2.37	0.46
1:A:639:LYS:HD3	1:A:639:LYS:HA	1.72	0.46
1:D:501:ARG:HD3	1:D:876:GLU:HB2	1.98	0.46
1:C:718:VAL:HG22	1:C:738:MSE:HE2	1.97	0.46
1:C:730:THR:OG1	1:C:733:GLY:O	2.34	0.46
1:E:585:VAL:HA	1:E:795:VAL:HG23	1.98	0.46
1:D:764:SER:O	1:D:798:ILE:HA	2.16	0.46
1:D:767:LEU:HD13	1:D:794:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:817:ASP:HB2	1:D:818:PRO:HD3	1.98	0.46
1:A:445:SER:OG	1:A:447:LEU:O	2.33	0.45
1:A:879:GLY:O	1:A:965:LEU:HD11	2.16	0.45
1:E:647:GLU:OE2	1:E:731:PRO:HG3	2.16	0.45
1:E:647:GLU:HG3	1:E:650:GLN:HB2	1.98	0.45
1:A:710:GLU:O	1:A:718:VAL:HG23	2.17	0.45
1:B:675:LYS:HE3	1:B:680:ARG:HG3	1.97	0.45
1:C:718:VAL:CG1	1:C:720:THR:O	2.65	0.45
1:E:704:THR:HG22	1:E:705:LEU:N	2.26	0.45
1:F:908:PRO:HA	1:F:923:ALA:HA	1.99	0.45
1:F:521:VAL:HG23	1:F:536:GLU:O	2.17	0.45
1:B:908:PRO:HA	1:B:923:ALA:HB2	1.98	0.45
1:D:551:LYS:HG2	1:D:553:THR:HG23	1.98	0.45
1:E:639:LYS:HE2	1:E:643:LEU:HD22	1.97	0.45
1:E:608:GLU:HB2	1:E:623:LYS:HB3	1.99	0.45
1:A:837:ILE:N	1:A:846:THR:OG1	2.37	0.45
1:C:544:LEU:HD21	1:C:767:LEU:HD12	1.99	0.45
1:D:579:LYS:HB3	1:D:807:ALA:HB1	1.97	0.45
1:E:518:GLY:H	1:E:860:PRO:HA	1.81	0.45
1:C:678:ILE:HD11	1:E:709:GLY:HA3	1.98	0.45
1:A:620:GLU:OE2	1:A:772:ARG:NH1	2.50	0.45
1:A:764:SER:O	1:A:798:ILE:HA	2.17	0.45
1:A:932:ALA:CB	1:A:944:LEU:HD13	2.47	0.45
1:B:640:ASP:HA	1:B:678:ILE:HA	1.98	0.45
1:B:752:VAL:HG22	1:B:769:ALA:HB3	1.99	0.45
1:C:836:ASP:OD1	1:C:848:THR:HG23	2.17	0.45
1:A:858:ILE:HG23	1:A:862:ALA:HB3	1.98	0.45
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.85	0.44
1:E:511:THR:HG23	1:E:867:THR:OG1	2.17	0.44
1:A:464:ARG:H	1:A:464:ARG:HG3	1.44	0.44
1:A:692:VAL:HG23	1:A:713:LEU:HD11	2.00	0.44
1:A:953:SER:H	1:A:975:LEU:HD22	1.81	0.44
1:E:835:ARG:HG2	1:E:836:ASP:OD2	2.17	0.44
1:C:486:TYR:CD1	1:C:508:MSE:HE1	2.52	0.44
1:E:771:GLN:HG2	1:E:792:THR:HG22	1.99	0.44
1:B:451:VAL:HG13	1:B:478:ILE:HG23	1.99	0.44
1:C:848:THR:HG22	1:C:867:THR:OG1	2.18	0.44
1:B:881:VAL:HB	1:B:887:VAL:HA	2.00	0.44
1:C:555:GLN:OE1	1:C:555:GLN:N	2.50	0.44
1:C:719:ASP:N	1:C:719:ASP:OD2	2.47	0.44
1:D:724:VAL:HG22	1:D:738:MSE:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:ILE:HD12	1:A:960:ILE:HA	1.88	0.44
