



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:15 AM UTC

PDB ID : 8EMB / pdb_00008emb
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

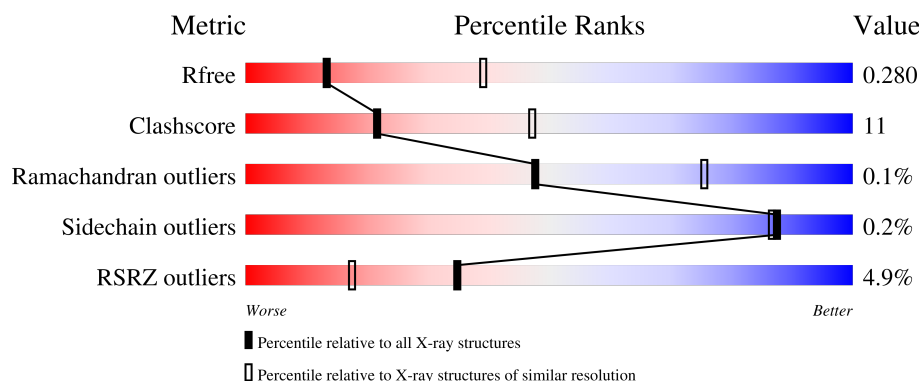
1 Overall quality at a glance

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}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (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 $\leq 5\%$. 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	4% 77% 20% .
1	C	553	2% 71% 25% .
1	D	553	5% 72% 26% .
1	E	553	9% 44% 21% 35%

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Mol	Chain	Length	Quality of chain
1	F	553	2% 34% 10% 56%

2 Entry composition

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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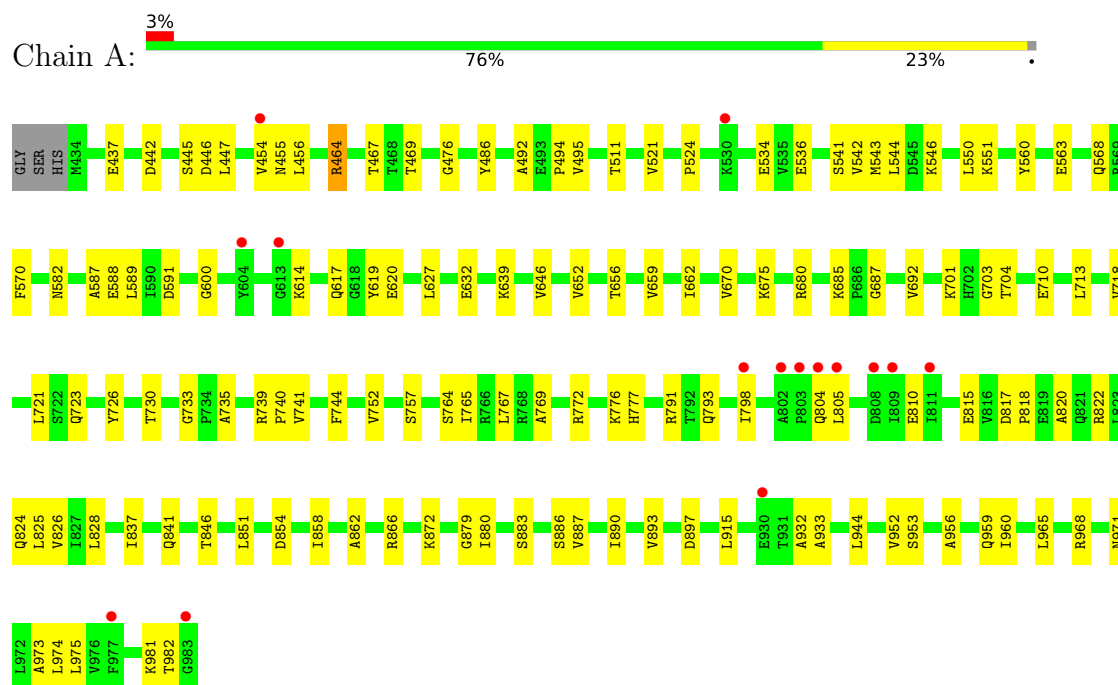
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Chain	Residue	Modelled	Actual	Comment	Reference
C	434	MSE	-	expression tag	UNP Q8DL57
C	508	MSE	LEU	engineered mutation	UNP Q8DL57
C	738	MSE	LEU	engineered mutation	UNP Q8DL57
C	922	MSE	LEU	engineered mutation	UNP Q8DL57
D	431	GLY	-	expression tag	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

