



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:50 PM UTC

PDB ID : 2JFD / pdb_00002jfd
Title : Structure of the MAT domain of human FAS
Authors : Bunkoczi, G.; Kavanagh, K.; Hozjan, V.; Rojkova, A.; Wu, X.; Arrowsmith, C.H.; Edwards, A.; Sundstrom, M.; Weigelt, J.; Smith, S.; Oppermann, U.
Deposited on : 2007-01-31
Resolution : 2.81 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
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

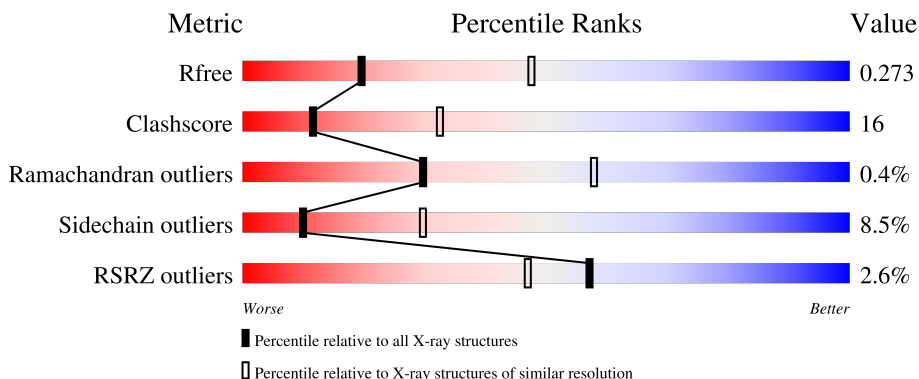
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	425	0% 69% 23% • 5%
1	B	425	4% 66% 27% • 6%
1	C	425	2% 68% 23% • 5%
1	D	425	3% 70% 22% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11392 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 FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			2929	1869	503	537	20			
1	B	400	Total	C	N	O	S	0	0	0
			2840	1823	475	523	19			
1	C	403	Total	C	N	O	S	0	1	0
			2899	1856	504	520	19			
1	D	399	Total	C	N	O	S	0	0	0
			2709	1708	476	508	17			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	MET	-	expression tag	UNP P49327
A	400	HIS	-	expression tag	UNP P49327
A	401	HIS	-	expression tag	UNP P49327
A	402	HIS	-	expression tag	UNP P49327
A	403	HIS	-	expression tag	UNP P49327
A	404	HIS	-	expression tag	UNP P49327
A	405	HIS	-	expression tag	UNP P49327
A	406	SER	-	expression tag	UNP P49327
A	407	SER	-	expression tag	UNP P49327
A	408	GLY	-	expression tag	UNP P49327
A	409	VAL	-	expression tag	UNP P49327
A	410	ASP	-	expression tag	UNP P49327
A	411	LEU	-	expression tag	UNP P49327
A	412	GLY	-	expression tag	UNP P49327
A	413	THR	-	expression tag	UNP P49327
A	414	GLU	-	expression tag	UNP P49327
A	415	ASN	-	expression tag	UNP P49327
A	416	LEU	-	expression tag	UNP P49327
A	417	TYR	-	expression tag	UNP P49327
A	418	PHE	-	expression tag	UNP P49327
A	419	GLN	-	expression tag	UNP P49327

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Chain	Residue	Modelled	Actual	Comment	Reference
A	420	SER	-	expression tag	UNP P49327
A	421	MET	-	expression tag	UNP P49327
B	399	MET	-	expression tag	UNP P49327
B	400	HIS	-	expression tag	UNP P49327
B	401	HIS	-	expression tag	UNP P49327
B	402	HIS	-	expression tag	UNP P49327
B	403	HIS	-	expression tag	UNP P49327
B	404	HIS	-	expression tag	UNP P49327
B	405	HIS	-	expression tag	UNP P49327
B	406	SER	-	expression tag	UNP P49327
B	407	SER	-	expression tag	UNP P49327
B	408	GLY	-	expression tag	UNP P49327
B	409	VAL	-	expression tag	UNP P49327
B	410	ASP	-	expression tag	UNP P49327
B	411	LEU	-	expression tag	UNP P49327
B	412	GLY	-	expression tag	UNP P49327
B	413	THR	-	expression tag	UNP P49327
B	414	GLU	-	expression tag	UNP P49327
B	415	ASN	-	expression tag	UNP P49327
B	416	LEU	-	expression tag	UNP P49327
B	417	TYR	-	expression tag	UNP P49327
B	418	PHE	-	expression tag	UNP P49327
B	419	GLN	-	expression tag	UNP P49327
B	420	SER	-	expression tag	UNP P49327
B	421	MET	-	expression tag	UNP P49327
C	399	MET	-	expression tag	UNP P49327
C	400	HIS	-	expression tag	UNP P49327
C	401	HIS	-	expression tag	UNP P49327
C	402	HIS	-	expression tag	UNP P49327
C	403	HIS	-	expression tag	UNP P49327
C	404	HIS	-	expression tag	UNP P49327
C	405	HIS	-	expression tag	UNP P49327
C	406	SER	-	expression tag	UNP P49327
C	407	SER	-	expression tag	UNP P49327
C	408	GLY	-	expression tag	UNP P49327
C	409	VAL	-	expression tag	UNP P49327
C	410	ASP	-	expression tag	UNP P49327
C	411	LEU	-	expression tag	UNP P49327
C	412	GLY	-	expression tag	UNP P49327
C	413	THR	-	expression tag	UNP P49327
C	414	GLU	-	expression tag	UNP P49327
C	415	ASN	-	expression tag	UNP P49327

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Chain	Residue	Modelled	Actual	Comment	Reference
C	416	LEU	-	expression tag	UNP P49327
C	417	TYR	-	expression tag	UNP P49327
C	418	PHE	-	expression tag	UNP P49327
C	419	GLN	-	expression tag	UNP P49327
C	420	SER	-	expression tag	UNP P49327
C	421	MET	-	expression tag	UNP P49327
D	399	MET	-	expression tag	UNP P49327
D	400	HIS	-	expression tag	UNP P49327
D	401	HIS	-	expression tag	UNP P49327
D	402	HIS	-	expression tag	UNP P49327
D	403	HIS	-	expression tag	UNP P49327
D	404	HIS	-	expression tag	UNP P49327
D	405	HIS	-	expression tag	UNP P49327
D	406	SER	-	expression tag	UNP P49327
D	407	SER	-	expression tag	UNP P49327
D	408	GLY	-	expression tag	UNP P49327
D	409	VAL	-	expression tag	UNP P49327
D	410	ASP	-	expression tag	UNP P49327
D	411	LEU	-	expression tag	UNP P49327
D	412	GLY	-	expression tag	UNP P49327
D	413	THR	-	expression tag	UNP P49327
D	414	GLU	-	expression tag	UNP P49327
D	415	ASN	-	expression tag	UNP P49327
D	416	LEU	-	expression tag	UNP P49327
D	417	TYR	-	expression tag	UNP P49327
D	418	PHE	-	expression tag	UNP P49327
D	419	GLN	-	expression tag	UNP P49327
D	420	SER	-	expression tag	UNP P49327
D	421	MET	-	expression tag	UNP P49327