1:C:776:LYS:HB3	1:C:779:GLU:HB2	2.00	0.44
1:B:446:ASP:C	1:B:968:ARG:HG3	2.38	0.44
1:B:815:GLU:HG3	1:B:820:ALA:C	2.38	0.44
1:F:839:ALA:HB1	1:F:872:LYS:HG2	1.99	0.44
1:B:932:ALA:CB	1:B:944:LEU:HD13	2.47	0.43
1:D:524:PRO:HD2	1:D:534:GLU:O	2.17	0.43
1:D:903:THR:HG21	1:D:908:PRO:HG3	2.00	0.43
1:E:547:ALA:HA	1:E:563:GLU:O	2.18	0.43
1:A:851:LEU:HD21	1:A:866:ARG:NH1	2.33	0.43
1:E:727:LEU:HB2	1:E:735:ALA:HB3	1.99	0.43
1:D:640:ASP:HA	1:D:678:ILE:HG22	2.00	0.43
1:D:644:LEU:HD23	1:D:644:LEU:HA	1.78	0.43
1:B:604:TYR:OH	1:B:775:TYR:O	2.36	0.43
1:B:489:PRO:HG2	1:B:511:THR:HG21	1.99	0.43
1:B:796:LEU:HD13	1:B:825:LEU:HD22	2.01	0.43
1:D:817:ASP:OD1	1:D:817:ASP:N	2.51	0.43
1:B:486:TYR:CD2	1:B:508:MSE:HE1	2.54	0.43
1:B:536:GLU:HG2	1:B:828:LEU:HD13	2.01	0.43
1:B:951:LEU:HG	1:B:952:VAL:N	2.33	0.43
1:B:960:ILE:HD12	1:B:960:ILE:HA	1.89	0.43
1:C:921:GLU:OE1	1:C:921:GLU:N	2.52	0.43
1:D:831:LEU:HD11	1:D:864:ILE:HD11	1.99	0.43
1:E:851:LEU:HD21	1:E:866:ARG:HH12	1.83	0.43
1:A:495:VAL:HG22	1:A:495:VAL:O	2.19	0.43
1:D:803:PRO:HB2	1:D:806:ALA:H	1.84	0.43
1:E:523:LEU:HD21	1:E:535:VAL:HG22	2.01	0.43
1:E:635:HIS:HB2	1:E:682:ILE:CG1	2.49	0.43
1:B:882:ARG:O	1:B:883:SER:HB3	2.19	0.43
1:E:637:VAL:CG2	1:E:679:LEU:HB2	2.49	0.43
1:C:481:LEU:HB3	1:C:945:ARG:NE	2.31	0.43
1:C:538:ILE:HD12	1:C:826:VAL:HB	2.00	0.43
1:C:604:TYR:OH	1:C:775:TYR:O	2.35	0.43
1:D:594:TYR:HB3	1:D:789:LEU:HD12	2.00	0.43
1:D:883:SER:HB3	1:D:886:SER:HB2	2.00	0.43
1:A:442:ASP:HA	1:A:974:LEU:HA	2.01	0.42
1:B:561:ILE:HD12	1:B:590:ILE:HD11	2.00	0.42
1:C:592:ASP:O	1:C:595:HIS:HB2	2.19	0.42
1:C:651:TYR:HB2	1:C:689:LEU:HD12	2.01	0.42
1:C:695:PRO:HB3	1:C:726:TYR:OH	2.19	0.42
1:C:909:THR:N	1:C:922:MSE:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:535:VAL:HB	1:F:831:LEU:HB2	2.01	0.42
1:A:442:ASP:HB2	1:A:971:ASN:OD1	2.19	0.42
1:D:620:GLU:OE1	1:D:620:GLU:N	2.46	0.42
1:D:908:PRO:HG2	1:D:938:ALA:O	2.18	0.42
1:C:646:VAL:HG11	1:C:670:VAL:HG11	2.01	0.42
1:C:951:LEU:HD23	1:C:952:VAL:N	2.34	0.42
1:D:474:LYS:HE3	1:D:474:LYS:HB3	1.78	0.42
1:D:563:GLU:HA	1:D:568:GLN:O	2.19	0.42
