Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 10:07 pm GMT

PDB ID	:	4BLA
Title	:	Crystal structure of full-length human Suppressor of fused (SUFU) mutant lacking a regulatory subdomain (crystal form II)
Authors	:	Cherry, A.L.; Finta, C.; Karlstrom, M.; Toftgard, R.; Jovine, L.
Deposited on	:	2013-05-02
Resolution	:	3.50 Å(reported)

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

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

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

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

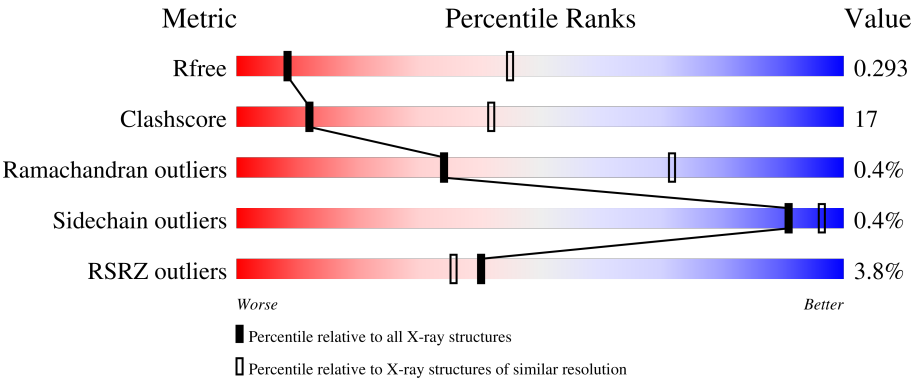
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	756	74% 22%
1	B	756	4% 79% 17%
1	C	756	4% 78% 17%
1	D	756	6% 69% 27%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22889 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 MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5718	3668	949	1083	18			
1	B	733	Total	C	N	O	S	0	0	0
			5734	3673	954	1089	18			
1	C	724	Total	C	N	O	S	0	0	0
			5665	3632	942	1073	18			
1	D	738	Total	C	N	O	S	0	0	0
			5772	3696	960	1098	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P0AEX9
A	3	THR	ILE	engineered mutation	UNP P0AEX9
A	360	ALA	GLU	engineered mutation	UNP P0AEX9
A	363	ALA	LYS	engineered mutation	UNP P0AEX9
A	364	ALA	ASP	engineered mutation	UNP P0AEX9
A	368	ASN	ARG	engineered mutation	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	371	ALA	-	linker	UNP P0AEX9
A	619	PRO	-	linker	UNP Q9UMX1
A	620	SER	-	linker	UNP Q9UMX1
A	621	ARG	-	linker	UNP Q9UMX1
A	622	GLY	-	linker	UNP Q9UMX1
A	623	GLU	-	linker	UNP Q9UMX1
A	624	ASP	-	linker	UNP Q9UMX1
A	625	PRO	-	linker	UNP Q9UMX1
A	749	VAL	-	expression tag	UNP Q9UMX1
A	750	GLU	-	expression tag	UNP Q9UMX1
A	751	HIS	-	expression tag	UNP Q9UMX1
A	752	HIS	-	expression tag	UNP Q9UMX1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	753	HIS	-	expression tag	UNP Q9UMX1
A	754	HIS	-	expression tag	UNP Q9UMX1
A	755	HIS	-	expression tag	UNP Q9UMX1
A	756	HIS	-	expression tag	UNP Q9UMX1
B	1	MET	-	expression tag	UNP P0AEX9
B	3	THR	ILE	engineered mutation	UNP P0AEX9
B	360	ALA	GLU	engineered mutation	UNP P0AEX9
B	363	ALA	LYS	engineered mutation	UNP P0AEX9
B	364	ALA	ASP	engineered mutation	UNP P0AEX9
B	368	ASN	ARG	engineered mutation	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
B	371	ALA	-	linker	UNP P0AEX9
B	619	PRO	-	linker	UNP Q9UMX1
B	620	SER	-	linker	UNP Q9UMX1
B	621	ARG	-	linker	UNP Q9UMX1
B	622	GLY	-	linker	UNP Q9UMX1
B	623	GLU	-	linker	UNP Q9UMX1
B	624	ASP	-	linker	UNP Q9UMX1
B	625	PRO	-	linker	UNP Q9UMX1
B	749	VAL	-	expression tag	UNP Q9UMX1
B	750	GLU	-	expression tag	UNP Q9UMX1
B	751	HIS	-	expression tag	UNP Q9UMX1
B	752	HIS	-	expression tag	UNP Q9UMX1
B	753	HIS	-	expression tag	UNP Q9UMX1
B	754	HIS	-	expression tag	UNP Q9UMX1
B	755	HIS	-	expression tag	UNP Q9UMX1
B	756	HIS	-	expression tag	UNP Q9UMX1
C	1	MET	-	expression tag	UNP P0AEX9
C	3	THR	ILE	engineered mutation	UNP P0AEX9
C	360	ALA	GLU	engineered mutation	UNP P0AEX9
C	363	ALA	LYS	engineered mutation	UNP P0AEX9
C	364	ALA	ASP	engineered mutation	UNP P0AEX9
C	368	ASN	ARG	engineered mutation	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
C	370	ALA	-	linker	UNP P0AEX9
C	371	ALA	-	linker	UNP P0AEX9
C	619	PRO	-	linker	UNP Q9UMX1
C	620	SER	-	linker	UNP Q9UMX1
C	621	ARG	-	linker	UNP Q9UMX1
C	622	GLY	-	linker	UNP Q9UMX1
C	623	GLU	-	linker	UNP Q9UMX1

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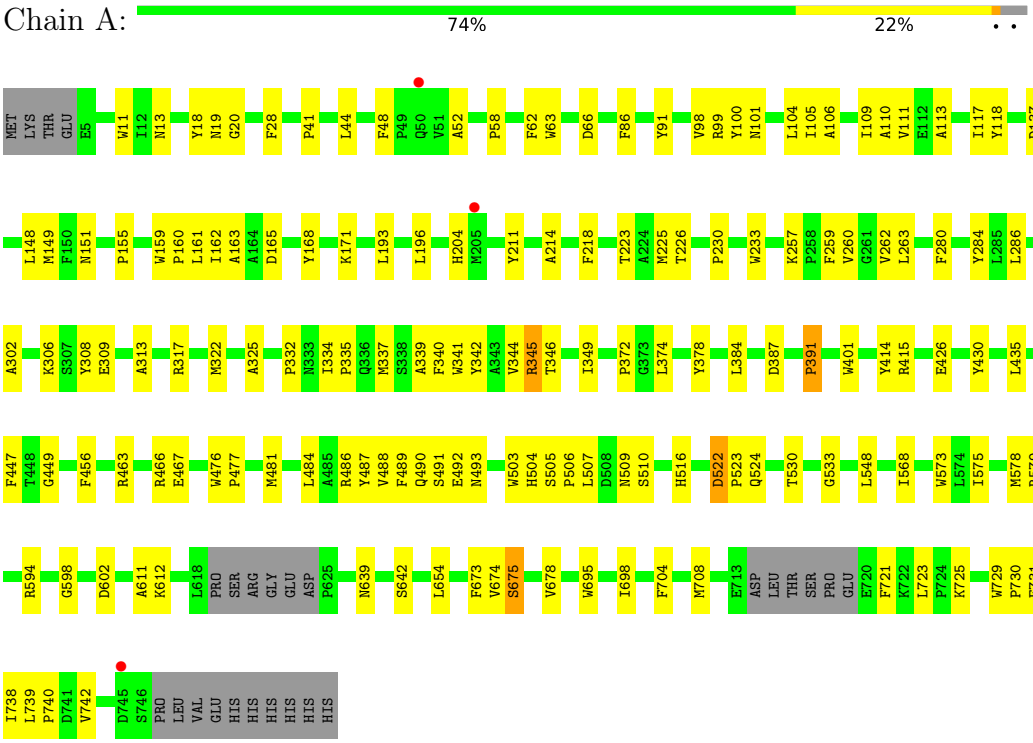
Chain	Residue	Modelled	Actual	Comment	Reference
C	624	ASP	-	linker	UNP Q9UMX1
C	625	PRO	-	linker	UNP Q9UMX1
C	749	VAL	-	expression tag	UNP Q9UMX1
C	750	GLU	-	expression tag	UNP Q9UMX1
C	751	HIS	-	expression tag	UNP Q9UMX1
C	752	HIS	-	expression tag	UNP Q9UMX1
C	753	HIS	-	expression tag	UNP Q9UMX1
C	754	HIS	-	expression tag	UNP Q9UMX1
C	755	HIS	-	expression tag	UNP Q9UMX1
C	756	HIS	-	expression tag	UNP Q9UMX1
D	1	MET	-	expression tag	UNP P0AEX9
D	3	THR	ILE	engineered mutation	UNP P0AEX9
D	360	ALA	GLU	engineered mutation	UNP P0AEX9
D	363	ALA	LYS	engineered mutation	UNP P0AEX9
D	364	ALA	ASP	engineered mutation	UNP P0AEX9
D	368	ASN	ARG	engineered mutation	UNP P0AEX9
D	369	ALA	-	linker	UNP P0AEX9
D	370	ALA	-	linker	UNP P0AEX9
D	371	ALA	-	linker	UNP P0AEX9
D	619	PRO	-	linker	UNP Q9UMX1
D	620	SER	-	linker	UNP Q9UMX1
D	621	ARG	-	linker	UNP Q9UMX1
D	622	GLY	-	linker	UNP Q9UMX1
D	623	GLU	-	linker	UNP Q9UMX1
D	624	ASP	-	linker	UNP Q9UMX1
D	625	PRO	-	linker	UNP Q9UMX1
D	749	VAL	-	expression tag	UNP Q9UMX1
D	750	GLU	-	expression tag	UNP Q9UMX1
D	751	HIS	-	expression tag	UNP Q9UMX1
D	752	HIS	-	expression tag	UNP Q9UMX1
D	753	HIS	-	expression tag	UNP Q9UMX1
D	754	HIS	-	expression tag	UNP Q9UMX1
D	755	HIS	-	expression tag	UNP Q9UMX1
D	756	HIS	-	expression tag	UNP Q9UMX1

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.