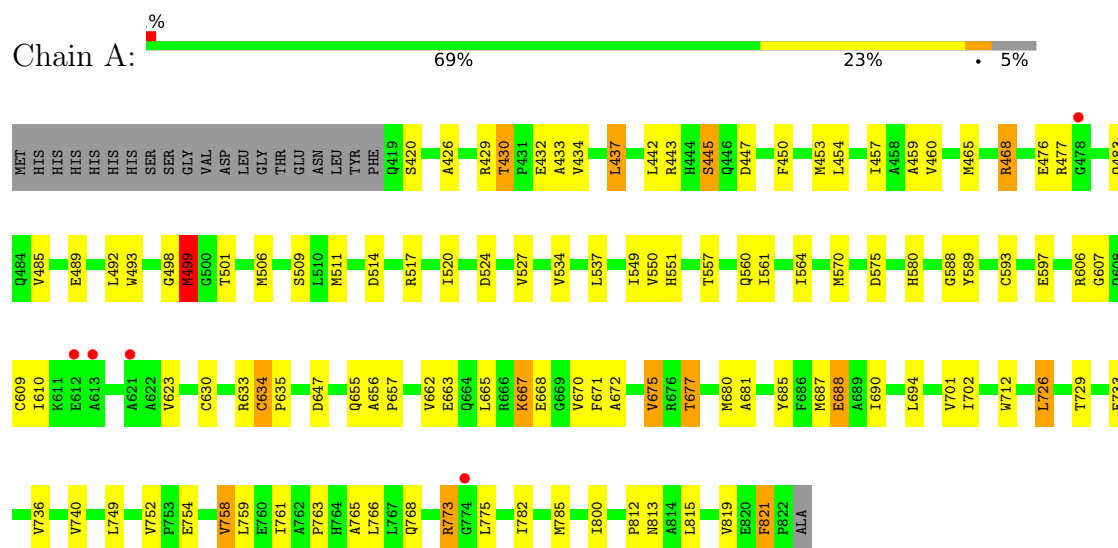
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	3	Total O 3 3	0	0
2	C	9	Total O 9 9	0	0