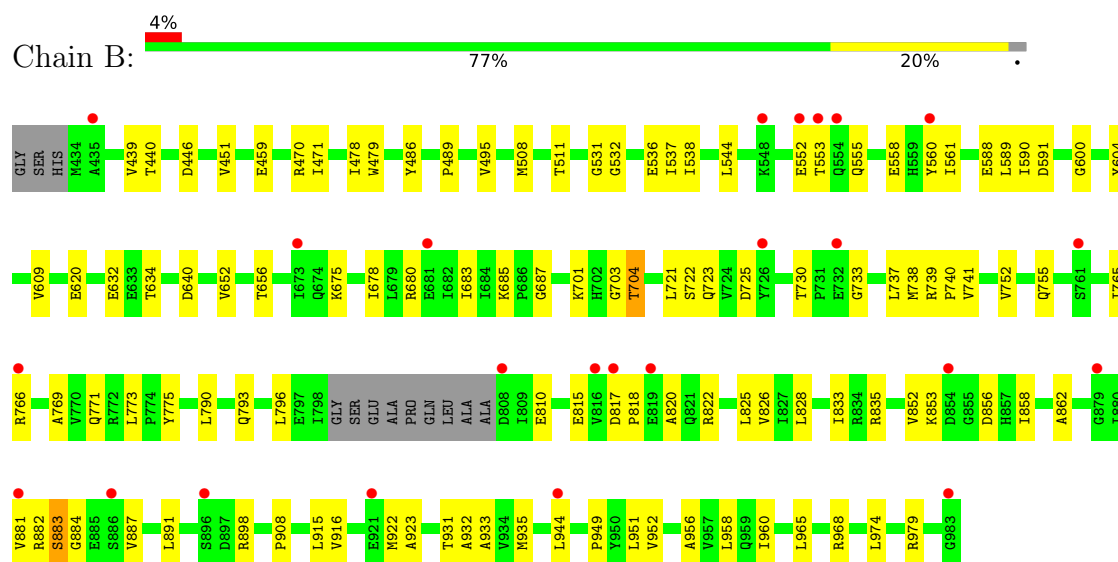
3 Residue-property plots [i](#)

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.

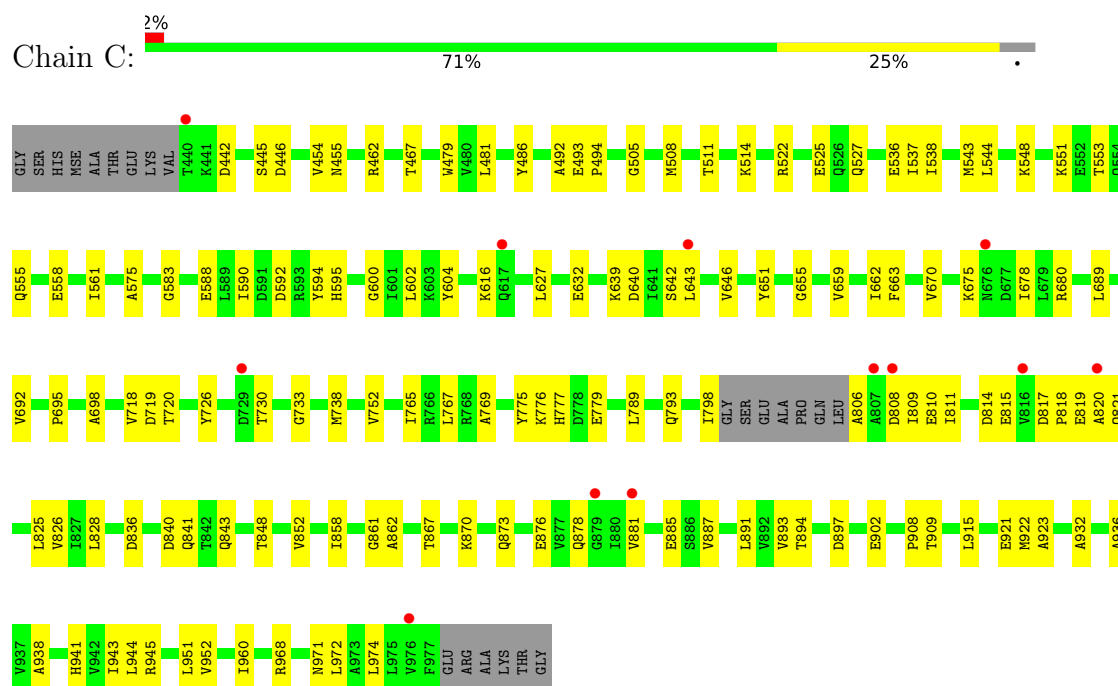
- Molecule 1: DNA-directed RNA polymerase subunit beta'