1:F:462:ARG:HG2	1:F:468:THR:HG22	2.00	0.42
1:B:439:VAL:HG21	1:B:979:ARG:HD2	2.00	0.42
1:C:561:ILE:HD12	1:C:590:ILE:HD11	2.02	0.42
1:C:594:TYR:HB3	1:C:789:LEU:HD12	2.00	0.42
1:E:708:PRO:HD3	1:E:721:LEU:HG	2.01	0.42
1:F:899:LEU:O	1:F:944:LEU:HD23	2.20	0.42
1:A:627:LEU:HG	1:A:744:PHE:HB2	2.00	0.42
1:B:459:GLU:HB3	1:B:471:ILE:HG22	2.01	0.42
1:B:470:ARG:HG2	1:B:958:LEU:HD12	2.01	0.42
1:B:815:GLU:OE2	1:B:820:ALA:HB3	2.19	0.42
1:D:695:PRO:HB3	1:D:726:TYR:OH	2.20	0.42
1:A:614:LYS:HE2	1:A:619:TYR:OH	2.19	0.42
1:A:652:VAL:HG22	1:A:656:THR:OG1	2.20	0.42
1:A:730:THR:OG1	1:A:733:GLY:O	2.35	0.42
1:A:765:ILE:HA	1:A:798:ILE:HG22	2.02	0.42
1:B:555:GLN:HB3	1:B:558:GLU:HG3	2.01	0.42
1:C:809:ILE:HG13	1:C:828:LEU:HD21	2.01	0.42
1:E:765:ILE:HG21	1:E:808:ASP:OD2	2.20	0.42
1:F:459:GLU:OE2	1:F:473:PRO:HG3	2.19	0.42
1:F:852:VAL:HG11	1:F:864:ILE:HG22	2.00	0.42
1:A:582:ASN:HB3	1:A:805:LEU:HD13	2.01	0.42
1:B:773:LEU:CD2	1:B:790:LEU:HD23	2.48	0.42
1:D:553:THR:C	1:D:555:GLN:H	2.22	0.42
1:D:604:TYR:OH	1:D:775:TYR:O	2.35	0.42
1:C:876:GLU:O	1:C:893:VAL:HG12	2.20	0.42
1:C:960:ILE:HD12	1:C:960:ILE:HA	1.89	0.42
1:A:952:VAL:HG13	1:A:956:ALA:HB3	2.02	0.42
1:C:479:TRP:CZ3	1:C:915:LEU:HD12	2.55	0.42
1:C:505:GLY:O	1:C:870:LYS:HD3	2.19	0.42
1:E:603:LYS:O	1:E:627:LEU:HD12	2.20	0.41
1:A:959:GLN:HG2	1:A:973:ALA:HA	2.02	0.41
1:B:552:GLU:HA	1:B:560:TYR:CE1	2.55	0.41
1:A:880:ILE:HG22	1:A:890:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:811:ILE:HD11	1:C:826:VAL:HG21	2.02	0.41
1:C:815:GLU:OE2	1:D:463:ASP:CB	2.68	0.41
1:D:446:ASP:C	1:D:968:ARG:HG3	2.41	0.41
1:D:952:VAL:HG13	1:D:956:ALA:HB3	2.03	0.41
1:E:602:LEU:HD13	1:E:629:TRP:CE3	2.50	0.41
1:E:698:ALA:HB2	1:E:713:LEU:HD13	2.03	0.41
1:E:721:LEU:HD13	1:E:743:GLU:OE2	2.21	0.41
1:F:894:THR:OG1	1:F:897:ASP:OD2	2.31	0.41
1:F:960:ILE:HG13	1:F:964:ASP:HB2	2.02	0.41
1:C:655:GLY:O	1:C:663:PHE:HD2	2.03	0.41
1:D:801:GLU:O	1:D:803:PRO:HD3	2.20	0.41
1:D:815:GLU:CG	1:D:822:ARG:HG3	2.47	0.41
1:A:776:LYS:HG2	1:A:777:HIS:H	1.84	0.41
1:D:580:VAL:HG13	1:D:584:GLN:CD	2.40	0.41
1:D:716:LEU:HD23	1:D:716:LEU:HA	1.88	0.41
1:A:692:VAL:HG21	1:A:713:LEU:HD11	2.01	0.41