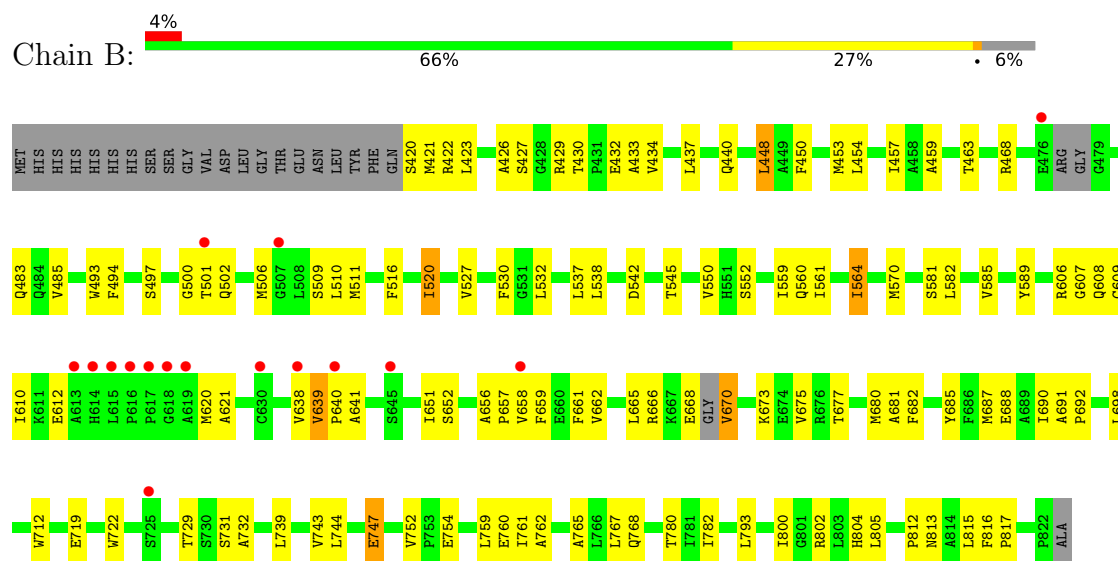
3 Residue-property plots

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: FATTY ACID SYNTHASE

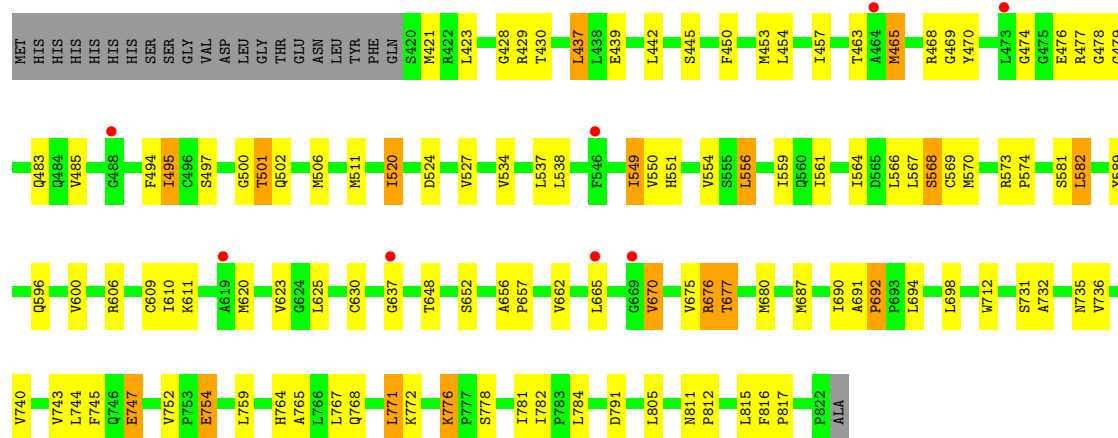


• Molecule 1: FATTY ACID SYNTHASE

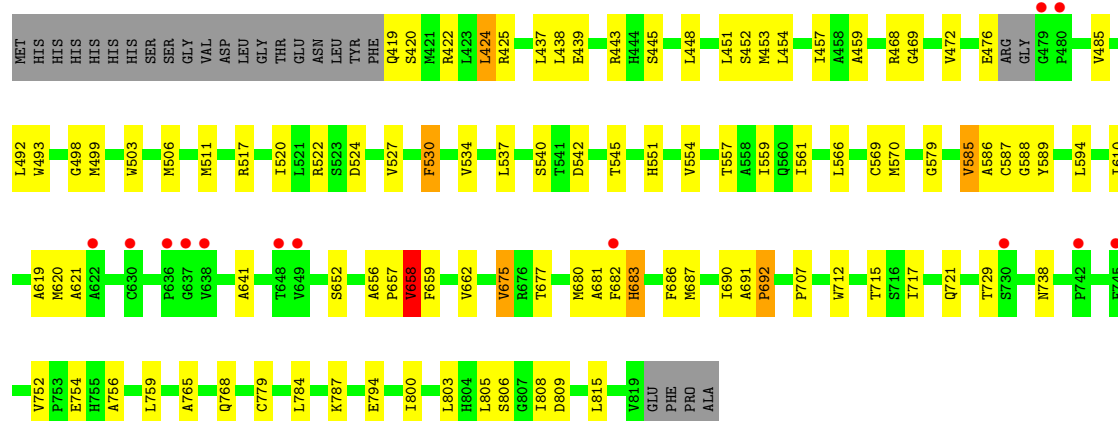


• Molecule 1: FATTY ACID SYNTHASE





• Molecule 1: FATTY ACID SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.98Å 92.69Å 259.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.22 – 2.81 45.22 – 2.81	Depositor EDS
% Data completeness (in resolution range)	81.0 (45.22-2.81) 81.0 (45.22-2.81)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.273 0.221 , 0.273	Depositor DCC
R_{free} test set	2074 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	74.5	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11392	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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

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	0.73	0/3003	0.95	4/4107 (0.1%)
1	B	0.65	0/2910	0.89	1/3985 (0.0%)
1	C	0.76	2/2975 (0.1%)	0.92	3/4069 (0.1%)
1	D	0.63	0/2769	0.86	2/3799 (0.1%)
All	All	0.70	2/11657 (0.0%)	0.91	10/15960 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	495	ILE	CA-CB	-5.90	1.47	1.54
1	C	782	ILE	CA-CB	-5.50	1.49	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	ARG	N-CA-C	-6.97	101.07	111.81
1	C	477	ARG	N-CA-C	-6.10	102.42	111.81
1	B	754	GLU	N-CA-C	5.93	117.42	111.07
1	A	754	GLU	N-CA-C	5.84	117.73	111.36
1	C	754	GLU	N-CA-C	5.40	117.25	111.36
1	D	692	PRO	N-CA-C	5.37	117.25	110.70
1	A	420	SER	N-CA-C	5.23	116.98	111.28
1	C	692	PRO	N-CA-C	5.12	116.95	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	754	GLU	N-CA-C	5.07	116.49	111.07
1	A	821	PHE	N-CA-C	5.03	120.94	109.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	476	GLU	Peptide
1	C	476	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2929	0	2774	94	0
1	B	2840	0	2643	108	0
1	C	2899	0	2757	88	0
1	D	2709	0	2400	76	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	9	0	0	0	0
All	All	11392	0	10574	351	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 16.