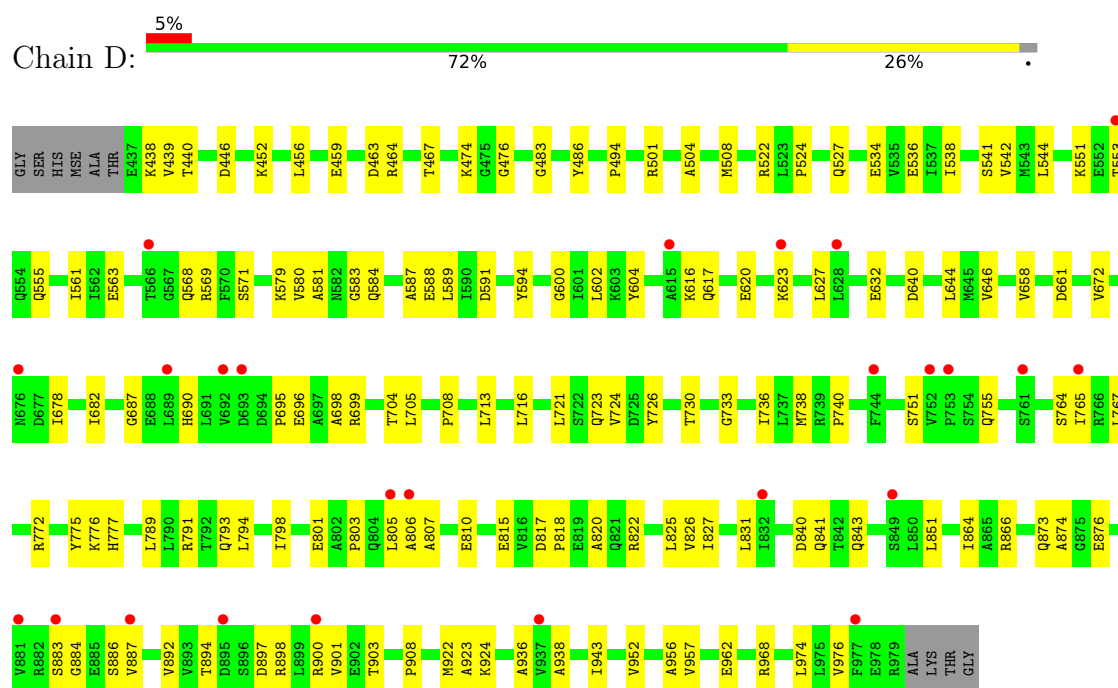
- Molecule 1: DNA-directed RNA polymerase subunit beta'



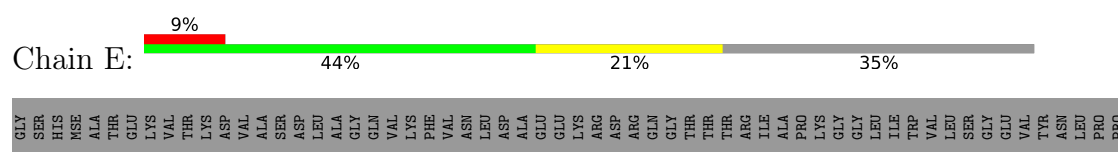
• Molecule 1: DNA-directed RNA polymerase subunit beta'



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



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





Chain F: 

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 0.267 , 0.280	Depositor DCC
R_{free} test set	1998 reflections (2.04%)	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 , 79.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.18	0/4233	0.44	0/5731
1	B	0.15	0/4173	0.41	0/5647
1	C	0.19	0/4093	0.46	0/5542
1	D	0.15	0/4188	0.44	0/5671
1	E	0.13	0/2787	0.35	0/3777
1	F	0.11	0/1850	0.33	0/2500
All	All	0.16	0/21324	0.42	0/28868

There are no bond length outliers.