1:A:982:THR:HA	1:B:495:VAL:HA	2.03	0.41
1:A:659:VAL:HB	1:A:662:ILE:HB	2.02	0.41
1:B:538:ILE:HG23	1:B:826:VAL:HB	2.01	0.41
1:C:932:ALA:HB3	1:C:944:LEU:HD13	2.02	0.41
1:D:452:LYS:HD3	1:D:962:GLU:OE2	2.21	0.41
1:D:463:ASP:OD1	1:D:467:THR:N	2.53	0.41
1:D:504:ALA:N	1:D:874:ALA:HB2	2.35	0.41
1:D:616:LYS:HD2	1:D:772:ARG:NH2	2.35	0.41
1:D:851:LEU:HD21	1:D:866:ARG:NH1	2.36	0.41
1:E:604:TYR:HE1	1:E:773:LEU:HD13	1.84	0.41
1:D:439:VAL:HG22	1:D:440:THR:H	1.85	0.41
1:D:730:THR:OG1	1:D:733:GLY:O	2.37	0.41
1:A:546:LYS:H	1:A:822:ARG:NH2	2.19	0.41
1:A:854:ASP:N	1:A:854:ASP:OD1	2.54	0.41
1:E:644:LEU:HD12	1:E:644:LEU:HA	1.82	0.41
1:A:646:VAL:HG11	1:A:670:VAL:HG11	2.02	0.41
1:B:765:ILE:HG13	1:B:796:LEU:HD11	2.03	0.41
1:C:604:TYR:CE1	1:C:777:HIS:HA	2.56	0.41
1:D:815:GLU:CB	1:D:818:PRO:HD2	2.50	0.41
1:C:878:GLN:O	1:C:891:LEU:HB3	2.21	0.40
1:A:932:ALA:HB3	1:A:944:LEU:HD13	2.03	0.40
1:C:536:GLU:HG2	1:C:828:LEU:HD12	2.03	0.40
1:C:537:ILE:O	1:C:828:LEU:HA	2.22	0.40
1:C:445:SER:HB2	1:C:972:LEU:HD11	2.04	0.40
1:C:522:ARG:HH11	1:C:811:ILE:HD13	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:623:LYS:HD2	1:D:623:LYS:HA	1.96	0.40
1:D:876:GLU:OE1	1:D:898:ARG:NH1	2.54	0.40
1:A:701:LYS:HD2	1:A:701:LYS:HA	1.89	0.40
1:B:537:ILE:O	1:B:828:LEU:HA	2.22	0.40
1:B:701:LYS:HA	1:B:704:THR:CG2	2.51	0.40
1:B:932:ALA:HB3	1:B:944:LEU:HD13	2.02	0.40
1:D:810:GLU:HB3	1:D:825:LEU:HG	2.03	0.40
1:E:722:SER:HA	1:E:740:PRO:HA	2.03	0.40
1:C:536:GLU:CB	1:C:828:LEU:HD12	2.51	0.40
1:F:922:MSE:SE	1:F:944:LEU:HD13	2.71	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	548/553 (99%)	517 (94%)	31 (6%)	0	100	100
1	B	537/553 (97%)	504 (94%)	31 (6%)	2 (0%)	34	64
1	C	527/553 (95%)	503 (95%)	24 (5%)	0	100	100
1	D	541/553 (98%)	505 (93%)	36 (7%)	0	100	100
1	E	356/553 (64%)	325 (91%)	31 (9%)	0	100	100
1	F	242/553 (44%)	229 (95%)	13 (5%)	0	100	100
All	All	2751/3318 (83%)	2583 (94%)	166 (6%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	704	THR
1	B	883	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	456/452 (101%)	447 (98%)	9 (2%)	55	78
1	B	451/452 (100%)	445 (99%)	6 (1%)	69	86
1	C	442/452 (98%)	436 (99%)	6 (1%)	67	84