All (351) 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:B:453:MET:O	1:B:457:ILE:HD12	1.53	1.05
1:C:453:MET:HE3	1:D:437:LEU:HD23	1.35	1.05
1:A:468:ARG:HD3	1:A:485:VAL:HG21	1.37	1.03
1:A:694:LEU:HD23	1:A:736:VAL:HG22	1.38	1.02
1:D:570:MET:CE	1:D:815:LEU:HD11	1.92	0.98
1:C:453:MET:HE3	1:D:437:LEU:CD2	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:MET:CE	1:D:437:LEU:HD23	1.94	0.97
1:B:570:MET:HE2	1:B:812:PRO:HA	1.44	0.95
1:D:675:VAL:HG23	1:D:677:THR:HG23	1.47	0.94
1:C:468:ARG:HD3	1:C:485:VAL:HG21	1.50	0.94
1:A:450:PHE:O	1:A:454:LEU:HD12	1.72	0.90
1:B:468:ARG:HD3	1:B:485:VAL:HG21	1.53	0.89
1:C:506:MET:HE2	1:C:559:ILE:HD12	1.53	0.89
1:B:506:MET:HE3	1:B:559:ILE:HD12	1.57	0.87
1:A:570:MET:HE2	1:A:815:LEU:HD11	1.54	0.86
1:B:560:GLN:O	1:B:564:ILE:HD12	1.75	0.86
1:D:453:MET:CE	1:D:454:LEU:HD23	2.04	0.86
1:A:675:VAL:HG12	1:A:677:THR:HG22	1.56	0.85
1:A:749:LEU:HD22	1:A:775:LEU:HD21	1.61	0.79
1:D:527:VAL:HG12	1:D:527:VAL:O	1.81	0.79
1:D:765:ALA:HB1	1:D:768:GLN:HG2	1.63	0.78
1:C:511:MET:HE1	1:C:520:ILE:HG21	1.65	0.78
1:B:511:MET:HE1	1:B:520:ILE:HG21	1.67	0.78
1:A:457:ILE:CG2	1:B:457:ILE:HG21	2.13	0.77
1:B:570:MET:HE3	1:B:815:LEU:CG	2.15	0.77
1:C:423:LEU:HD23	1:C:812:PRO:HG3	1.66	0.77
1:D:656:ALA:HB3	1:D:657:PRO:HD3	1.70	0.74
1:A:457:ILE:HG23	1:B:457:ILE:HG21	1.68	0.73
1:D:570:MET:HE2	1:D:815:LEU:CD1	2.19	0.73
1:D:759:LEU:HD22	1:D:784:LEU:HD21	1.71	0.73
1:B:610:ILE:HG23	1:B:680:MET:CE	2.19	0.72
1:D:619:ALA:HB3	1:D:658:VAL:HG21	1.69	0.72
1:D:570:MET:HE2	1:D:815:LEU:HD11	1.69	0.72
1:D:468:ARG:HD3	1:D:485:VAL:HG21	1.70	0.72
1:C:754:GLU:O	1:C:778:SER:OG	2.04	0.72
1:B:570:MET:HE3	1:B:815:LEU:HG	1.72	0.71
1:A:527:VAL:HG12	1:A:527:VAL:O	1.89	0.71
1:D:453:MET:HE1	1:D:454:LEU:HD23	1.72	0.71
1:C:765:ALA:HB1	1:C:768:GLN:HG2	1.72	0.71
1:D:691:ALA:HB3	1:D:692:PRO:HD3	1.73	0.70
1:A:459:ALA:HB3	1:B:429:ARG:NH1	2.07	0.70
1:B:691:ALA:HB3	1:B:692:PRO:HD3	1.72	0.70
1:C:582:LEU:HD12	1:C:582:LEU:O	1.92	0.70
1:B:550:VAL:HG21	1:B:608:GLN:OE1	1.91	0.69
1:A:468:ARG:CD	1:A:485:VAL:HG21	2.19	0.69
1:B:453:MET:O	1:B:457:ILE:CD1	2.36	0.68
1:D:537:LEU:HD21	1:D:551:HIS:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:511:MET:HE1	1:D:520:ILE:HG21	1.74	0.68
1:C:675:VAL:HG12	1:C:675:VAL:O	1.93	0.68
1:C:694:LEU:HD23	1:C:736:VAL:HG22	1.75	0.67
1:B:527:VAL:HG12	1:B:532:LEU:HB2	1.77	0.67
1:B:570:MET:HE1	1:B:800:ILE:HG21	1.75	0.67
1:A:570:MET:CE	1:A:815:LEU:HD11	2.23	0.67
1:C:511:MET:HE1	1:C:520:ILE:CG2	2.24	0.67
1:A:588:GLY:HA2	1:A:712:TRP:CZ3	2.30	0.66
1:B:661:PHE:CZ	1:B:665:LEU:HD11	2.31	0.66
1:B:739:LEU:HD12	1:B:739:LEU:O	1.94	0.66
1:B:638:VAL:HG13	1:B:658:VAL:HG22	1.77	0.66
1:C:561:ILE:HG23	1:C:589:TYR:CE2	2.31	0.65
1:C:610:ILE:HA	1:C:690:ILE:HD13	1.79	0.65
1:B:765:ALA:HB1	1:B:768:GLN:HG2	1.77	0.65
1:A:450:PHE:CE2	1:A:454:LEU:HD11	2.31	0.64
1:A:610:ILE:HG23	1:A:680:MET:CE	2.27	0.64
1:A:570:MET:HE2	1:A:815:LEU:CD1	2.24	0.64
1:C:423:LEU:HD23	1:C:812:PRO:CG	2.27	0.64
1:C:759:LEU:HD22	1:C:784:LEU:HD21	1.79	0.64
1:A:450:PHE:HA	1:A:453:MET:HE2	1.79	0.64
1:A:454:LEU:HA	1:A:457:ILE:HD12	1.79	0.63
1:A:537:LEU:HD21	1:A:551:HIS:CD2	2.32	0.63
1:C:429:ARG:NH1	1:D:459:ALA:HB1	2.14	0.63
1:A:429:ARG:NH2	1:B:459:ALA:HB3	2.13	0.63
1:D:527:VAL:O	1:D:527:VAL:CG1	2.45	0.63
1:A:564:ILE:CD1	1:A:761:ILE:HG21	2.28	0.63
1:B:506:MET:O	1:B:538:LEU:HD22	1.99	0.63
1:B:610:ILE:HG23	1:B:680:MET:HE1	1.81	0.62
1:D:570:MET:HE2	1:D:815:LEU:CG	2.30	0.62
1:C:537:LEU:HD21	1:C:551:HIS:CD2	2.35	0.62
1:A:675:VAL:HG12	1:A:677:THR:CG2	2.30	0.62
1:B:759:LEU:HD23	1:B:782:ILE:HB	1.82	0.62
1:C:680:MET:HE3	1:C:687:MET:HE1	1.81	0.62
1:B:621:ALA:HA	1:B:675:VAL:HG23	1.82	0.61
1:A:606:ARG:O	1:A:610:ILE:HD12	2.01	0.61
1:A:662:VAL:HG13	1:A:672:ALA:HB1	1.82	0.61
1:A:610:ILE:HG23	1:A:680:MET:HE1	1.80	0.61
1:C:556:LEU:O	1:C:556:LEU:HD12	2.01	0.61
1:A:647:ASP:OD1	1:A:773:ARG:NH1	2.33	0.61
1:A:819:VAL:HG12	1:A:819:VAL:O	2.00	0.60