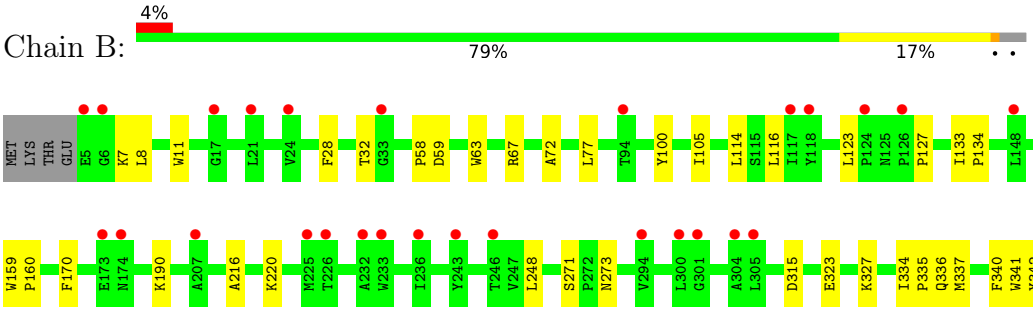
• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

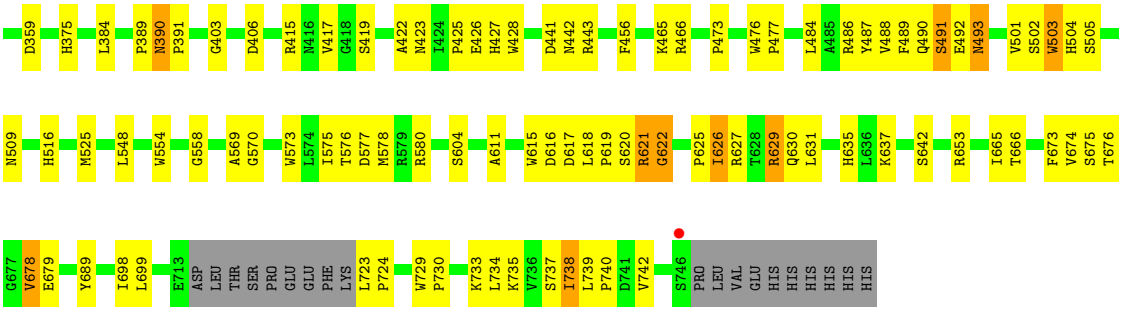
Chain A:



• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

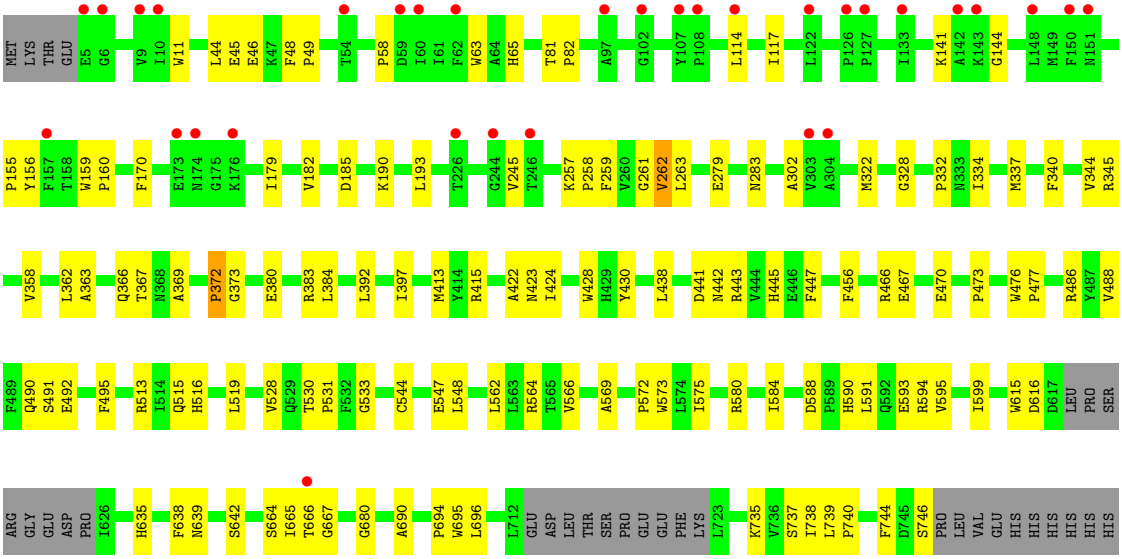
Chain B:





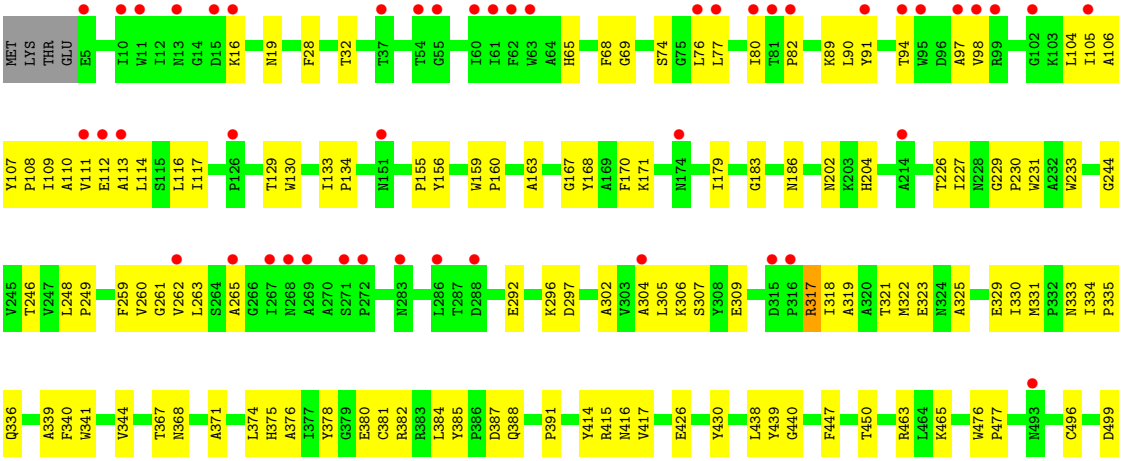
• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

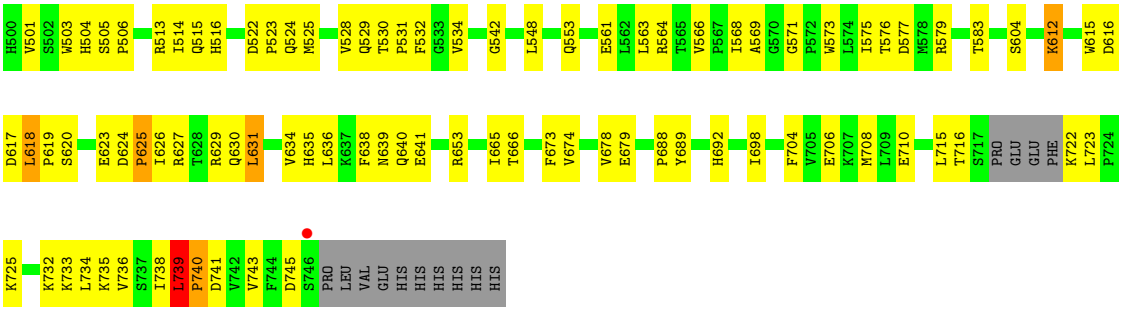
Chain C:



• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

Chain D:




H500 V501 S502 W503 H504 S505 P506 R513 I514 Q515 H516 D522 P523 Q524 M525 V528 Q529 T530 P531 F532 G533 V534 G542 L548 Q553 E561 L562 L563 R564 T565 V566 P567 I568 A569 G570 G571 P572 W573 L574 I575 T576 D577 M578 R579 T583 S604 K612 W615 D616
D617 L618 P619 S620 E623 D624 P625 I626 R627 T628 R629 Q630 L631 V634 H635 L636 K637 F638 N639 Q640 E641 R653 I665 T666 F673 V674 V678 E679 P688 Y689 H692 I698 F704 V705 E706 K707 M708 L709 E710 L715 T716 S717 PRO GLU GLU PHE K722 L723 P724
K725 K732 K733 L734 K735 V736 S737 I738 L739 P740 D741 V742 V743 F744 D745 S746 PRO LEU VAL GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	117.92Å 372.57Å 86.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.58 – 3.50 39.58 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.58-3.50) 99.5 (39.58-3.50)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.259 , 0.293 0.259 , 0.293	Depositor DCC
R_{free} test set	2462 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	110.8	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 76.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22889	wwPDB-VP
Average B, all atoms (Å^2)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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	0.48	1/5871 (0.0%)	0.64	1/7984 (0.0%)
1	B	0.48	1/5888 (0.0%)	0.61	0/8011
1	C	0.46	0/5816	0.63	1/7911 (0.0%)
1	D	0.49	1/5926 (0.0%)	0.63	1/8062 (0.0%)
All	All	0.48	3/23501 (0.0%)	0.63	3/31968 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	678	VAL	CB-CG2	-5.64	1.41	1.52
1	A	675	SER	CB-OG	-5.56	1.35	1.42
1	D	740	PRO	N-CD	5.16	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	739	LEU	C-N-CD	5.96	140.92	128.40
1	C	415	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	522	ASP	CB-CG-OD2	5.02	122.82	118.30

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	5718	0	5580	194	0
1	B	5734	0	5590	167	0
1	C	5665	0	5527	131	0
1	D	5772	0	5630	318	0
All	All	22889	0	22327	776	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 17.