1	D	452/452 (100%)	448 (99%)	4 (1%)	78	90
1	E	305/452 (68%)	300 (98%)	5 (2%)	62	83
1	F	196/452 (43%)	194 (99%)	2 (1%)	76	89
All	All	2302/2712 (85%)	2270 (99%)	32 (1%)	67	84

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	434	MSE
1	A	464	ARG
1	A	467	THR
1	A	469	THR
1	A	677	ASP
1	A	757	SER
1	A	834	ARG
1	A	854	ASP
1	A	945	ARG
1	B	461	LYS
1	B	674	GLN
1	B	677	ASP
1	B	835	ARG
1	B	853	LYS
1	B	948	ARG
1	C	582	ASN
1	C	623	LYS
1	C	677	ASP
1	C	711	GLU
1	C	745	SER
1	C	902	GLU
1	D	606	ASP

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Mol	Chain	Res	Type
1	D	674	GLN
1	D	680	ARG
1	D	817	ASP
1	E	560	TYR
1	E	606	ASP
1	E	663	PHE
1	E	688	GLU
1	E	778	ASP
1	F	854	ASP
1	F	897	ASP

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

Mol	Chain	Res	Type
1	C	595	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	544/553 (98%)	0.23	14 (2%) 56 30	57, 122, 177, 218	0
1	B	535/553 (96%)	0.26	10 (1%) 66 43	43, 109, 165, 199	0
1	C	526/553 (95%)	0.19	8 (1%) 73 51	45, 75, 139, 200	0
1	D	538/553 (97%)	0.40	36 (6%) 17 7	58, 144, 192, 216	0
1	E	356/553 (64%)	1.76	130 (36%) 0 0	119, 190, 242, 272	0
1	F	243/553 (43%)	1.90	92 (37%) 0 0	162, 192, 221, 252	0
All	All	2742/3318 (82%)	0.61	290 (10%) 6 2	43, 126, 208, 272	0

All (290) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	664	CYS	9.1
1	B	554	GLN	7.3
1	F	929	PRO	7.0
1	E	808	ASP	7.0
1	E	841	GLN	6.9
1	E	839	ALA	6.7
1	F	887	VAL	6.4
1	F	857	HIS	6.3
1	E	655	GLY	6.2
1	F	908	PRO	6.2
1	E	838	ALA	6.1
1	E	850	LEU	5.8
1	F	865	ALA	5.8
1	E	805	LEU	5.8
1	F	903	THR	5.8
1	F	856	ASP	5.7
1	D	676	ASN	5.7
1	F	942	VAL	5.7
1	E	786	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	840	ASP	5.6
1	E	857	HIS	5.6
1	F	904	ASN	5.4
1	B	552	GLU	5.4
1	F	880	ILE	5.3
1	E	773	LEU	5.3
1	F	890	ILE	5.3
1	E	634	THR	5.3
1	F	521	VAL	5.2
1	E	635	HIS	5.2
1	F	907	LYS	5.2
1	E	834	ARG	5.1
1	E	665	GLN	5.1
1	E	529	SER	5.0
1	E	704	THR	5.0
1	F	464	ARG	4.9
1	E	864	ILE	4.9
1	E	532	GLY	4.9
1	E	727	LEU	4.9
1	E	515	THR	4.8
1	E	750	PRO	4.8
1	E	528	ASP	4.8
1	E	705	LEU	4.8
1	B	553	THR	4.7
1	E	843	GLN	4.7
1	F	462	ARG	4.7
1	E	852	VAL	4.7
1	F	526	GLN	4.6
1	E	592	ASP	4.6