1:D:621:ALA:HA	1:D:675:VAL:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ALA:HB1	1:A:768:GLN:HG2	1.81	0.60
1:C:570:MET:HE2	1:C:815:LEU:HD21	1.83	0.60
1:D:453:MET:HE3	1:D:457:ILE:CD1	2.32	0.60
1:A:460:VAL:HG11	1:A:465:MET:SD	2.41	0.59
1:A:457:ILE:HG23	1:B:457:ILE:CG2	2.32	0.59
1:D:453:MET:HE3	1:D:454:LEU:HD23	1.83	0.59
1:B:610:ILE:CG2	1:B:680:MET:CE	2.81	0.59
1:D:610:ILE:HA	1:D:690:ILE:HD13	1.83	0.59
1:D:469:GLY:HA2	1:D:805:LEU:HD21	1.85	0.59
1:B:620:MET:HE3	1:B:652:SER:HB2	1.84	0.59
1:A:429:ARG:HH22	1:B:459:ALA:HB3	1.68	0.59
1:A:570:MET:HE1	1:A:800:ILE:HG13	1.85	0.58
1:B:690:ILE:HG22	1:B:690:ILE:O	2.03	0.58
1:B:610:ILE:CG2	1:B:680:MET:HE2	2.33	0.58
1:D:424:LEU:HD12	1:D:425:ARG:N	2.18	0.58
1:C:506:MET:HE2	1:C:559:ILE:CD1	2.29	0.58
1:D:511:MET:HE1	1:D:520:ILE:CG2	2.34	0.58
1:B:426:ALA:HB1	1:B:437:LEU:HD23	1.85	0.57
1:B:570:MET:HE3	1:B:815:LEU:CD1	2.34	0.57
1:C:680:MET:CE	1:C:687:MET:HE1	2.34	0.57
1:D:570:MET:HE2	1:D:815:LEU:HG	1.86	0.57
1:B:570:MET:HE3	1:B:815:LEU:HD11	1.86	0.57
1:D:492:LEU:HD11	1:D:759:LEU:HD12	1.86	0.57
1:C:469:GLY:HA2	1:C:805:LEU:HD21	1.86	0.57
1:B:620:MET:HB2	1:B:677:THR:HG21	1.87	0.57
1:B:639:VAL:HG22	1:B:640:PRO:HD2	1.86	0.57
1:D:570:MET:CE	1:D:815:LEU:CD1	2.72	0.57
1:A:561:ILE:HG23	1:A:589:TYR:CE1	2.40	0.56
1:B:527:VAL:HG12	1:B:527:VAL:O	2.05	0.56
1:D:503:TRP:CE2	1:D:787:LYS:HA	2.40	0.56
1:B:610:ILE:HG21	1:B:680:MET:HE2	1.87	0.56
1:C:675:VAL:O	1:C:677:THR:HG22	2.05	0.56
1:B:719:GLU:HA	1:B:722:TRP:CD2	2.41	0.55
1:C:691:ALA:HB3	1:C:692:PRO:HD3	1.88	0.55
1:D:453:MET:CE	1:D:454:LEU:CD2	2.83	0.55
1:A:457:ILE:HG21	1:B:457:ILE:HG21	1.86	0.55
1:A:759:LEU:HD23	1:A:782:ILE:HB	1.88	0.55
1:C:429:ARG:HH12	1:D:459:ALA:HB1	1.71	0.55
1:A:511:MET:HE1	1:A:520:ILE:HG21	1.88	0.55
1:A:609:CYS:HB3	1:A:690:ILE:CG2	2.36	0.55
1:C:752:VAL:O	1:C:776:LYS:HE3	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:LEU:O	1:C:445:SER:OG	2.23	0.55
1:B:432:GLU:CD	1:B:432:GLU:H	2.15	0.55
1:D:453:MET:HE1	1:D:454:LEU:CD2	2.37	0.55
1:D:641:ALA:HB2	1:D:652:SER:HB3	1.88	0.54
1:A:437:LEU:CD2	1:A:454:LEU:HD23	2.37	0.54
1:B:638:VAL:CG1	1:B:658:VAL:HG22	2.38	0.54
1:D:542:ASP:O	1:D:545:THR:HG22	2.07	0.54
1:D:422:ARG:NH2	1:D:448:LEU:HD23	2.23	0.54
1:C:468:ARG:HD3	1:C:485:VAL:CG2	2.32	0.54
1:B:656:ALA:HB3	1:B:657:PRO:HD3	1.88	0.54
1:A:610:ILE:CG2	1:A:680:MET:HE2	2.38	0.54
1:A:610:ILE:HG21	1:A:680:MET:HE2	1.90	0.54
1:B:527:VAL:CG1	1:B:532:LEU:HB2	2.37	0.54
1:A:749:LEU:HD22	1:A:775:LEU:CD2	2.32	0.54
1:C:494:PHE:CD1	1:C:574:PRO:HB3	2.43	0.54
1:C:421:MET:HE2	1:C:474:GLY:O	2.08	0.54
1:A:610:ILE:CG2	1:A:680:MET:CE	2.86	0.53
1:C:665:LEU:O	1:C:670:VAL:HG23	2.07	0.53
1:A:450:PHE:CD2	1:A:454:LEU:HD11	2.44	0.53
1:A:570:MET:HE2	1:A:815:LEU:CG	2.37	0.53
1:A:511:MET:HE1	1:A:520:ILE:CG2	2.38	0.53
1:B:680:MET:HB3	1:B:682:PHE:CE1	2.44	0.53
1:B:816:PHE:HB3	1:B:817:PRO:CD	2.38	0.53
1:C:767:LEU:O	1:C:771:LEU:HB2	2.08	0.53
1:B:511:MET:HE1	1:B:520:ILE:CG2	2.38	0.53
1:B:608:GLN:O	1:B:612:GLU:HG3	2.09	0.53
1:B:638:VAL:CG1	1:B:651:ILE:HD12	2.39	0.53
1:B:497:SER:OG	1:B:767:LEU:HD23	2.10	0.52
1:C:501:THR:HG21	1:C:764:HIS:O	2.10	0.52
1:A:524:ASP:OD1	1:A:534:VAL:HG23	2.09	0.52
1:C:442:LEU:O	1:C:442:LEU:HD12	2.09	0.52
1:B:485:VAL:HG22	1:B:805:LEU:O	2.09	0.52
1:B:570:MET:CE	1:B:815:LEU:HD11	2.39	0.52
1:C:524:ASP:OD2	1:C:534:VAL:N	2.42	0.52
1:D:675:VAL:CG2	1:D:677:THR:HG23	2.29	0.52
1:D:658:VAL:HG12	1:D:659:PHE:N	2.24	0.52
1:B:494:PHE:HB3	1:B:761:ILE:HD12	1.91	0.51
1:C:500:GLY:C	1:C:502:GLN:H	2.18	0.51
1:D:468:ARG:CD	1:D:485:VAL:HG21	2.37	0.51
1:D:681:ALA:O	1:D:687:MET:HE3	2.11	0.51
1:B:680:MET:HG2	1:B:682:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:620:MET:O	1:D:675:VAL:HG22	2.11	0.51
1:A:426:ALA:HB3	1:A:434:VAL:HG13	1.92	0.51
1:A:430:THR:HG22	1:A:433:ALA:H	1.75	0.51
1:A:560:GLN:O	1:A:564:ILE:HD13	2.11	0.51
1:C:791:ASP:C	1:C:791:ASP:OD1	2.53	0.51
1:C:439:GLU:OE2	1:C:439:GLU:HA	2.11	0.51