All (776) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:TYR:CE2	1:D:171:LYS:HB2	1.54	1.40
1:A:507:LEU:HB2	1:A:578:MET:CE	1.56	1.33
1:D:112:GLU:CG	1:D:262:VAL:HB	1.59	1.30
1:D:111:VAL:HB	1:D:322:MET:SD	1.79	1.22
1:A:723:LEU:HD13	1:A:738:ILE:HD11	1.24	1.12
1:A:507:LEU:HB2	1:A:578:MET:HE2	1.15	1.10
1:D:722:LYS:O	1:D:725:LYS:HG3	1.49	1.09
1:D:80:ILE:HD12	1:D:107:TYR:CE1	1.88	1.08
1:B:674:VAL:HG13	1:B:678:VAL:HG21	1.28	1.08
1:D:168:TYR:HE2	1:D:171:LYS:CB	1.66	1.07
1:D:112:GLU:HG3	1:D:262:VAL:CB	1.86	1.05
1:D:112:GLU:HG3	1:D:262:VAL:HB	1.35	1.01
1:A:507:LEU:HB2	1:A:578:MET:HE1	1.43	1.00
1:B:355:ARG:NH1	1:B:389:PRO:HG3	1.74	1.00
1:D:111:VAL:CB	1:D:322:MET:SD	2.49	1.00
1:D:113:ALA:HA	1:D:260:VAL:HG11	1.46	0.98
1:D:112:GLU:CG	1:D:262:VAL:CB	2.43	0.96
1:D:579:ARG:CZ	1:D:579:ARG:HA	1.94	0.96
1:B:733:LYS:HE2	1:B:735:LYS:HE3	1.45	0.96
1:B:456:PHE:HE2	1:B:489:PHE:CE1	1.83	0.96
1:A:738:ILE:N	1:A:738:ILE:HD12	1.78	0.96
1:C:193:LEU:HD23	1:C:362:LEU:HD21	1.48	0.94
1:D:112:GLU:HG2	1:D:262:VAL:HB	1.46	0.94
1:D:612:LYS:NZ	1:D:739:LEU:HD13	1.81	0.94
1:D:111:VAL:HG21	1:D:322:MET:HA	1.48	0.94
1:D:715:LEU:O	1:D:716:THR:OG1	1.86	0.94
1:C:182:VAL:HB	1:C:366:GLN:NE2	1.82	0.93
1:D:440:GLY:HA3	1:D:532:PHE:CE1	2.04	0.93
1:D:80:ILE:HB	1:D:107:TYR:OH	1.69	0.92
1:B:72:ALA:CB	1:B:105:ILE:HD13	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:VAL:HG13	1:B:678:VAL:CG2	1.98	0.92
1:A:507:LEU:CB	1:A:578:MET:HE2	2.01	0.90
1:B:72:ALA:HB2	1:B:105:ILE:HD13	1.53	0.90
1:D:159:TRP:CE2	1:D:259:PHE:CE2	2.60	0.90
1:C:182:VAL:HB	1:C:366:GLN:HE21	1.35	0.90
1:A:374:LEU:HD21	1:A:378:TYR:CZ	2.07	0.90
1:D:168:TYR:CE2	1:D:171:LYS:CB	2.47	0.89
1:D:168:TYR:HE2	1:D:171:LYS:HB2	0.80	0.89
1:B:390:ASN:O	1:B:390:ASN:ND2	2.05	0.88
1:A:723:LEU:CD1	1:A:738:ILE:HD11	2.02	0.88
1:D:259:PHE:CD1	1:D:329:GLU:HB2	2.08	0.88
1:C:358:VAL:O	1:C:362:LEU:HG	1.74	0.88
1:B:620:SER:O	1:B:621:ARG:HG2	1.73	0.87
1:A:446:GLU:OE1	1:A:446:GLU:N	2.06	0.87
1:D:80:ILE:HB	1:D:107:TYR:CZ	2.09	0.86
1:D:113:ALA:HA	1:D:260:VAL:CG1	2.05	0.86
1:D:629:ARG:NH1	1:D:631:LEU:HD23	1.89	0.86
1:D:524:GLN:NE2	1:D:573:TRP:CZ2	2.44	0.86
1:A:729:TRP:HB3	1:A:730:PRO:HD2	1.56	0.85
1:D:114:LEU:HG	1:D:230:PRO:HD3	1.59	0.85
1:B:617:ASP:HB3	1:B:619:PRO:HD2	1.59	0.84
1:A:374:LEU:HD21	1:A:378:TYR:CE2	2.11	0.84
1:D:82:PRO:HG3	1:D:107:TYR:HE1	1.41	0.84
1:A:674:VAL:HG13	1:A:678:VAL:HG21	1.59	0.84
1:B:155:PRO:HG2	1:B:341:TRP:CE3	2.13	0.84
1:D:740:PRO:HD2	1:D:741:ASP:OD1	1.75	0.84
1:B:503:TRP:CE2	1:D:738:ILE:HG21	2.12	0.83
1:D:617:ASP:O	1:D:618:LEU:HG	1.79	0.83
1:C:441:ASP:OD2	1:C:443:ARG:NE	2.12	0.83
1:D:465:LYS:HG3	1:D:575:ILE:HG22	1.60	0.82
1:D:167:GLY:HA2	1:D:186:ASN:HD21	1.41	0.82
1:D:159:TRP:CE2	1:D:259:PHE:CZ	2.68	0.82
1:B:441:ASP:OD2	1:B:443:ARG:NH2	2.12	0.82
1:D:465:LYS:HG3	1:D:575:ILE:CG2	2.09	0.82
1:D:80:ILE:CD1	1:D:107:TYR:CE1	2.63	0.82
1:D:465:LYS:HD2	1:D:577:ASP:HB2	1.60	0.82
1:B:504:HIS:O	1:B:504:HIS:ND1	2.13	0.81
1:B:733:LYS:HE2	1:B:735:LYS:CE	2.10	0.81
1:D:722:LYS:O	1:D:725:LYS:CG	2.27	0.81
1:D:624:ASP:OD2	1:D:627:ARG:NH2	2.13	0.81
1:D:159:TRP:CZ2	1:D:259:PHE:CZ	2.68	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LEU:CB	1:A:578:MET:CE	2.52	0.80
1:C:190:LYS:HG2	1:C:362:LEU:HD12	1.62	0.79
1:D:111:VAL:CG1	1:D:322:MET:SD	2.71	0.79
1:C:738:ILE:HG23	1:C:739:LEU:N	1.98	0.79
1:D:259:PHE:CE1	1:D:329:GLU:HB2	2.18	0.79
1:D:612:LYS:HZ2	1:D:739:LEU:HD13	1.48	0.78
1:A:467:GLU:HG3	1:A:579:ARG:NH2	1.99	0.78
1:D:564:ARG:HG3	1:D:564:ARG:HH11	1.48	0.78
1:D:110:ALA:HB1	1:D:302:ALA:CB	2.14	0.77
1:D:415:ARG:NH1	1:D:426:GLU:OE2	2.17	0.77
1:B:456:PHE:CE2	1:B:489:PHE:CE1	2.73	0.77
1:A:505:SER:OG	1:A:506:PRO:HD2	1.84	0.77
1:A:522:ASP:OD1	1:A:523:PRO:HD2	1.85	0.76
1:C:665:ILE:HG13	1:C:666:THR:N	2.00	0.76
1:A:506:PRO:HG2	1:A:509:ASN:HA	1.66	0.76
1:A:487:TYR:O	1:A:491:SER:HB3	1.85	0.76
1:B:674:VAL:CG1	1:B:678:VAL:HG21	2.12	0.76
1:D:170:PHE:HE1	1:D:179:ILE:HA	1.51	0.75
1:D:566:VAL:HB	1:D:569:ALA:CB	2.15	0.75
1:D:112:GLU:HG3	1:D:262:VAL:CA	2.14	0.75
1:B:738:ILE:HG21	1:D:503:TRP:C	2.07	0.75
1:D:116:LEU:HD23	1:D:248:LEU:HD23	1.69	0.75
1:A:654:LEU:HA	1:A:675:SER:OG	1.86	0.75
1:D:110:ALA:HB1	1:D:302:ALA:HB3	1.67	0.75
1:D:159:TRP:NE1	1:D:259:PHE:CZ	2.55	0.75
1:D:566:VAL:HB	1:D:569:ALA:HB3	1.69	0.74
1:A:260:VAL:HG21	1:A:325:ALA:HA	1.69	0.74
1:B:615:TRP:O	1:B:621:ARG:NH1	2.21	0.74
1:B:626:ILE:HG12	1:B:627:ARG:H	1.53	0.74
1:D:739:LEU:HD23	1:D:739:LEU:N	2.03	0.74
1:D:639:ASN:OD1	1:D:640:GLN:N	2.19	0.74
1:A:159:TRP:CD1	1:A:259:PHE:CZ	2.75	0.74
1:C:363:ALA:O	1:C:367:THR:HG23	1.88	0.73
1:D:530:THR:HG23	1:D:531:PRO:HD2	1.71	0.73
1:D:116:LEU:HD11	1:D:246:THR:HG23	1.69	0.73
1:B:28:PHE:CE2	1:B:32:THR:HG21	2.23	0.73
1:C:738:ILE:HG23	1:C:739:LEU:H	1.52	0.73
1:D:738:ILE:O	1:D:740:PRO:HD3	1.88	0.72
1:D:69:GLY:HA3	1:D:333:ASN:HB3	1.71	0.72
1:C:615:TRP:CE3	1:C:696:LEU:HD22	2.25	0.71
1:D:440:GLY:HA3	1:D:532:PHE:CZ	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:LYS:HG2	1:C:362:LEU:CD1	2.19	0.71
1:C:665:ILE:HG13	1:C:666:THR:HG23	1.74	0.70
1:D:715:LEU:C	1:D:716:THR:HG1	1.92	0.70
1:A:415:ARG:NH1	1:A:426:GLU:OE2	2.25	0.70
1:A:730:PRO:HG2	1:A:731:GLU:OE1	1.92	0.70
1:B:406:ASP:OD1	1:B:486:ARG:NH2	2.25	0.70
1:D:94:THR:HB	1:D:108:PRO:HB3	1.73	0.70
1:D:617:ASP:OD1	1:D:620:SER:N	2.25	0.70
1:B:630:GLN:O	1:B:631:LEU:HD23	1.92	0.69
1:D:387:ASP:OD2	1:D:388:GLN:NE2	2.25	0.69
1:D:722:LYS:N	1:D:725:LYS:HE2	2.07	0.69
1:A:456:PHE:CE2	1:A:488:VAL:HG12	2.26	0.69
1:A:739:LEU:N	1:A:740:PRO:CD	2.56	0.69
1:B:487:TYR:HE2	1:D:740:PRO:HB2	1.57	0.69
1:D:259:PHE:HD1	1:D:329:GLU:HB2	1.58	0.69
1:C:185:ASP:HB2	1:C:366:GLN:OE1	1.92	0.69
1:D:113:ALA:HB2	1:D:325:ALA:HA	1.74	0.69
1:B:723:LEU:HB2	1:B:724:PRO:HA	1.76	0.68
1:D:111:VAL:HG11	1:D:322:MET:SD	2.33	0.68
1:D:94:THR:HB	1:D:108:PRO:CB	2.23	0.68
1:A:492:GLU:HA	1:A:492:GLU:OE1	1.92	0.68
1:B:618:LEU:HD21	1:C:665:ILE:CG2	2.23	0.68
1:C:635:HIS:CE1	1:C:735:LYS:HD3	2.28	0.68
1:B:422:ALA:O	1:B:423:ASN:ND2	2.27	0.68
1:C:513:ARG:HD2	1:C:544:CYS:SG	2.34	0.68
1:C:392:LEU:HD21	1:C:473:PRO:HD2	1.75	0.68
1:B:492:GLU:OE2	1:D:745:ASP:OD1	2.13	0.67
1:A:487:TYR:CE1	1:A:491:SER:HB2	2.30	0.67
1:B:28:PHE:O	1:B:32:THR:HG22	1.93	0.67
1:B:734:LEU:C	1:B:734:LEU:HD12	2.14	0.67
1:A:137:ASP:OD2	1:A:204:HIS:ND1	2.26	0.67
1:C:443:ARG:NH2	1:D:679:GLU:OE1	2.28	0.67
1:D:116:LEU:HB3	1:D:227:ILE:HG12	1.77	0.67
1:A:708:MET:CE	1:A:732:LYS:NZ	2.58	0.67
1:D:440:GLY:HA3	1:D:532:PHE:CD1	2.29	0.67
1:C:495:PHE:CD2	1:C:519:LEU:HD11	2.30	0.67
1:D:524:GLN:NE2	1:D:573:TRP:CE2	2.63	0.67
1:A:477:PRO:O	1:A:481:MET:HG3	1.95	0.66
1:B:72:ALA:HB1	1:B:105:ILE:HD13	1.74	0.66
1:D:113:ALA:CA	1:D:260:VAL:HG11	2.23	0.66
1:B:155:PRO:HG2	1:B:341:TRP:CZ3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ASN:HD22	1:B:390:ASN:C	1.95	0.66
1:D:465:LYS:CG	1:D:575:ILE:CG2	2.73	0.66