1	D	883	SER	4.6
1	E	825	LEU	4.4
1	F	883	SER	4.4
1	E	673	ILE	4.4
1	E	527	GLN	4.3
1	B	555	GLN	4.3
1	F	930	GLU	4.3
1	E	842	THR	4.3
1	E	663	PHE	4.2
1	F	910	VAL	4.2
1	E	696	GLU	4.2
1	E	831	LEU	4.2
1	E	535	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	670	VAL	4.2
1	E	674	GLN	4.2
1	E	784	VAL	4.2
1	F	864	ILE	4.2
1	D	761	SER	4.1
1	F	924	LYS	4.1
1	D	977	PHE	4.1
1	E	736	ILE	4.1
1	F	863	VAL	4.1
1	C	882	ARG	4.1
1	F	533	ARG	4.1
1	E	804	GLN	4.0
1	F	950	TYR	4.0
1	F	494	PRO	3.9
1	E	845	SER	3.9
1	F	506	ALA	3.9
1	F	515	THR	3.9
1	F	510	GLU	3.9
1	F	965	LEU	3.9
1	E	712	VAL	3.8
1	F	520	VAL	3.8
1	F	507	VAL	3.8
1	E	783	SER	3.8
1	F	850	LEU	3.8
1	D	717	VAL	3.8
1	F	531	GLY	3.8
1	E	676	ASN	3.7
1	E	639	LYS	3.7
1	F	941	HIS	3.7
1	E	654	ALA	3.7
1	F	851	LEU	3.7
1	F	884	GLY	3.7
1	F	905	GLY	3.7
1	F	870	LYS	3.7
1	E	865	ALA	3.7
1	E	672	VAL	3.7
1	E	690	HIS	3.7
1	E	793	GLN	3.6
1	B	883	SER	3.6
1	E	619	TYR	3.6
1	A	808	ASP	3.6
1	E	580	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	673	ILE	3.6
1	F	869	ILE	3.5
1	F	866	ARG	3.5
1	F	849	SER	3.5
1	E	649	ASN	3.5
1	E	555	GLN	3.5
1	E	700	LEU	3.4
1	F	470	ARG	3.4
1	E	737	LEU	3.4
1	E	812	VAL	3.4
1	F	919	GLY	3.4
1	E	735	ALA	3.4
1	A	530	LYS	3.4
1	C	883	SER	3.4
1	E	835	ARG	3.4
1	F	902	GLU	3.4
1	F	909	THR	3.4
1	E	832	ILE	3.3
1	E	666	ASN	3.3
1	F	471	ILE	3.3
1	E	525	GLU	3.3
1	E	830	SER	3.3
1	F	873	GLN	3.3
1	C	464	ARG	3.2
1	E	837	ILE	3.2
1	E	868	ASP	3.2
1	E	833	ILE	3.2
1	E	669	VAL	3.2
1	F	522	ARG	3.2
1	F	484	GLU	3.2
1	F	858	ILE	3.2
1	E	846	THR	3.2
1	E	836	ASP	3.2
1	F	496	VAL	3.2
1	D	675	LYS	3.1
1	F	519	GLY	3.1
1	D	804	GLN	3.1
1	F	911	LYS	3.1
1	E	642	SER	3.1
1	E	751	SER	3.1
1	E	741	VAL	3.1
1	F	901	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	939	ASP	3.1
1	D	628	LEU	3.1
1	E	559	HIS	3.1
1	F	899	LEU	3.1
1	F	886	SER	3.1
1	C	808	ASP	3.0
1	F	943	ILE	3.0
1	E	679	LEU	3.0
1	E	701	LYS	3.0
1	F	458	ALA	3.0
1	E	656	THR	3.0
1	E	698	ALA	3.0
1	E	691	LEU	3.0
1	F	972	LEU	3.0
1	F	527	GLN	3.0
1	E	618	GLY	2.9
1	C	465	GLN	2.9
1	F	906	ALA	2.9
1	D	884	GLY	2.9
1	F	465	GLN	2.9
1	D	627	LEU	2.9
1	E	541	SER	2.8
1	C	466	GLY	2.8
1	D	682	ILE	2.8
1	D	770	VAL	2.8