1:A:663:GLU:O	1:A:667:LYS:HG2	2.11	0.51
1:A:681:ALA:O	1:A:687:MET:HE3	2.11	0.51
1:C:744:LEU:HB3	1:C:747:GLU:CG	2.41	0.51
1:B:561:ILE:HG23	1:B:589:TYR:CE2	2.46	0.50
1:A:499:MET:SD	1:A:580:HIS:HE1	2.35	0.50
1:B:641:ALA:HB2	1:B:652:SER:HB3	1.92	0.50
1:D:717:ILE:HG21	1:D:721:GLN:O	2.11	0.50
1:A:430:THR:CG2	1:A:433:ALA:H	2.25	0.50
1:A:570:MET:HE2	1:A:815:LEU:HD21	1.94	0.50
1:C:556:LEU:HD12	1:C:556:LEU:C	2.36	0.50
1:C:620:MET:HE3	1:C:652:SER:HB2	1.93	0.50
1:D:453:MET:HE3	1:D:457:ILE:HD12	1.92	0.50
1:B:497:SER:HB2	1:B:762:ALA:HB2	1.94	0.50
1:B:681:ALA:O	1:B:687:MET:HE3	2.11	0.50
1:C:581:SER:OG	1:C:582:LEU:N	2.44	0.50
1:B:582:LEU:O	1:B:585:VAL:HG23	2.12	0.50
1:B:457:ILE:O	1:B:457:ILE:HG22	2.12	0.49
1:A:690:ILE:O	1:A:690:ILE:HG22	2.11	0.49
1:A:702:ILE:N	1:A:702:ILE:HD12	2.27	0.49
1:C:623:VAL:HG12	1:C:625:LEU:H	1.78	0.49
1:B:506:MET:HE3	1:B:559:ILE:CD1	2.37	0.49
1:C:596:GLN:O	1:C:600:VAL:HG23	2.12	0.48
1:A:668:GLU:HG3	1:A:670:VAL:HG23	1.95	0.48
1:D:492:LEU:HD11	1:D:759:LEU:CD1	2.43	0.48
1:C:675:VAL:O	1:C:676:ARG:C	2.55	0.48
1:A:468:ARG:HD3	1:A:485:VAL:CG2	2.27	0.48
1:C:698:LEU:HB2	1:C:732:ALA:HB1	1.96	0.48
1:A:685:TYR:O	1:A:688:GLU:HB2	2.14	0.48
1:C:511:MET:HE1	1:C:520:ILE:CB	2.44	0.47
1:D:588:GLY:HA3	1:D:594:LEU:HD12	1.96	0.47
1:B:782:ILE:HD13	1:B:802:ARG:HB2	1.97	0.47
1:D:472:VAL:HG11	1:D:794:GLU:HG3	1.97	0.47
1:C:609:CYS:HB3	1:C:690:ILE:HG23	1.97	0.47
1:A:670:VAL:HG12	1:A:671:PHE:N	2.29	0.47
1:B:423:LEU:HD23	1:B:812:PRO:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:MET:O	1:B:675:VAL:N	2.46	0.47
1:C:485:VAL:HG22	1:C:805:LEU:O	2.15	0.47
1:C:564:ILE:O	1:C:568:SER:OG	2.31	0.47
1:D:469:GLY:CA	1:D:805:LEU:HD21	2.44	0.47
1:D:570:MET:HE1	1:D:800:ILE:HG21	1.96	0.47
1:A:506:MET:HE3	1:A:763:PRO:CG	2.44	0.47
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.96	0.47
1:B:483:GLN:HG2	1:B:805:LEU:HD13	1.95	0.47
1:B:685:TYR:CE2	1:C:637:GLY:HA2	2.50	0.47
1:B:542:ASP:O	1:B:545:THR:HG22	2.14	0.47
1:A:511:MET:HE1	1:A:520:ILE:HB	1.97	0.47
1:D:585:VAL:HG12	1:D:586:ALA:N	2.30	0.47
1:B:450:PHE:CZ	1:B:454:LEU:HD11	2.50	0.46
1:C:731:SER:O	1:C:735:ASN:OD1	2.33	0.46
1:A:437:LEU:HD22	1:A:454:LEU:HD23	1.97	0.46
1:C:437:LEU:HD12	1:C:437:LEU:O	2.15	0.46
1:C:453:MET:O	1:C:457:ILE:HD13	2.15	0.46
1:D:448:LEU:HD12	1:D:448:LEU:H	1.81	0.46
1:A:623:VAL:HG13	1:A:665:LEU:CD1	2.45	0.46
1:B:430:THR:HG23	1:B:433:ALA:H	1.79	0.46
1:B:581:SER:OG	1:B:582:LEU:N	2.39	0.46
1:D:579:GLY:O	1:D:715:THR:HG21	2.16	0.46
1:D:683:HIS:HD1	1:D:683:HIS:N	2.13	0.46
1:C:745:PHE:CZ	1:C:767:LEU:HD13	2.51	0.46
1:A:656:ALA:HB3	1:A:657:PRO:CD	2.46	0.46
1:B:638:VAL:HG11	1:B:651:ILE:HD12	1.97	0.46
1:C:550:VAL:HG23	1:C:611:LYS:HD3	1.98	0.46
1:A:459:ALA:HB3	1:B:429:ARG:HH12	1.76	0.46
1:B:570:MET:HE3	1:B:815:LEU:CD2	2.46	0.45
1:C:744:LEU:HB3	1:C:747:GLU:HG3	1.99	0.45
1:A:609:CYS:HB3	1:A:690:ILE:HG23	1.99	0.45
1:B:656:ALA:HB3	1:B:657:PRO:CD	2.46	0.45
1:C:620:MET:HG3	1:C:677:THR:HG21	1.98	0.45
1:B:739:LEU:HD12	1:B:739:LEU:C	2.41	0.45
1:C:610:ILE:HA	1:C:690:ILE:CD1	2.46	0.45
1:B:516:PHE:CZ	1:B:520:ILE:HD11	2.52	0.45
1:B:662:VAL:HG12	1:B:666:ARG:HG3	1.99	0.45
1:B:468:ARG:HG2	1:B:804:HIS:NE2	2.32	0.45
1:A:670:VAL:HG12	1:A:671:PHE:H	1.82	0.45
1:D:438:LEU:O	1:D:439:GLU:C	2.59	0.45
1:A:701:VAL:HB	1:A:702:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:LEU:HD21	1:A:733:GLU:C	2.41	0.45
1:D:511:MET:HE3	1:D:517:ARG:HA	1.99	0.45
1:A:549:ILE:CD1	1:A:610:ILE:HG21	2.47	0.45
1:A:634:CYS:HA	1:A:635:PRO:HD2	1.81	0.45
1:D:570:MET:HE1	1:D:815:LEU:HD11	1.89	0.45
1:D:524:ASP:OD2	1:D:534:VAL:HB	2.17	0.44
1:D:530:PHE:CD1	1:D:530:PHE:N	2.84	0.44
1:D:768:GLN:HA	1:D:768:GLN:NE2	2.32	0.44
1:A:655:GLN:O	1:A:656:ALA:C	2.59	0.44
1:B:421:MET:HE3	1:B:793:LEU:HG	1.98	0.44
1:B:448:LEU:N	1:B:448:LEU:HD23	2.33	0.44
1:B:511:MET:SD	1:B:520:ILE:HD13	2.56	0.44
1:D:680:MET:HE3	1:D:682:PHE:CE1	2.52	0.44
1:A:430:THR:HG23	1:A:432:GLU:H	1.83	0.44
1:D:561:ILE:HG12	1:D:589:TYR:CD2	2.52	0.44