1:A:486:ARG:O	1:A:490:GLN:HG3	1.95	0.66
1:B:616:ASP:OD2	1:B:637:LYS:NZ	2.25	0.66
1:A:507:LEU:CB	1:A:578:MET:HE1	2.23	0.66
1:A:708:MET:CE	1:A:732:LYS:HZ1	2.08	0.66
1:B:504:HIS:NE2	1:D:641:GLU:OE2	2.29	0.66
1:B:155:PRO:HG2	1:B:341:TRP:HE3	1.59	0.65
1:B:487:TYR:HE2	1:D:740:PRO:CB	2.09	0.65
1:A:374:LEU:CD2	1:A:378:TYR:CE2	2.79	0.65
1:A:524:GLN:NE2	1:A:573:TRP:CH2	2.65	0.65
1:C:182:VAL:C	1:C:366:GLN:HE22	1.99	0.65
1:D:636:LEU:HD12	1:D:734:LEU:HD12	1.78	0.65
1:A:491:SER:OG	1:A:493:ASN:HB2	1.96	0.65
1:A:487:TYR:CD1	1:A:491:SER:HB2	2.31	0.65
1:D:738:ILE:HD12	1:D:738:ILE:C	2.16	0.65
1:A:62:PHE:CE2	1:A:109:ILE:HD12	2.31	0.65
1:B:505:SER:HB2	1:D:723:LEU:HD12	1.78	0.65
1:C:566:VAL:HB	1:C:569:ALA:CB	2.26	0.65
1:A:345:ARG:NH1	1:A:345:ARG:HG2	2.12	0.65
1:D:82:PRO:HG3	1:D:107:TYR:CE1	2.30	0.65
1:D:465:LYS:HG2	1:D:575:ILE:HG21	1.79	0.64
1:D:522:ASP:OD1	1:D:523:PRO:HD2	1.97	0.64
1:B:28:PHE:CZ	1:B:32:THR:HG21	2.33	0.64
1:D:112:GLU:CD	1:D:262:VAL:HB	2.17	0.64
1:D:378:TYR:HB3	1:D:382:ARG:HH12	1.62	0.64
1:A:20:GLY:N	1:A:297:ASP:OD2	2.31	0.64
1:A:374:LEU:C	1:A:374:LEU:HD23	2.18	0.64
1:A:506:PRO:CG	1:A:509:ASN:HA	2.28	0.64
1:C:588:ASP:HB3	1:C:591:LEU:HD13	1.78	0.64
1:B:72:ALA:CB	1:B:105:ILE:CD1	2.76	0.64
1:D:387:ASP:OD2	1:D:388:GLN:CD	2.35	0.64
1:D:113:ALA:HB2	1:D:325:ALA:CA	2.27	0.63
1:A:111:VAL:HG23	1:A:262:VAL:HG22	1.79	0.63
1:D:159:TRP:NE1	1:D:259:PHE:CE1	2.65	0.63
1:A:100:TYR:CE1	1:A:101:ASN:HB2	2.34	0.63
1:B:105:ILE:HG22	1:B:105:ILE:O	1.99	0.63
1:D:387:ASP:OD2	1:D:388:GLN:OE1	2.17	0.63
1:A:704:PHE:CE2	1:A:708:MET:CE	2.82	0.63
1:A:729:TRP:HB3	1:A:730:PRO:CD	2.29	0.63
1:C:279:GLU:OE1	1:C:283:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:ARG:O	1:C:515:GLN:HG3	1.98	0.63
1:D:167:GLY:HA2	1:D:186:ASN:ND2	2.12	0.63
1:A:168:TYR:CE2	1:A:171:LYS:HE3	2.34	0.63
1:A:218:PHE:CZ	1:A:226:THR:HB	2.33	0.63
1:C:590:HIS:HA	1:C:593:GLU:HG3	1.80	0.63
1:C:185:ASP:O	1:C:190:LYS:NZ	2.32	0.62
1:C:566:VAL:HB	1:C:569:ALA:HB3	1.81	0.62
1:D:116:LEU:HD11	1:D:246:THR:CG2	2.28	0.62
1:A:723:LEU:HD13	1:A:738:ILE:CD1	2.14	0.62
1:A:345:ARG:CG	1:A:345:ARG:HH11	2.12	0.62
1:A:99:ARG:HG3	1:A:104:LEU:HD23	1.82	0.62
1:D:159:TRP:CZ2	1:D:259:PHE:CE2	2.87	0.62
1:A:467:GLU:HA	1:A:467:GLU:OE1	1.99	0.62
1:C:193:LEU:CD2	1:C:362:LEU:HD21	2.27	0.62
1:C:340:PHE:CZ	1:C:369:ALA:HB1	2.36	0.61
1:A:18:TYR:CE1	1:A:19:ASN:OD1	2.52	0.61
1:C:486:ARG:O	1:C:490:GLN:HG3	2.01	0.61
1:C:495:PHE:CD2	1:C:519:LEU:CD1	2.84	0.61
1:C:456:PHE:CE2	1:C:488:VAL:HG12	2.35	0.61
1:B:604:SER:O	1:B:653:ARG:NH1	2.34	0.61
1:B:738:ILE:HG21	1:D:503:TRP:O	2.01	0.61
1:D:723:LEU:CD2	1:D:736:VAL:HG12	2.30	0.61
1:A:345:ARG:HG2	1:A:345:ARG:HH11	1.64	0.61
1:D:91:TYR:CZ	1:D:306:LYS:HG2	2.36	0.61
1:B:355:ARG:NH1	1:B:389:PRO:CG	2.59	0.61
1:A:522:ASP:CG	1:A:523:PRO:HD2	2.21	0.60
1:B:734:LEU:HD12	1:B:734:LEU:O	2.01	0.60
1:D:465:LYS:CG	1:D:575:ILE:HG21	2.29	0.60
1:B:487:TYR:CE2	1:D:740:PRO:CB	2.84	0.60
1:A:110:ALA:O	1:A:263:LEU:N	2.34	0.60
1:A:737:SER:C	1:A:738:ILE:HD12	2.22	0.60
1:B:675:SER:O	1:B:678:VAL:HG22	2.01	0.60
1:C:114:LEU:HD11	1:C:156:TYR:CE2	2.36	0.60
1:A:374:LEU:HD23	1:A:374:LEU:O	2.02	0.60
1:D:577:ASP:OD1	1:D:579:ARG:N	2.32	0.60
1:B:355:ARG:CZ	1:B:389:PRO:HG3	2.32	0.60
1:B:389:PRO:HG2	1:B:390:ASN:H	1.66	0.60
1:A:86:PHE:HZ	1:A:286:LEU:CD1	2.15	0.60
1:C:595:VAL:O	1:C:599:ILE:HG13	2.01	0.60
1:D:629:ARG:HH11	1:D:631:LEU:HD23	1.65	0.60
1:B:739:LEU:N	1:B:740:PRO:CD	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:VAL:CB	1:C:366:GLN:NE2	2.62	0.59
1:D:109:ILE:HA	1:D:304:ALA:HB2	1.84	0.59
1:C:690:ALA:O	1:C:696:LEU:HD12	2.01	0.59
1:B:676:THR:HG22	1:B:699:LEU:HD21	1.84	0.59
1:A:738:ILE:N	1:A:738:ILE:CD1	2.57	0.59
1:D:447:PHE:CE1	1:D:532:PHE:CD1	2.91	0.59
1:D:579:ARG:HA	1:D:579:ARG:NE	2.17	0.59
1:A:654:LEU:CA	1:A:675:SER:OG	2.51	0.59
1:A:675:SER:O	1:A:678:VAL:HG22	2.02	0.59
1:D:89:LYS:HB3	1:D:305:LEU:CD1	2.32	0.59
1:B:7:LYS:O	1:B:273:ASN:ND2	2.35	0.59
1:B:72:ALA:HB1	1:B:105:ILE:CD1	2.33	0.58
1:D:391:PRO:HG2	1:D:414:TYR:CZ	2.38	0.58
1:D:723:LEU:HD22	1:D:736:VAL:HG12	1.85	0.58
1:A:612:LYS:HE2	1:A:742:VAL:HG22	1.84	0.58
1:D:168:TYR:CD1	1:D:183:GLY:HA3	2.38	0.58
1:A:334:ILE:CG2	1:A:335:PRO:HD2	2.34	0.58
1:D:114:LEU:HD23	1:D:229:GLY:CA	2.34	0.58
1:B:77:LEU:HD13	1:B:105:ILE:HG22	1.86	0.58
1:A:99:ARG:HE	1:A:104:LEU:HD21	1.68	0.58
1:B:487:TYR:CE2	1:D:740:PRO:HB2	2.38	0.58
1:D:112:GLU:HB2	1:D:260:VAL:HG23	1.86	0.58
1:D:233:TRP:CZ3	1:D:317:ARG:HB3	2.39	0.58
1:D:65:HIS:HE1	1:D:261:GLY:HA2	1.69	0.58
1:C:739:LEU:N	1:C:740:PRO:CD	2.67	0.57
1:D:168:TYR:HD2	1:D:170:PHE:O	1.87	0.57
1:B:492:GLU:CD	1:B:492:GLU:O	2.42	0.57
1:B:573:TRP:HB2	1:B:575:ILE:HD11	1.85	0.57
1:D:378:TYR:HB3	1:D:382:ARG:NH1	2.19	0.57
1:B:490:GLN:O	1:B:491:SER:HB2	2.04	0.57
1:C:262:VAL:HG12	1:C:263:LEU:N	2.19	0.57
1:B:739:LEU:HD22	1:D:501:VAL:HG13	1.86	0.57
1:A:739:LEU:N	1:A:740:PRO:HD3	2.20	0.57
1:B:618:LEU:HD21	1:C:665:ILE:HG21	1.85	0.57
1:C:358:VAL:CG1	1:C:362:LEU:HD11	2.35	0.57
1:D:113:ALA:C	1:D:114:LEU:HD12	2.24	0.57
1:B:575:ILE:N	1:B:575:ILE:HD12	2.20	0.56
1:C:738:ILE:CG2	1:C:739:LEU:H	2.18	0.56
1:D:625:PRO:O	1:D:626:ILE:HB	2.05	0.56
1:D:116:LEU:CD1	1:D:246:THR:CG2	2.83	0.56
1:D:380:GLU:HG2	1:D:525:MET:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:ARG:HH22	1:D:524:GLN:HB2	1.69	0.56
1:C:738:ILE:HG23	1:C:739:LEU:HG	1.87	0.56
1:B:618:LEU:HB3	1:B:619:PRO:HD3	1.88	0.56
1:B:77:LEU:HD12	1:B:105:ILE:HG21	1.87	0.56
1:B:629:ARG:HD2	1:B:631:LEU:HD21	1.88	0.56
1:D:259:PHE:CE1	1:D:329:GLU:CB	2.88	0.56
1:C:392:LEU:HD21	1:C:473:PRO:CG	2.36	0.56
1:B:77:LEU:CD1	1:B:105:ILE:CG2	2.84	0.56
1:C:513:ARG:CD	1:C:544:CYS:SG	2.94	0.56
1:D:80:ILE:CD1	1:D:107:TYR:CD1	2.89	0.56
1:D:159:TRP:NE1	1:D:259:PHE:CE2	2.73	0.56
1:A:426:GLU:CD	1:A:466:ARG:HD3	2.26	0.56
1:D:110:ALA:HB1	1:D:302:ALA:HB1	1.86	0.56
1:D:114:LEU:CD2	1:D:231:TRP:CH2	2.89	0.56
1:C:392:LEU:HD12	1:C:392:LEU:O	2.06	0.56
1:A:111:VAL:HG11	1:A:322:MET:SD	2.46	0.55
1:B:456:PHE:HE2	1:B:489:PHE:CD1	2.23	0.55
1:D:112:GLU:HB2	1:D:260:VAL:CG2	2.36	0.55
1:A:163:ALA:HB1	1:A:257:LYS:HD2	1.88	0.55
1:B:630:GLN:C	1:B:631:LEU:HD23	2.26	0.55
1:D:688:PRO:HB2	1:D:689:TYR:CE1	2.42	0.55
1:B:476:TRP:CG	1:B:477:PRO:HD3	2.42	0.55
1:D:65:HIS:HE2	1:D:331:MET:HB2	1.72	0.55
1:A:708:MET:HG2	1:A:729:TRP:CZ2	2.42	0.55
1:C:584:ILE:HD12	1:C:591:LEU:HD23	1.88	0.55
1:C:516:HIS:ND1	1:C:548:LEU:HD22	2.20	0.55
1:D:114:LEU:HD21	1:D:231:TRP:CH2	2.42	0.55
1:A:443:ARG:HG3	1:A:444:VAL:HG23	1.88	0.55
1:A:704:PHE:CE2	1:A:708:MET:HE1	2.42	0.55
1:C:362:LEU:HD23	1:C:362:LEU:N	2.21	0.55
1:C:392:LEU:HD21	1:C:473:PRO:CD	2.37	0.55
1:D:68:PHE:HB3	1:D:105:ILE:HD13	1.88	0.55
1:D:530:THR:CG2	1:D:531:PRO:HD2	2.37	0.55
1:A:487:TYR:O	1:A:491:SER:N	2.36	0.55
1:A:704:PHE:HE2	1:A:708:MET:HE1	1.72	0.55
1:A:165:ASP:OD1	1:A:165:ASP:O	2.25	0.55