1	E	844	GLY	2.8
1	E	699	ARG	2.8
1	D	698	ALA	2.8
1	F	479	TRP	2.8
1	D	625	GLY	2.8
1	F	456	LEU	2.8
1	E	629	TRP	2.7
1	F	885	GLU	2.7
1	F	537	ILE	2.7
1	E	591	ASP	2.7
1	E	806	ALA	2.7
1	D	607	ILE	2.7
1	E	524	PRO	2.7
1	E	587	ALA	2.7
1	D	744	PHE	2.7
1	D	802	ALA	2.7
1	F	892	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	611	LYS	2.7
1	E	614	LYS	2.7
1	F	855	GLY	2.7
1	E	534	GLU	2.7
1	E	512	THR	2.7
1	E	814	ASP	2.6
1	F	493	GLU	2.6
1	A	529	SER	2.6
1	F	502	ILE	2.6
1	F	882	ARG	2.6
1	F	505	GLY	2.6
1	E	680	ARG	2.6
1	A	798	ILE	2.6
1	E	620	GLU	2.6
1	E	785	ASP	2.6
1	A	555	GLN	2.6
1	B	681	GLU	2.6
1	F	916	VAL	2.6
1	E	856	ASP	2.6
1	F	535	VAL	2.6
1	E	604	TYR	2.6
1	F	478	ILE	2.6
1	F	944	LEU	2.6
1	D	828	LEU	2.5
1	E	689	LEU	2.5
1	F	852	VAL	2.5
1	E	716	LEU	2.5
1	E	866	ARG	2.5
1	F	441	LYS	2.5
1	C	884	GLY	2.5
1	F	900	ARG	2.5
1	E	858	ILE	2.5
1	D	823	LEU	2.5
1	E	740	PRO	2.5
1	F	830	SER	2.5
1	F	949	PRO	2.5
1	E	710	GLU	2.5
1	E	810	GLU	2.5
1	E	581	ALA	2.4
1	E	742	GLN	2.4
1	E	867	THR	2.4
1	D	554	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	871	ALA	2.4
1	A	937	VAL	2.4
1	A	554	GLN	2.4
1	D	674	GLN	2.4
1	A	553	THR	2.4
1	F	455	ASN	2.4
1	D	766	ARG	2.4
1	E	554	GLN	2.3
1	E	824	GLN	2.3
1	A	858	ILE	2.3
1	F	889	ARG	2.3
1	E	526	GLN	2.3
1	D	882	ARG	2.3
1	B	823	LEU	2.3
1	E	652	VAL	2.3
1	C	468	THR	2.3
1	E	553	THR	2.3
1	D	816	VAL	2.3
1	D	696	GLU	2.3
1	E	813	THR	2.2
1	E	667	SER	2.2
1	A	528	ASP	2.2
1	A	852	VAL	2.2
1	F	485	VAL	2.2
1	E	627	LEU	2.2
1	E	542	VAL	2.2
1	F	442	ASP	2.2
1	E	530	LYS	2.2
1	D	773	LEU	2.2
1	D	746	VAL	2.2
1	E	668	GLY	2.2
1	A	563	GLU	2.2
1	E	823	LEU	2.2
1	E	765	ILE	2.2
1	E	801	GLU	2.2
1	F	486	TYR	2.1
1	D	742	GLN	2.1
1	E	853	LYS	2.1
1	F	476	GLY	2.1
1	D	817	ASP	2.1
1	A	575	ALA	2.1
1	B	882	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	658	VAL	2.1
1	A	550	LEU	2.1
1	E	847	PHE	2.1
1	D	743	GLU	2.1
1	D	937	VAL	2.1
1	B	611	LYS	2.1
1	E	645	MET	2.1
1	F	938	ALA	2.1
1	F	920	ASP	2.1
1	D	769	ALA	2.0
1	D	643	LEU	2.0
1	D	716	LEU	2.0
1	D	805	LEU	2.0
1	E	616	LYS	2.0
1	E	533	ARG	2.0
1	E	675	LYS	2.0
1	F	829	GLU	2.0
1	D	658	VAL	2.0
1	E	697	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.