1:C:656:ALA:HB3	1:C:657:PRO:HD3	2.00	0.44
1:C:743:VAL:HG12	1:C:745:PHE:HB2	2.00	0.44
1:B:621:ALA:HB1	1:B:673:LYS:O	2.18	0.44
1:C:437:LEU:HD12	1:C:437:LEU:C	2.42	0.44
1:D:511:MET:HE1	1:D:520:ILE:CB	2.48	0.44
1:D:803:LEU:HD22	1:D:808:ILE:HG21	1.99	0.44
1:B:812:PRO:O	1:B:813:ASN:C	2.60	0.44
1:A:426:ALA:CB	1:A:434:VAL:HG13	2.48	0.43
1:A:447:ASP:OD1	1:A:447:ASP:C	2.61	0.43
1:C:428:GLY:C	1:C:465:MET:HG2	2.43	0.43
1:A:749:LEU:HD21	1:A:775:LEU:HD11	2.00	0.43
1:B:457:ILE:HD12	1:B:457:ILE:H	1.82	0.43
1:C:470:TYR:CD2	1:C:470:TYR:C	2.96	0.43
1:C:811:ASN:HA	1:C:812:PRO:HD3	1.92	0.43
1:A:527:VAL:O	1:A:527:VAL:CG1	2.60	0.43
1:C:450:PHE:CE1	1:C:454:LEU:CD1	3.01	0.43
1:C:457:ILE:O	1:C:457:ILE:CG2	2.65	0.43
1:C:582:LEU:HD12	1:C:582:LEU:C	2.42	0.43
1:B:712:TRP:C	1:B:712:TRP:CD1	2.95	0.43
1:B:550:VAL:HG22	1:B:607:GLY:C	2.43	0.43
1:C:606:ARG:HA	1:C:694:LEU:CD1	2.48	0.43
1:A:514:ASP:O	1:A:517:ARG:HG3	2.18	0.43
1:B:516:PHE:CE1	1:B:520:ILE:CD1	3.02	0.43
1:C:712:TRP:CD1	1:C:712:TRP:C	2.97	0.43
1:A:493:TRP:CE3	1:A:752:VAL:HG22	2.54	0.42
1:B:609:CYS:HB3	1:B:690:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:687:MET:N	1:D:687:MET:HE2	2.34	0.42
1:A:524:ASP:OD1	1:A:534:VAL:N	2.52	0.42
1:B:430:THR:O	1:B:433:ALA:HB3	2.19	0.42
1:C:691:ALA:HB3	1:C:692:PRO:CD	2.48	0.42
1:D:493:TRP:CE3	1:D:752:VAL:HG22	2.54	0.42
1:D:756:ALA:HB3	1:D:779:CYS:SG	2.59	0.42
1:C:495:ILE:HG13	1:C:771:LEU:HD21	2.00	0.42
1:C:501:THR:CG2	1:C:764:HIS:O	2.67	0.42
1:A:499:MET:O	1:A:766:LEU:HD22	2.20	0.42
1:A:758:VAL:O	1:A:758:VAL:HG12	2.18	0.42
1:B:516:PHE:CE1	1:B:520:ILE:HD11	2.54	0.42
1:B:560:GLN:O	1:B:564:ILE:CD1	2.59	0.42
1:A:492:LEU:N	1:A:575:ASP:OD2	2.41	0.42
1:B:668:GLU:C	1:B:670:VAL:HG23	2.44	0.42
1:C:520:ILE:HD13	1:C:538:LEU:HD12	2.00	0.42
1:A:511:MET:HE1	1:A:520:ILE:CB	2.49	0.42
1:D:686:PHE:C	1:D:687:MET:HE2	2.45	0.42
1:C:494:PHE:CZ	1:C:567:LEU:HD23	2.55	0.42
1:A:430:THR:HG23	1:A:432:GLU:N	2.34	0.42
1:B:658:VAL:O	1:B:659:PHE:C	2.63	0.42
1:C:816:PHE:HB3	1:C:817:PRO:CD	2.50	0.42
1:C:478:GLY:O	1:C:479:GLY:C	2.63	0.41
1:D:619:ALA:CB	1:D:658:VAL:HG11	2.49	0.41
1:B:570:MET:HE3	1:B:815:LEU:HD21	2.01	0.41
1:D:579:GLY:HA3	1:D:587:CYS:SG	2.61	0.41
1:A:550:VAL:HG22	1:A:607:GLY:C	2.44	0.41
1:B:744:LEU:HB3	1:B:747:GLU:CG	2.51	0.41
1:B:760:GLU:OE1	1:B:765:ALA:HB1	2.20	0.41
1:C:453:MET:HE3	1:D:437:LEU:HD21	1.95	0.41
1:C:511:MET:HE1	1:C:520:ILE:HB	2.03	0.41
1:C:772:LYS:HG3	1:C:781:ILE:HD12	2.02	0.41
1:D:588:GLY:HA2	1:D:712:TRP:CZ3	2.56	0.41
1:C:511:MET:CE	1:C:520:ILE:HG21	2.43	0.41
1:B:493:TRP:CZ3	1:B:752:VAL:HG22	2.56	0.41
1:B:510:LEU:CD2	1:B:793:LEU:HA	2.51	0.41
1:C:610:ILE:HG12	1:C:690:ILE:HD12	2.03	0.41
1:B:454:LEU:HA	1:B:457:ILE:HD13	2.02	0.41
1:D:658:VAL:O	1:D:662:VAL:HG23	2.20	0.41
1:A:763:PRO:HA	1:A:785:MET:SD	2.61	0.41
1:B:434:VAL:O	1:B:437:LEU:N	2.53	0.41
1:B:500:GLY:C	1:B:502:GLN:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:MET:SD	1:C:520:ILE:HD12	2.60	0.41
1:A:442:LEU:O	1:A:445:SER:OG	2.33	0.41
1:A:765:ALA:HB1	1:A:768:GLN:CG	2.48	0.41
1:B:698:LEU:HB2	1:B:732:ALA:HB1	2.03	0.41
1:C:609:CYS:HB3	1:C:690:ILE:CG2	2.50	0.41
1:A:812:PRO:O	1:A:813:ASN:C	2.64	0.40
1:D:445:SER:O	1:D:451:LEU:HD11	2.21	0.40
1:B:606:ARG:O	1:B:610:ILE:HD12	2.19	0.40
1:D:557:THR:HG21	1:D:585:VAL:HG11	2.02	0.40
1:D:707:PRO:HA	1:D:729:THR:HG22	2.03	0.40
1:C:549:ILE:HD12	1:C:610:ILE:HG21	2.03	0.40
1:A:564:ILE:HD11	1:A:761:ILE:HG21	2.03	0.40
1:B:422:ARG:CZ	1:B:448:LEU:HD13	2.51	0.40
1:A:506:MET:HE3	1:A:763:PRO:HG2	2.03	0.40
1:B:680:MET:HG2	1:B:682:PHE:CE2	2.57	0.40
1:B:690:ILE:O	1:B:690:ILE:CG2	2.68	0.40
1:B:719:GLU:HA	1:B:722:TRP:CG	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	402/425 (95%)	379 (94%)	20 (5%)	3 (1%)	18	45
1	B	394/425 (93%)	370 (94%)	24 (6%)	0	100	100
1	C	402/425 (95%)	374 (93%)	27 (7%)	1 (0%)	43	71
1	D	395/425 (93%)	376 (95%)	16 (4%)	3 (1%)	16	41
All	All	1593/1700 (94%)	1499 (94%)	87 (6%)	7 (0%)	30	58