1:C:392:LEU:HD21	1:C:473:PRO:HG2	1.89	0.55
1:D:612:LYS:HZ3	1:D:739:LEU:HD13	1.71	0.55
1:A:486:ARG:NH1	1:D:623:GLU:CD	2.60	0.54
1:C:159:TRP:N	1:C:160:PRO:CD	2.70	0.54
1:D:112:GLU:HG3	1:D:262:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LEU:HD21	1:D:231:TRP:CZ3	2.42	0.54
1:D:627:ARG:HB3	1:D:627:ARG:NH1	2.22	0.54
1:A:111:VAL:HG12	1:A:302:ALA:O	2.07	0.54
1:B:389:PRO:CG	1:B:390:ASN:H	2.20	0.54
1:D:116:LEU:CD1	1:D:246:THR:HG23	2.37	0.54
1:D:722:LYS:N	1:D:725:LYS:CE	2.69	0.54
1:C:495:PHE:HD2	1:C:519:LEU:HD11	1.73	0.54
1:A:486:ARG:HH12	1:D:623:GLU:CD	2.11	0.54
1:D:112:GLU:O	1:D:114:LEU:CD1	2.55	0.54
1:D:114:LEU:HD23	1:D:229:GLY:HA3	1.90	0.54
1:D:612:LYS:NZ	1:D:739:LEU:CD1	2.64	0.54
1:D:68:PHE:HB3	1:D:105:ILE:CD1	2.38	0.54
1:A:708:MET:HE1	1:A:732:LYS:HE2	1.90	0.53
1:C:495:PHE:HD2	1:C:519:LEU:CD1	2.22	0.53
1:D:440:GLY:CA	1:D:532:PHE:CE1	2.85	0.53
1:D:564:ARG:HG3	1:D:564:ARG:NH1	2.19	0.53
1:B:456:PHE:CE2	1:B:489:PHE:CD1	2.96	0.53
1:D:334:ILE:CG1	1:D:335:PRO:HD2	2.38	0.53
1:C:170:PHE:CZ	1:C:340:PHE:CE1	2.97	0.53
1:D:116:LEU:HD21	1:D:249:PRO:HD3	1.89	0.53
1:C:441:ASP:O	1:C:442:ASN:HB2	2.08	0.53
1:C:564:ARG:NH1	1:C:572:PRO:O	2.42	0.53
1:C:694:PRO:HG2	1:C:695:TRP:CE3	2.43	0.53
1:A:334:ILE:HG23	1:A:335:PRO:HD2	1.91	0.53
1:C:491:SER:O	1:C:492:GLU:HB3	2.09	0.53
1:D:524:GLN:NE2	1:D:573:TRP:CH2	2.76	0.53
1:D:674:VAL:CG1	1:D:678:VAL:HG21	2.39	0.53
1:A:401:TRP:NE1	1:B:679:GLU:O	2.33	0.53
1:D:447:PHE:CD1	1:D:532:PHE:CD1	2.97	0.53
1:D:629:ARG:NH1	1:D:631:LEU:CD2	2.69	0.53
1:A:160:PRO:HA	1:A:257:LYS:O	2.09	0.53
1:A:467:GLU:HG3	1:A:579:ARG:CZ	2.38	0.53
1:A:113:ALA:HB2	1:A:260:VAL:HG22	1.91	0.53
1:A:28:PHE:CE1	1:A:284:TYR:HB2	2.44	0.52
1:A:291:LEU:HB3	1:A:308:TYR:CE2	2.44	0.52
1:D:566:VAL:HB	1:D:569:ALA:HB2	1.90	0.52
1:A:467:GLU:CD	1:A:579:ARG:CZ	2.77	0.52
1:B:337:MET:CE	1:B:341:TRP:NE1	2.72	0.52
1:C:372:PRO:HB2	1:C:531:PRO:HG2	1.91	0.52
1:C:422:ALA:O	1:C:423:ASN:HB2	2.09	0.52
1:B:315:ASP:N	1:B:315:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:HIS:NE2	1:D:331:MET:HB2	2.24	0.52
1:C:615:TRP:CZ2	1:C:694:PRO:O	2.63	0.52
1:C:738:ILE:CG2	1:C:739:LEU:N	2.68	0.52
1:D:112:GLU:HG3	1:D:262:VAL:HA	1.89	0.52
1:B:77:LEU:HD12	1:B:105:ILE:CG2	2.40	0.52
1:B:505:SER:CB	1:D:723:LEU:HD12	2.39	0.52
1:B:573:TRP:HB2	1:B:575:ILE:CD1	2.39	0.52
1:D:80:ILE:CB	1:D:107:TYR:CZ	2.88	0.52
1:D:516:HIS:ND1	1:D:548:LEU:HD22	2.24	0.52
1:D:159:TRP:CE2	1:D:163:ALA:HB2	2.45	0.52
1:D:615:TRP:CE3	1:D:616:ASP:HA	2.45	0.52
1:A:708:MET:HE2	1:A:732:LYS:NZ	2.25	0.52
1:D:155:PRO:HG2	1:D:341:TRP:CE3	2.45	0.52
1:D:334:ILE:HG12	1:D:335:PRO:HD2	1.92	0.52
1:A:260:VAL:CG2	1:A:325:ALA:HA	2.37	0.52
1:B:509:ASN:ND2	1:D:722:LYS:HB2	2.24	0.52
1:C:372:PRO:CB	1:C:531:PRO:HG2	2.39	0.52
1:C:547:GLU:OE2	1:C:580:ARG:NH2	2.43	0.52
1:D:375:HIS:HA	1:D:378:TYR:HB2	1.91	0.52
1:A:335:PRO:HB3	1:A:447:PHE:CE1	2.45	0.52
1:B:426:GLU:OE2	1:B:466:ARG:HD3	2.10	0.52
1:D:80:ILE:HG21	1:D:107:TYR:CE2	2.45	0.52
1:A:309:GLU:O	1:A:313:ALA:N	2.42	0.52
1:A:218:PHE:CE2	1:A:226:THR:HB	2.45	0.51
1:B:738:ILE:HD12	1:B:738:ILE:N	2.25	0.51
1:D:339:ALA:HA	1:D:375:HIS:NE2	2.25	0.51
1:D:19:ASN:HB2	1:D:297:ASP:OD2	2.10	0.51
1:D:674:VAL:HG13	1:D:678:VAL:HG21	1.92	0.51
1:A:674:VAL:HG13	1:A:678:VAL:CG2	2.37	0.51
1:C:615:TRP:HZ2	1:C:694:PRO:O	1.94	0.51
1:D:105:ILE:C	1:D:105:ILE:HD12	2.31	0.51
1:D:673:PHE:CE2	1:D:698:ILE:HD11	2.45	0.51
1:D:732:LYS:HG2	1:D:733:LYS:N	2.24	0.51
1:D:89:LYS:HB3	1:D:305:LEU:HD13	1.92	0.51
1:C:302:ALA:HB1	1:C:322:MET:SD	2.51	0.51
1:A:530:THR:HG22	1:A:533:GLY:O	2.11	0.51
1:A:230:PRO:HA	1:A:233:TRP:CD1	2.46	0.51
1:A:673:PHE:CE2	1:A:698:ILE:HD11	2.46	0.51
1:B:665:ILE:HG13	1:B:666:THR:HG23	1.91	0.51
1:B:337:MET:HE2	1:B:341:TRP:HE1	1.76	0.51
1:D:339:ALA:HB1	1:D:375:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:PRO:HB3	1:A:447:PHE:CZ	2.46	0.51
1:C:65:HIS:ND1	1:C:262:VAL:HB	2.26	0.50
1:C:262:VAL:CG1	1:C:263:LEU:N	2.74	0.50
1:C:665:ILE:HG13	1:C:666:THR:CG2	2.40	0.50
1:D:159:TRP:N	1:D:160:PRO:CD	2.74	0.50
1:A:28:PHE:CE1	1:A:280:PHE:CG	2.99	0.50
1:A:391:PRO:HG3	1:A:414:TYR:CZ	2.46	0.50
1:D:522:ASP:OD2	1:D:525:MET:HG2	2.11	0.50
1:C:358:VAL:HG12	1:C:362:LEU:HD11	1.94	0.50
1:D:447:PHE:HE1	1:D:532:PHE:CD1	2.30	0.50
1:A:168:TYR:CD2	1:A:171:LYS:HE3	2.46	0.50
1:A:516:HIS:ND1	1:A:548:LEU:HD22	2.27	0.50
1:B:11:TRP:CD2	1:B:58:PRO:HG2	2.47	0.50
1:D:529:GLN:OE1	1:D:534:VAL:HG22	2.12	0.50
1:A:161:LEU:HD23	1:A:196:LEU:HG	1.94	0.50
1:D:618:LEU:N	1:D:619:PRO:HD2	2.27	0.50
1:B:487:TYR:CD2	1:D:740:PRO:HB3	2.47	0.50
1:C:476:TRP:CG	1:C:477:PRO:HD3	2.47	0.50
1:D:80:ILE:HD12	1:D:107:TYR:CD1	2.42	0.50
1:D:447:PHE:CD1	1:D:532:PHE:HD1	2.30	0.49
1:D:617:ASP:CG	1:D:619:PRO:HG2	2.32	0.49
1:A:111:VAL:HG23	1:A:262:VAL:CG2	2.41	0.49
1:D:112:GLU:CB	1:D:260:VAL:HG23	2.41	0.49
1:D:688:PRO:HB2	1:D:689:TYR:CD1	2.47	0.49
1:B:427:HIS:HB3	1:B:465:LYS:HA	1.93	0.49
1:D:381:CYS:HB3	1:D:414:TYR:CZ	2.47	0.49
1:D:496:CYS:N	1:D:499:ASP:OD2	2.39	0.49
1:C:744:PHE:CD1	1:C:746:SER:C	2.86	0.49
1:D:89:LYS:O	1:D:305:LEU:HD12	2.13	0.49
1:D:635:HIS:CE1	1:D:735:LYS:HE2	2.48	0.49
1:A:345:ARG:CD	1:A:349:ILE:HD12	2.42	0.49
1:D:98:VAL:HG21	1:D:106:ALA:HB3	1.95	0.49
1:A:332:PRO:HG2	1:A:337:MET:SD	2.53	0.49
1:A:435:LEU:HD23	1:A:489:PHE:HE1	1.78	0.49
1:B:487:TYR:CE2	1:D:740:PRO:HB3	2.47	0.49
1:A:100:TYR:CD1	1:A:100:TYR:C	2.84	0.48
1:A:723:LEU:HD23	1:A:725:LYS:HG3	1.94	0.48
1:D:168:TYR:O	1:D:183:GLY:CA	2.61	0.48
1:B:738:ILE:HD12	1:B:738:ILE:H	1.79	0.48
1:D:109:ILE:HG22	1:D:109:ILE:O	2.13	0.48
1:A:41:PRO:HG2	1:A:44:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:PHE:CZ	1:A:708:MET:HE3	2.48	0.48
1:B:389:PRO:CG	1:B:390:ASN:N	2.76	0.48
1:D:97:ALA:HA	1:D:330:ILE:HG12	1.95	0.48
1:A:111:VAL:CG2	1:A:260:VAL:CG1	2.91	0.48
1:A:111:VAL:CG2	1:A:262:VAL:HG22	2.44	0.48
1:A:611:ALA:HB1	1:A:642:SER:HB3	1.96	0.48
1:B:487:TYR:C	1:B:487:TYR:CD1	2.87	0.48
1:C:392:LEU:HD12	1:C:392:LEU:C	2.34	0.48
1:D:114:LEU:HD22	1:D:156:TYR:OH	2.13	0.48
1:D:732:LYS:CG	1:D:733:LYS:N	2.76	0.48
1:C:591:LEU:O	1:C:595:VAL:HG23	2.12	0.48
1:D:74:SER:HB2	1:D:76:LEU:HG	1.96	0.48
1:D:330:ILE:N	1:D:330:ILE:HD12	2.29	0.48
1:B:159:TRP:N	1:B:160:PRO:CD	2.76	0.48
1:B:484:LEU:HD21	1:B:501:VAL:HG11	1.95	0.48
1:A:105:ILE:HG22	1:A:105:ILE:O	2.14	0.48
1:B:334:ILE:HG23	1:B:335:PRO:HD2	1.96	0.48
1:D:376:ALA:HB1	1:D:528:VAL:HG11	1.96	0.48
1:B:739:LEU:N	1:B:740:PRO:HD3	2.28	0.47
1:D:65:HIS:HB3	1:D:262:VAL:HG13	1.96	0.47
1:D:689:TYR:CD1	1:D:689:TYR:N	2.78	0.47
1:A:695:TRP:HH2	1:B:403:GLY:O	1.97	0.47
1:B:504:HIS:HB3	1:D:739:LEU:HD21	1.96	0.47
1:B:729:TRP:HB3	1:B:730:PRO:HD2	1.96	0.47
1:C:397:ILE:HD13	1:D:692:HIS:CE1	2.49	0.47
1:D:615:TRP:HE3	1:D:616:ASP:CA	2.27	0.47
1:B:342:TYR:HD2	1:B:375:HIS:CD2	2.33	0.47
1:B:617:ASP:CB	1:B:619:PRO:HD2	2.38	0.47
1:A:11:TRP:CG	1:A:58:PRO:HG3	2.50	0.47
1:A:98:VAL:CG2	1:A:106:ALA:HB3	2.45	0.47