There are no bond angle outliers.

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	4185	0	4263	86	0
1	B	4127	0	4207	70	0
1	C	4047	0	4121	99	0
1	D	4140	0	4214	104	0
1	E	2752	0	2781	80	0
1	F	1835	0	1879	36	0
All	All	21086	0	21465	461	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 (461) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:551:LYS:NZ	1:E:757:SER:O	2.35	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: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:B:446:ASP:C	1:B:968:ARG:HG3	2.38	0.48
1:B:815:GLU:HG3	1:B:820:ALA:C	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:553:THR:C	1:D:555:GLN:H	2.22	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:446:ASP:C	1:D:968:ARG:HG3	2.41	0.46
1:D:501:ARG:HD3	1:D:876:GLU:HB2	1.98	0.46
1:D:580:VAL:HG13	1:D:584:GLN:CD	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:640:ASP:OD1	1:C:642:SER:OG	2.32	0.45
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.85	0.44
1:D:841:GLN:CD	1:D:841:GLN:H	2.24	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:C:446:ASP:C	1:C:968:ARG:HG3	2.42	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:D:604:TYR:OH	1:D:775:TYR:O	2.35	0.44
1:C:555:GLN:OE1	1:C:555:GLN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:701:LYS:C	1:A:703:GLY:H	2.25	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:815:GLU:HG3	1:D:820:ALA:C	2.43	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:837:ILE:H	1:A:846:THR:HG1	1.63	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: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:D:884:GLY:C	1:D:886:SER:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:951:LEU:HG	1:B:952:VAL:N	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:GLU:HA	1:B:560:TYR:CE1	2.55	0.41
1:A:446:ASP:C	1:A:968:ARG:HG3	2.45	0.41
1:A:880:ILE:HG22	1:A:890:ILE:HG12	2.01	0.41
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: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: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:D:730:THR:OG1	1:D:733:GLY:O	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:ARG:HH11	1:C:811:ILE:HD13	1.85	0.40
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%)	30	57
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%)	48	75

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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%)	453 (99%)	3 (1%)	76	80
1	B	451/452 (100%)	451 (100%)	0	100	100
1	C	442/452 (98%)	441 (100%)	1 (0%)	87	87
1	D	452/452 (100%)	452 (100%)	0	100	100
1	E	305/452 (68%)	304 (100%)	1 (0%)	86	85
1	F	196/452 (43%)	196 (100%)	0	100	100
All	All	2302/2712 (85%)	2297 (100%)	5 (0%)	87	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	ARG
1	A	467	THR
1	A	469	THR
1	C	902	GLU
1	E	688	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	568	GLN
1	A	702	HIS
1	A	941	HIS
1	B	650	GLN
1	B	873	GLN
1	C	517	HIS
1	C	676	ASN
1	C	763	GLN
1	C	878	GLN
1	C	941	HIS
1	D	554	GLN
1	D	690	HIS