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	499	MET
1	D	499	MET
1	C	676	ARG
1	A	498	GLY
1	D	498	GLY
1	A	821	PHE
1	D	658	VAL

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	290/352 (82%)	265 (91%)	25 (9%)	10	29
1	B	272/352 (77%)	252 (93%)	20 (7%)	13	36
1	C	282/352 (80%)	256 (91%)	26 (9%)	8	26
1	D	237/352 (67%)	216 (91%)	21 (9%)	9	27
All	All	1081/1408 (77%)	989 (92%)	92 (8%)	10	30

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	430	THR
1	A	437	LEU
1	A	443	ARG
1	A	445	SER
1	A	468	ARG
1	A	483	GLN
1	A	489	GLU
1	A	499	MET
1	A	501	THR
1	A	509	SER
1	A	557	THR
1	A	593	CYS
1	A	597	GLU
1	A	630	CYS
1	A	633	ARG

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Mol	Chain	Res	Type
1	A	634	CYS
1	A	667	LYS
1	A	675	VAL
1	A	677	THR
1	A	688	GLU
1	A	726	LEU
1	A	729	THR
1	A	740	VAL
1	A	758	VAL
1	A	773	ARG
1	B	420	SER
1	B	427	SER
1	B	440	GLN
1	B	448	LEU
1	B	463	THR
1	B	501	THR
1	B	509	SER
1	B	520	ILE
1	B	530	PHE
1	B	537	LEU
1	B	552	SER
1	B	564	ILE
1	B	639	VAL
1	B	670	VAL
1	B	688	GLU
1	B	729	THR
1	B	731	SER
1	B	743	VAL
1	B	747	GLU
1	B	780	THR
1	C	430	THR
1	C	437	LEU
1	C	463	THR
1	C	465	MET
1	C	483	GLN
1	C	497	SER
1	C	501	THR
1	C	520	ILE
1	C	527	VAL
1	C	549	ILE
1	C	554	VAL
1	C	556	LEU

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Mol	Chain	Res	Type
1	C	566	LEU
1	C	568	SER
1	C	569	CYS
1	C	573	ARG
1	C	582	LEU
1	C	630	CYS
1	C	648	THR
1	C	662	VAL
1	C	670	VAL
1	C	677	THR
1	C	740	VAL
1	C	747	GLU
1	C	771	LEU
1	C	776	LYS
1	D	419	GLN
1	D	420	SER
1	D	424	LEU
1	D	443	ARG
1	D	452	SER
1	D	476	GLU
1	D	506	MET
1	D	522	ARG
1	D	530	PHE
1	D	540	SER
1	D	554	VAL
1	D	559	ILE
1	D	566	LEU
1	D	569	CYS
1	D	585	VAL
1	D	658	VAL
1	D	675	VAL
1	D	683	HIS
1	D	738	ASN
1	D	806	SER
1	D	809	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	440	GLN
1	B	444	HIS
1	B	483	GLN

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Mol	Chain	Res	Type
1	B	560	GLN
1	B	643	HIS
1	B	644	ASN
1	C	440	GLN
1	C	608	GLN
1	D	444	HIS
1	D	484	GLN

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	404/425 (95%)	0.19	5 (1%) 76 68	23, 42, 61, 79	0
1	B	400/425 (94%)	0.30	16 (4%) 42 33	22, 42, 57, 72	0
1	C	403/425 (94%)	0.32	8 (1%) 65 55	19, 42, 59, 82	1 (0%)
1	D	399/425 (93%)	0.36	13 (3%) 49 39	22, 42, 60, 70	0
All	All	1606/1700 (94%)	0.29	42 (2%) 57 47	19, 42, 60, 82	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	617	PRO	4.0
1	C	464	ALA	3.9
1	D	730	SER	3.9
1	C	637	GLY	3.5
1	B	615	LEU	3.5
1	D	648	THR	3.3
1	D	479	GLY	3.2
1	A	612	GLU	3.0
1	A	478	GLY	2.9
1	C	488	GLY	2.9
1	A	621	ALA	2.8
1	B	616	PRO	2.7
1	D	638	VAL	2.7
1	B	613	ALA	2.7
1	A	774	GLY	2.7
1	A	613	ALA	2.6
1	B	638	VAL	2.5
1	C	546	PHE	2.5
1	D	622	ALA	2.4
1	C	473	LEU	2.4
1	C	669	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	645	SER	2.4
1	B	507	GLY	2.3
1	D	637	GLY	2.3
1	B	725	SER	2.3
1	D	682	PHE	2.3
1	B	619	ALA	2.2
1	B	630	CYS	2.2
1	C	665	LEU	2.2
1	B	501	THR	2.2
1	C	619	ALA	2.1
1	B	476	GLU	2.1
1	B	658	VAL	2.1
1	D	649	VAL	2.1
1	D	745	PHE	2.1
1	B	640	PRO	2.1
1	D	480	PRO	2.1
1	D	636	PRO	2.1
1	D	742	PRO	2.1
1	B	618	GLY	2.1
1	B	614	HIS	2.0
1	D	630	CYS	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.