1:A:117:ILE:HB	1:A:226:THR:HG23	1.95	0.47
1:D:65:HIS:CE1	1:D:261:GLY:HA2	2.47	0.47
1:B:423:ASN:O	1:B:425:PRO:HD3	2.14	0.47
1:A:44:LEU:HB3	1:A:48:PHE:CZ	2.49	0.47
1:A:476:TRP:N	1:A:477:PRO:CD	2.77	0.47
1:A:486:ARG:NH1	1:D:623:GLU:OE2	2.48	0.47
1:B:105:ILE:O	1:B:105:ILE:CG2	2.62	0.47
1:C:413:MET:HG2	1:C:430:TYR:CD2	2.49	0.47
1:C:441:ASP:OD2	1:C:443:ARG:NH2	2.47	0.47
1:D:69:GLY:CA	1:D:333:ASN:HB3	2.42	0.47
1:B:59:ASP:OD1	1:B:271:SER:OG	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:PRO:HG2	1:B:390:ASN:N	2.30	0.47
1:B:570:GLY:HA2	1:B:575:ILE:O	2.15	0.47
1:D:629:ARG:HH12	1:D:631:LEU:HD23	1.75	0.47
1:B:569:ALA:HB1	1:B:580:ARG:NH1	2.30	0.47
1:D:112:GLU:CG	1:D:262:VAL:CA	2.89	0.47
1:C:615:TRP:CE3	1:C:616:ASP:O	2.67	0.47
1:D:318:ILE:O	1:D:322:MET:HG2	2.15	0.47
1:A:149:MET:HG3	1:A:223:THR:HG21	1.97	0.46
1:A:159:TRP:N	1:A:160:PRO:CD	2.78	0.46
1:C:44:LEU:HD11	1:C:63:TRP:CE3	2.50	0.46
1:D:109:ILE:C	1:D:304:ALA:HB2	2.36	0.46
1:D:506:PRO:HA	1:D:514:ILE:O	2.15	0.46
1:D:665:ILE:HG13	1:D:666:THR:HG23	1.97	0.46
1:D:113:ALA:HB3	1:D:321:THR:O	2.15	0.46
1:D:371:ALA:CB	1:D:439:TYR:HA	2.45	0.46
1:D:447:PHE:CE1	1:D:532:PHE:CE1	3.04	0.46
1:B:415:ARG:NH1	1:B:417:VAL:HG12	2.29	0.46
1:C:155:PRO:HD3	1:C:345:ARG:HG2	1.97	0.46
1:C:392:LEU:HD11	1:C:413:MET:SD	2.56	0.46
1:A:233:TRP:CZ3	1:A:317:ARG:HB3	2.51	0.46
1:A:374:LEU:CD2	1:A:374:LEU:C	2.84	0.46
1:A:374:LEU:CD2	1:A:378:TYR:CD2	2.99	0.46
1:A:476:TRP:CG	1:A:477:PRO:HD3	2.50	0.46
1:C:467:GLU:OE1	1:C:467:GLU:HA	2.15	0.46
1:D:262:VAL:HG22	1:D:263:LEU:O	2.15	0.46
1:D:309:GLU:HG2	1:D:318:ILE:CG2	2.46	0.46
1:D:553:GLN:O	1:D:604:SER:OG	2.23	0.46
1:B:577:ASP:OD2	1:B:580:ARG:HB2	2.14	0.46
1:B:723:LEU:HA	1:B:724:PRO:C	2.35	0.46
1:C:441:ASP:OD2	1:C:443:ARG:CZ	2.64	0.46
1:B:155:PRO:HB3	1:B:344:VAL:HG12	1.98	0.46
1:C:392:LEU:CD2	1:C:473:PRO:HD2	2.46	0.46
1:D:16:LYS:HE2	1:D:263:LEU:HD22	1.97	0.46
1:D:168:TYR:CE1	1:D:183:GLY:HA3	2.50	0.46
1:B:422:ALA:C	1:B:423:ASN:ND2	2.69	0.46
1:A:148:LEU:HD23	1:A:225:MET:HB2	1.97	0.46
1:A:233:TRP:CD1	1:A:233:TRP:N	2.82	0.46
1:B:617:ASP:OD1	1:B:631:LEU:HD13	2.15	0.46
1:C:476:TRP:N	1:C:477:PRO:CD	2.79	0.46
1:B:133:ILE:N	1:B:134:PRO:CD	2.79	0.46
1:B:334:ILE:HG22	1:B:336:GLN:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:TRP:CD2	1:D:738:ILE:HG21	2.51	0.46
1:C:65:HIS:HD1	1:C:262:VAL:HB	1.81	0.46
1:D:504:HIS:N	1:D:515:GLN:O	2.48	0.46
1:A:41:PRO:C	1:A:44:LEU:HD21	2.37	0.46
1:A:345:ARG:HD2	1:A:349:ILE:HD12	1.98	0.46
1:B:611:ALA:HB1	1:B:642:SER:HB3	1.98	0.46
1:D:113:ALA:CB	1:D:325:ALA:N	2.79	0.46
1:D:639:ASN:ND2	1:D:641:GLU:HB2	2.30	0.46
1:D:743:VAL:HG23	1:D:743:VAL:O	2.16	0.46
1:A:704:PHE:CE2	1:A:708:MET:SD	3.09	0.45
1:D:463:ARG:HH22	1:D:524:GLN:CG	2.29	0.45
1:D:618:LEU:HB2	1:D:619:PRO:CD	2.46	0.45
1:B:77:LEU:CD1	1:B:105:ILE:HG22	2.45	0.45
1:B:575:ILE:N	1:B:575:ILE:CD1	2.79	0.45
1:C:44:LEU:HD12	1:C:45:GLU:N	2.31	0.45
1:D:77:LEU:HD13	1:D:105:ILE:HD13	1.98	0.45
1:D:476:TRP:CG	1:D:477:PRO:HD3	2.51	0.45
1:A:738:ILE:C	1:A:740:PRO:HD2	2.37	0.45
1:B:7:LYS:HG2	1:B:8:LEU:N	2.31	0.45
1:B:426:GLU:CD	1:B:466:ARG:HD3	2.37	0.45
1:B:738:ILE:HG12	1:D:503:TRP:O	2.15	0.45
1:C:373:GLY:HA3	1:C:438:LEU:HA	1.97	0.45
1:D:259:PHE:HE1	1:D:329:GLU:CB	2.28	0.45
1:A:591:LEU:CD2	1:A:594:ARG:NH1	2.79	0.45
1:C:45:GLU:HG2	1:C:46:GLU:N	2.30	0.45
1:D:706:GLU:O	1:D:710:GLU:HG3	2.16	0.45
1:A:111:VAL:CB	1:A:262:VAL:HG22	2.47	0.45
1:B:441:ASP:O	1:B:442:ASN:HB3	2.16	0.45
1:D:476:TRP:N	1:D:477:PRO:CD	2.79	0.45
1:A:98:VAL:HG21	1:A:106:ALA:HB3	1.97	0.45
1:B:504:HIS:O	1:D:640:GLN:OE1	2.35	0.45
1:D:615:TRP:CE3	1:D:616:ASP:CA	3.00	0.45
1:A:721:PHE:O	1:A:725:LYS:CE	2.65	0.45
1:B:190:LYS:HE2	1:B:359:ASP:HA	1.98	0.45
1:C:392:LEU:HD11	1:C:413:MET:HB2	1.98	0.45
1:C:562:LEU:HD21	1:C:594:ARG:HD2	1.98	0.45
1:D:117:ILE:HA	1:D:244:GLY:O	2.17	0.45
1:A:342:TYR:O	1:A:346:THR:HG23	2.16	0.45
1:B:504:HIS:HB2	1:D:739:LEU:HD11	1.98	0.45
1:C:466:ARG:NH2	1:C:470:GLU:O	2.50	0.45
1:C:566:VAL:HB	1:C:569:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:THR:HG22	1:D:531:PRO:HA	1.99	0.45
1:D:638:PHE:HE2	1:D:734:LEU:HD11	1.82	0.45
1:A:491:SER:HG	1:A:493:ASN:HB2	1.82	0.45
1:C:48:PHE:N	1:C:49:PRO:HD2	2.32	0.45
1:D:105:ILE:HD12	1:D:106:ALA:CB	2.46	0.45
1:D:112:GLU:HB3	1:D:261:GLY:O	2.17	0.45
1:D:130:TRP:CD1	1:D:249:PRO:HB2	2.52	0.45
1:D:259:PHE:HB3	1:D:331:MET:SD	2.57	0.45
1:D:513:ARG:HH11	1:D:583:THR:HG23	1.82	0.45
1:A:387:ASP:OD1	1:A:387:ASP:N	2.49	0.44
1:C:332:PRO:HB2	1:C:337:MET:SD	2.57	0.44
1:D:440:GLY:O	1:D:532:PHE:CE1	2.71	0.44
1:A:86:PHE:HZ	1:A:286:LEU:HD12	1.81	0.44
1:A:506:PRO:HB3	1:A:510:SER:O	2.17	0.44
1:C:81:THR:N	1:C:82:PRO:HD3	2.32	0.44
1:C:562:LEU:HB3	1:C:591:LEU:HD23	1.99	0.44
1:B:337:MET:CE	1:B:341:TRP:HE1	2.30	0.44
1:B:635:HIS:HA	1:B:733:LYS:O	2.17	0.44
1:C:430:TYR:CZ	1:C:477:PRO:HG2	2.53	0.44
1:D:111:VAL:H	1:D:302:ALA:HB1	1.82	0.44
1:B:114:LEU:HD11	1:B:156:TYR:CE2	2.53	0.44
1:B:502:SER:HB3	1:B:548:LEU:HD21	1.99	0.44
1:D:159:TRP:NE1	1:D:163:ALA:HB2	2.33	0.44
1:D:604:SER:O	1:D:653:ARG:NH1	2.50	0.44
1:A:708:MET:HE1	1:A:732:LYS:CE	2.47	0.44
1:B:11:TRP:CG	1:B:58:PRO:HG2	2.53	0.44
1:B:389:PRO:CD	1:B:390:ASN:H	2.30	0.44
1:B:737:SER:HB3	1:B:740:PRO:HG2	1.99	0.44
1:D:80:ILE:CD1	1:D:107:TYR:CZ	3.00	0.44
1:B:425:PRO:HG3	1:B:465:LYS:HD2	1.99	0.44
1:D:305:LEU:HD23	1:D:307:SER:OG	2.17	0.44
1:A:48:PHE:O	1:A:52:ALA:HB2	2.18	0.44
1:A:463:ARG:NH2	1:A:524:GLN:HG2	2.32	0.44
1:A:575:ILE:HD12	1:A:575:ILE:N	2.33	0.44
1:B:576:THR:HG22	1:B:578:MET:HE2	2.00	0.44
1:D:463:ARG:NH2	1:D:524:GLN:HB2	2.32	0.44
1:D:564:ARG:O	1:D:571:GLY:HA2	2.18	0.44
1:D:741:ASP:OD1	1:D:741:ASP:N	2.50	0.44
1:A:487:TYR:O	1:A:491:SER:CB	2.62	0.44
1:A:704:PHE:CZ	1:A:708:MET:CE	3.01	0.44
1:C:664:SER:OG	1:C:667:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:VAL:HG23	1:D:325:ALA:CB	2.47	0.44
1:D:133:ILE:N	1:D:134:PRO:CD	2.81	0.44
1:D:522:ASP:OD1	1:D:523:PRO:CD	2.66	0.44
1:D:542:GLY:HA3	1:D:576:THR:HG21	1.98	0.44
1:C:141:LYS:C	1:C:144:GLY:H	2.21	0.44
1:D:368:ASN:HA	1:D:374:LEU:HD13	1.99	0.44
1:A:430:TYR:CZ	1:A:477:PRO:HG2	2.53	0.43
1:B:63:TRP:CD1	1:B:67:ARG:HG3	2.52	0.43
1:B:476:TRP:CD2	1:B:477:PRO:HD3	2.53	0.43
1:D:112:GLU:OE2	1:D:262:VAL:HB	2.17	0.43
1:A:568:ILE:HD11	1:A:587:ILE:HD13	1.99	0.43
1:B:576:THR:HG22	1:B:578:MET:CE	2.48	0.43
1:B:737:SER:CB	1:B:740:PRO:HG2	2.48	0.43
1:C:193:LEU:CD2	1:C:362:LEU:CD2	2.95	0.43
1:D:116:LEU:HB2	1:D:226:THR:O	2.17	0.43
1:D:564:ARG:HH11	1:D:564:ARG:CG	2.24	0.43
1:A:334:ILE:CG2	1:A:335:PRO:CD	2.96	0.43
1:B:569:ALA:CB	1:B:580:ARG:HH11	2.31	0.43
1:D:391:PRO:HG3	1:D:414:TYR:CE2	2.53	0.43
1:A:505:SER:OG	1:A:506:PRO:CD	2.63	0.43
1:C:179:ILE:HG22	1:C:334:ILE:HD13	2.01	0.43
1:D:114:LEU:HD23	1:D:229:GLY:HA2	2.01	0.43
1:D:170:PHE:CE1	1:D:179:ILE:HA	2.41	0.43
1:A:111:VAL:CG1	1:A:322:MET:SD	3.06	0.43