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Mol	Chain	Res	Type
1	D	723	GLN
1	D	878	GLN
1	E	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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	544/553 (98%)	0.37	15 (2%)	55	32	57, 122, 177, 218	0
1	B	535/553 (96%)	0.34	24 (4%)	38	20	43, 109, 165, 199	0
1	C	526/553 (95%)	0.19	12 (2%)	61	38	45, 75, 139, 200	0
1	D	538/553 (97%)	0.50	25 (4%)	37	19	58, 144, 192, 216	0
1	E	356/553 (64%)	0.99	48 (13%)	7	4	119, 190, 242, 272	0
1	F	243/553 (43%)	0.63	10 (4%)	41	22	162, 192, 221, 252	0
All	All	2742/3318 (82%)	0.46	134 (4%)	35	17	43, 126, 208, 272	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	808	ASP	5.9
1	A	808	ASP	4.7
1	F	976	VAL	3.9
1	D	977	PHE	3.8
1	B	983	GLY	3.8
1	E	809	ILE	3.7
1	E	643	LEU	3.7
1	E	828	LEU	3.7
1	B	881	VAL	3.5
1	E	635	HIS	3.4
1	B	886	SER	3.4
1	E	750	PRO	3.3
1	E	808	ASP	3.2
1	C	881	VAL	3.2
1	D	676	ASN	3.2
1	B	726	TYR	3.2
1	D	744	PHE	3.2
1	E	658	VAL	3.2
1	F	901	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	530	LYS	3.1
1	C	440	THR	3.1
1	B	554	GLN	3.1
1	E	634	THR	3.1
1	D	752	VAL	3.0
1	A	809	ILE	3.0
1	E	646	VAL	3.0
1	D	806	ALA	3.0
1	B	854	ASP	3.0
1	E	811	ILE	3.0
1	A	803	PRO	2.9
1	B	552	GLU	2.9
1	E	806	ALA	2.9
1	E	656	THR	2.9
1	F	440	THR	2.8
1	E	622	LEU	2.8
1	D	883	SER	2.8
1	F	929	PRO	2.8
1	F	912	VAL	2.8
1	B	761	SER	2.8
1	B	553	THR	2.8
1	E	801	GLU	2.8
1	E	673	ILE	2.7
1	B	435	ALA	2.7
1	C	816	VAL	2.7
1	E	833	ILE	2.6
1	E	550	LEU	2.6
1	E	553	THR	2.6
1	E	679	LEU	2.6
1	E	805	LEU	2.6
1	D	937	VAL	2.6
1	A	454	VAL	2.6
1	C	807	ALA	2.6
1	F	535	VAL	2.6
1	B	816	VAL	2.5
1	B	560	TYR	2.5
1	E	639	LYS	2.5
1	C	879	GLY	2.5
1	B	921	GLU	2.5
1	C	676	ASN	2.5
1	E	751	SER	2.5
1	E	767	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	718	VAL	2.5
1	E	682	ILE	2.4
1	B	681	GLU	2.4
1	D	693	ASP	2.4
1	B	673	ILE	2.4
1	F	850	LEU	2.4
1	E	676	ASN	2.4
1	E	775	TYR	2.4
1	D	628	LEU	2.4
1	E	649	ASN	2.4
1	F	865	ALA	2.4
1	A	805	LEU	2.4
1	D	895	ASP	2.4
1	E	544	LEU	2.4
1	C	643	LEU	2.3
1	E	691	LEU	2.3
1	E	794	LEU	2.3
1	E	825	LEU	2.3
1	B	732	GLU	2.3
1	D	753	PRO	2.3
1	D	553	THR	2.3
1	B	817	ASP	2.3
1	A	613	GLY	2.3
1	A	798	ILE	2.3
1	F	520	VAL	2.3
1	C	729	ASP	2.3
1	D	900	ARG	2.3
1	A	802	ALA	2.3
1	D	761	SER	2.3
1	B	879	GLY	2.2
1	E	831	LEU	2.2
1	A	983	GLY	2.2
1	D	881	VAL	2.2
1	E	784	VAL	2.2
1	A	804	GLN	2.2
1	C	820	ALA	2.2
1	C	976	VAL	2.2
1	D	887	VAL	2.2
1	C	617	GLN	2.2
1	B	944	LEU	2.2
1	E	727	LEU	2.2
1	A	811	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	713	LEU	2.2
1	D	615	ALA	2.2
1	E	781	VAL	2.1
1	D	689	LEU	2.1
1	D	849	SER	2.1
1	E	761	SER	2.1
1	E	753	PRO	2.1
1	A	977	PHE	2.1
1	E	596	THR	2.1
1	E	783	SER	2.1
1	B	808	ASP	2.1
1	E	629	TRP	2.1
1	D	566	THR	2.1
1	D	805	LEU	2.1
1	E	789	LEU	2.1
1	B	819	GLU	2.1
1	B	896	SER	2.1
1	E	850	LEU	2.1
1	B	766	ARG	2.1
1	F	490	PRO	2.1
1	E	571	SER	2.1
1	B	548	LYS	2.1
1	E	662	ILE	2.1
1	A	604	TYR	2.1
1	A	930	GLU	2.1
1	D	692	VAL	2.0
1	D	765	ILE	2.0
1	E	785	ASP	2.0
1	E	681	GLU	2.0
1	D	832	ILE	2.0
1	D	623	LYS	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 oligosaccharides 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.