1:A:151:ASN:OD1	1:A:211:TYR:N	2.51	0.43
1:A:487:TYR:CZ	1:A:491:SER:OG	2.64	0.43
1:B:492:GLU:O	1:B:493:ASN:HB2	2.18	0.43
1:C:635:HIS:CE1	1:C:735:LYS:CD	3.00	0.43
1:D:387:ASP:CG	1:D:388:GLN:OE1	2.57	0.43
1:A:639:ASN:HA	1:A:737:SER:O	2.18	0.43
1:B:170:PHE:CE1	1:B:340:PHE:CZ	3.07	0.43
1:B:384:LEU:CD1	1:B:525:MET:HG2	2.49	0.43
1:C:65:HIS:ND1	1:C:261:GLY:O	2.51	0.43
1:A:118:TYR:CB	1:A:225:MET:SD	3.07	0.43
1:A:148:LEU:O	1:A:149:MET:HG2	2.19	0.43
1:D:98:VAL:HG13	1:D:104:LEU:HD22	2.00	0.43
1:D:109:ILE:O	1:D:304:ALA:HB2	2.19	0.43
1:A:345:ARG:CD	1:A:345:ARG:C	2.85	0.43
1:A:708:MET:HE2	1:A:732:LYS:HZ3	1.84	0.43
1:B:673:PHE:CE2	1:B:698:ILE:HD11	2.54	0.43
1:D:105:ILE:HD12	1:D:106:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:GLU:OE2	1:D:296:LYS:NZ	2.38	0.43
1:A:729:TRP:CB	1:A:730:PRO:HD2	2.39	0.43
1:B:116:LEU:HB2	1:B:248:LEU:HD23	2.00	0.43
1:C:575:ILE:HD12	1:C:575:ILE:N	2.34	0.43
1:A:110:ALA:O	1:A:262:VAL:HG13	2.19	0.43
1:A:447:PHE:C	1:A:447:PHE:CD1	2.91	0.43
1:C:665:ILE:HG13	1:C:666:THR:H	1.82	0.43
1:D:116:LEU:HD21	1:D:248:LEU:HA	2.01	0.43
1:D:129:THR:C	1:D:249:PRO:HB3	2.39	0.43
1:D:380:GLU:CG	1:D:525:MET:HE3	2.48	0.43
1:A:41:PRO:HG2	1:A:44:LEU:HD21	2.00	0.42
1:A:340:PHE:O	1:A:344:VAL:HG23	2.19	0.42
1:A:598:GLY:O	1:A:602:ASP:HB2	2.18	0.42
1:C:193:LEU:HD23	1:C:362:LEU:CD2	2.32	0.42
1:D:563:LEU:HD23	1:D:569:ALA:HB1	2.01	0.42
1:A:708:MET:HE3	1:A:732:LYS:HZ1	1.83	0.42
1:B:323:GLU:O	1:B:327:LYS:HG3	2.19	0.42
1:C:380:GLU:HG3	1:C:528:VAL:CG2	2.49	0.42
1:D:90:LEU:HD22	1:D:304:ALA:O	2.19	0.42
1:A:384:LEU:HD21	1:A:524:GLN:HG3	2.01	0.42
1:B:216:ALA:O	1:B:220:LYS:HB2	2.20	0.42
1:B:415:ARG:CZ	1:B:417:VAL:HG12	2.50	0.42
1:D:384:LEU:HD23	1:D:385:TYR:CE2	2.53	0.42
1:D:505:SER:N	1:D:515:GLN:HB3	2.34	0.42
1:A:503:TRP:O	1:A:504:HIS:HB2	2.19	0.42
1:C:442:ASN:OD1	1:C:447:PHE:N	2.52	0.42
1:D:109:ILE:CA	1:D:304:ALA:HB2	2.48	0.42
1:D:417:VAL:O	1:D:426:GLU:HA	2.20	0.42
1:B:77:LEU:CB	1:B:105:ILE:HG23	2.49	0.42
1:D:80:ILE:CG2	1:D:107:TYR:CE2	3.03	0.42
1:D:430:TYR:CZ	1:D:477:PRO:HG2	2.55	0.42
1:A:28:PHE:CE1	1:A:284:TYR:CB	3.02	0.42
1:A:214:ALA:O	1:A:218:PHE:CD2	2.72	0.42
1:A:415:ARG:HH12	1:A:466:ARG:NE	2.17	0.42
1:B:428:TRP:CE3	1:B:473:PRO:HB3	2.54	0.42
1:C:170:PHE:CZ	1:C:340:PHE:CZ	3.08	0.42
1:D:371:ALA:HB1	1:D:438:LEU:O	2.19	0.42
1:D:385:TYR:OH	1:D:416:ASN:ND2	2.48	0.42
1:A:13:ASN:HB2	1:A:63:TRP:CZ2	2.55	0.42
1:C:117:ILE:HG12	1:C:245:VAL:HG22	2.02	0.42
1:C:141:LYS:O	1:C:144:GLY:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:PHE:CD2	1:D:105:ILE:HD13	2.55	0.42
1:D:741:ASP:O	1:D:743:VAL:HG13	2.20	0.42
1:A:155:PRO:HG2	1:A:341:TRP:CE3	2.55	0.42
1:C:261:GLY:O	1:C:262:VAL:HB	2.20	0.42
1:C:428:TRP:CH2	1:C:466:ARG:NH1	2.88	0.42
1:C:639:ASN:HA	1:C:737:SER:O	2.20	0.42
1:C:680:GLY:HA2	1:D:367:THR:HG21	2.01	0.42
1:D:309:GLU:CG	1:D:322:MET:HG3	2.50	0.42
1:D:465:LYS:NZ	1:D:568:ILE:HA	2.35	0.42
1:D:704:PHE:CE2	1:D:708:MET:CE	3.03	0.42
1:B:426:GLU:OE2	1:B:466:ARG:CD	2.68	0.42
1:B:689:TYR:CD1	1:B:689:TYR:N	2.84	0.42
1:D:334:ILE:HA	1:D:335:PRO:HD3	1.92	0.42
1:D:335:PRO:C	1:D:336:GLN:HG3	2.40	0.42
1:C:11:TRP:CE2	1:C:58:PRO:HG3	2.54	0.41
1:C:155:PRO:HB3	1:C:344:VAL:HG12	2.02	0.41
1:D:113:ALA:CB	1:D:325:ALA:HB2	2.50	0.41
1:D:159:TRP:CD1	1:D:259:PHE:CG	3.08	0.41
1:D:380:GLU:CG	1:D:525:MET:CE	2.98	0.41
1:A:612:LYS:HB2	1:A:639:ASN:HB2	2.02	0.41
1:C:185:ASP:CB	1:C:366:GLN:OE1	2.64	0.41
1:D:639:ASN:HD21	1:D:641:GLU:HB2	1.85	0.41
1:D:738:ILE:O	1:D:738:ILE:HD12	2.20	0.41
1:A:732:LYS:HG2	1:A:733:LYS:N	2.35	0.41
1:B:554:TRP:CH2	1:B:558:GLY:HA3	2.56	0.41
1:C:372:PRO:CB	1:C:531:PRO:CG	2.98	0.41
1:C:442:ASN:HA	1:C:445:HIS:O	2.21	0.41
1:C:635:HIS:HE1	1:C:735:LYS:HD3	1.82	0.41
1:D:97:ALA:HA	1:D:330:ILE:CG2	2.50	0.41
1:D:319:ALA:O	1:D:323:GLU:HG3	2.20	0.41
1:D:615:TRP:HE3	1:D:616:ASP:N	2.18	0.41
1:A:118:TYR:HB3	1:A:225:MET:SD	2.60	0.41
1:A:334:ILE:HG22	1:A:335:PRO:HD2	2.01	0.41
1:B:123:LEU:HD21	1:B:127:PRO:HD3	2.01	0.41
1:C:694:PRO:HG2	1:C:695:TRP:HE3	1.83	0.41
1:A:66:ASP:OD1	1:A:66:ASP:N	2.51	0.41
1:A:111:VAL:HA	1:A:262:VAL:HA	2.01	0.41
1:B:415:ARG:NH1	1:B:415:ARG:HG2	2.36	0.41
1:B:441:ASP:CG	1:B:443:ARG:HE	2.24	0.41
1:D:617:ASP:OD2	1:D:619:PRO:HG2	2.20	0.41
1:D:629:ARG:HG2	1:D:630:GLN:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PRO:CB	1:A:44:LEU:HD21	2.49	0.41
1:A:484:LEU:O	1:A:488:VAL:HG23	2.21	0.41
1:B:516:HIS:ND1	1:B:548:LEU:HD22	2.36	0.41
1:B:625:PRO:O	1:B:626:ILE:HG22	2.21	0.41
1:C:383:ARG:NH2	1:C:384:LEU:HD11	2.35	0.41
1:A:447:PHE:CE1	1:A:449:GLY:N	2.89	0.41
1:A:486:ARG:NH1	1:D:623:GLU:OE1	2.48	0.41
1:B:170:PHE:CZ	1:B:340:PHE:CZ	3.09	0.41
1:B:337:MET:HE2	1:B:341:TRP:NE1	2.35	0.41
1:B:509:ASN:OD1	1:D:722:LYS:HD3	2.21	0.41
1:B:516:HIS:CG	1:B:548:LEU:HD22	2.56	0.41
1:C:160:PRO:HG3	1:C:258:PRO:HA	2.03	0.41
1:D:371:ALA:HB2	1:D:439:TYR:HA	2.01	0.41
1:A:332:PRO:HB2	1:A:337:MET:SD	2.60	0.41
1:B:476:TRP:N	1:B:477:PRO:CD	2.83	0.41
1:B:100:TYR:HB3	1:B:105:ILE:HD12	2.02	0.41
1:C:302:ALA:HB1	1:C:322:MET:CG	2.51	0.41
1:C:530:THR:HG22	1:C:533:GLY:O	2.20	0.41
1:B:419:SER:O	1:B:419:SER:OG	2.32	0.41
1:B:484:LEU:O	1:B:488:VAL:HG23	2.20	0.41
1:C:638:PHE:HB3	1:C:642:SER:OG	2.21	0.41
1:D:463:ARG:NH2	1:D:524:GLN:CG	2.84	0.41
1:D:634:VAL:HG21	1:D:689:TYR:HB3	2.03	0.41
1:A:28:PHE:CZ	1:A:284:TYR:HB2	2.55	0.40
1:A:91:TYR:CZ	1:A:306:LYS:HG2	2.56	0.40
1:A:139:GLU:O	1:A:142:ALA:HB3	2.21	0.40
1:A:161:LEU:HD23	1:A:196:LEU:CD2	2.50	0.40
1:B:505:SER:HB2	1:D:640:GLN:OE1	2.21	0.40
1:B:625:PRO:C	1:B:626:ILE:HG22	2.42	0.40
1:D:202:ASN:HB2	1:D:204:HIS:CD2	2.57	0.40
1:D:465:LYS:CG	1:D:575:ILE:HG22	2.39	0.40
1:C:424:ILE:HD13	1:C:573:TRP:CD2	2.57	0.40
1:D:340:PHE:CZ	1:D:344:VAL:HG21	2.56	0.40
1:D:561:GLU:O	1:D:564:ARG:HB2	2.22	0.40
1:D:618:LEU:HB2	1:D:619:PRO:HD3	2.03	0.40
1:A:162:ILE:HD11	1:A:193:LEU:HD21	2.03	0.40
1:A:467:GLU:CD	1:A:579:ARG:NH1	2.74	0.40
1:B:621:ARG:O	1:B:622:GLY:C	2.58	0.40
1:B:739:LEU:HD12	1:B:742:VAL:CG2	2.51	0.40
1:D:106:ALA:HB1	1:D:265:ALA:O	2.21	0.40
1:D:638:PHE:CE2	1:D:734:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TYR:CZ	1:A:171:LYS:HE3	2.55	0.40
1:D:114:LEU:CD1	1:D:114:LEU:N	2.85	0.40
1:D:292:GLU:HG2	1:D:296:LYS:HE3	2.02	0.40
1:A:339:ALA:HB1	1:A:372:PRO:HG2	2.02	0.40
1:A:487:TYR:O	1:A:488:VAL:C	2.59	0.40
1:B:503:TRP:CZ2	1:D:738:ILE:HG21	2.53	0.40
1:C:257:LYS:HA	1:C:328:GLY:HA2	2.03	0.40
1:D:28:PHE:O	1:D:32:THR:HB	2.21	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	724/756 (96%)	709 (98%)	14 (2%)	1 (0%)	51	84
1	B	729/756 (96%)	707 (97%)	16 (2%)	6 (1%)	19	58
1	C	718/756 (95%)	701 (98%)	15 (2%)	2 (0%)	41	75
1	D	734/756 (97%)	713 (97%)	19 (3%)	2 (0%)	41	75
All	All	2905/3024 (96%)	2830 (97%)	64 (2%)	11 (0%)	34	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	262	VAL
1	D	618	LEU
1	B	491	SER
1	B	626	ILE
1	B	621	ARG
1	B	622	GLY
1	B	391	PRO

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Mol	Chain	Res	Type
1	B	493	ASN
1	C	372	PRO
1	D	625	PRO
1	A	391	PRO

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	604/629 (96%)	603 (100%)	1 (0%)	93 98
1	B	606/629 (96%)	602 (99%)	4 (1%)	84 93
1	C	598/629 (95%)	597 (100%)	1 (0%)	93 98
1	D	611/629 (97%)	607 (99%)	4 (1%)	84 93
All	All	2419/2516 (96%)	2409 (100%)	10 (0%)	91 96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	ARG
1	B	390	ASN
1	B	503	TRP
1	B	629	ARG
1	B	738	ILE
1	C	259	PHE
1	D	317	ARG
1	D	612	LYS
1	D	631	LEU
1	D	739	LEU

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	730/756 (96%)	-0.37	3 (0%)	92	90	62, 133, 202, 298	0
1	B	733/756 (96%)	-0.08	29 (3%)	38	33	60, 158, 353, 503	0
1	C	724/756 (95%)	-0.02	32 (4%)	34	30	56, 171, 346, 474	0
1	D	738/756 (97%)	0.05	48 (6%)	18	17	57, 184, 398, 518	0
All	All	2925/3024 (96%)	-0.11	112 (3%)	40	36	56, 152, 360, 518	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	174	ASN	7.4
1	D	82	PRO	7.4
1	D	5	GLU	7.3
1	B	5	GLU	6.7
1	D	112	GLU	6.5
1	D	94	THR	6.1
1	D	76	LEU	6.1
1	D	105	ILE	5.8
1	B	304	ALA	5.5
1	D	80	ILE	5.5
1	C	127	PRO	5.5
1	B	21	LEU	5.4
1	C	10	ILE	5.4
1	D	174	ASN	5.4
1	C	304	ALA	5.2
1	B	232	ALA	5.2
1	D	269	ALA	4.8
1	B	233	TRP	4.8
1	D	81	THR	4.8
1	C	173	GLU	4.7
1	B	126	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	60	ILE	4.6
1	D	268	ASN	4.6
1	B	17	GLY	4.6
1	B	174	ASN	4.5
1	B	300	LEU	4.4
1	B	305	LEU	4.2
1	D	91	TYR	4.0
1	B	226	THR	3.9
1	B	246	THR	3.9
1	D	15	ASP	3.9
1	D	98	VAL	3.9
1	D	55	GLY	3.7
1	D	10	ILE	3.7
1	D	61	ILE	3.7
1	C	157	PHE	3.6
1	C	59	ASP	3.6
1	D	77	LEU	3.5
1	C	6	GLY	3.4
1	C	143	LYS	3.4
1	D	13	ASN	3.3
1	D	97	ALA	3.3
1	D	16	LYS	3.3
1	C	9	VAL	3.3
1	B	746	SER	3.3
1	C	150	PHE	3.3
1	D	304	ALA	3.2
1	D	286	LEU	3.2
1	D	262	VAL	3.2
1	B	301	GLY	3.2
1	D	272	PRO	3.2
1	C	107	TYR	3.1
1	D	746	SER	3.1
1	D	62	PHE	3.0
1	B	117	ILE	3.0
1	D	214	ALA	3.0
1	C	60	ILE	2.9
1	B	158	THR	2.9
1	D	95	TRP	2.9
1	B	294	VAL	2.9
1	D	267	ILE	2.9
1	B	173	GLU	2.8
1	C	126	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	244	GLY	2.8
1	A	205	MET	2.8
1	C	133	ILE	2.8
1	D	113	ALA	2.7
1	D	63	TRP	2.7
1	D	54	THR	2.7
1	D	126	PRO	2.6
1	B	33	GLY	2.6
1	B	207	ALA	2.6
1	B	94	THR	2.6
1	C	62	PHE	2.6
1	B	24	VAL	2.6
1	B	148	LEU	2.6
1	D	493	ASN	2.6
1	D	102	GLY	2.6
1	B	124	PRO	2.5
1	B	6	GLY	2.5
1	D	151	ASN	2.5
1	D	11	TRP	2.5
1	C	54	THR	2.5
1	D	283	ASN	2.4
1	D	111	VAL	2.4
1	A	50	GLN	2.4
1	A	745	ASP	2.4
1	C	97	ALA	2.4
1	C	303	VAL	2.4
1	C	5	GLU	2.4
1	D	99	ARG	2.4
1	D	265	ALA	2.4
1	C	176	LYS	2.3
1	C	108	PRO	2.3
1	C	114	LEU	2.2
1	C	148	LEU	2.2
1	D	37	THR	2.2
1	C	151	ASN	2.2
1	D	288	ASP	2.2
1	C	226	THR	2.2
1	D	315	ASP	2.2
1	B	236	ILE	2.2
1	C	142	ALA	2.2
1	D	316	PRO	2.2
1	B	118	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	122	LEU	2.1
1	B	243	TYR	2.1
1	C	246	THR	2.1
1	C	666	THR	2.0
1	B	225	MET	2.0
1	C	102	GLY	2.0
1	D	271	SER	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.