

Full wwPDB X-ray Structure Validation Report (i)

Sep 4, 2024 - 01:18 pm BST

PDB ID		8QFB	
Title	e of human MPP8 C-terminal region (resid	Crystal structure of human MP	(residues 565-860 $)$
Authors	Modis, Y.	Prigozhin, D.M.; Modis, Y.	
Deposited on		2023-09-04	
Resolution		3.04 Å(reported)	
Authors Deposited on Resolution	of human MPP8 C-terminal region (resided) Modis, Y.	Orystal structure of human MP Prigozhin, D.M.; Modis, Y. 2023-09-04 3.04 Å(reported)	ι (residues 565-δ

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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.04 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.



Motria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	164625	3418 (3.08-3.00)
Clashscore	180529	3811 (3.08-3.00)
Ramachandran outliers	177936	3656 (3.08-3.00)
Sidechain outliers	177891	3658 (3.08-3.00)
RSRZ outliers	164620	3430 (3.08-3.00)

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	А	336	66%	23%	11%
1	В	336	^{2%} 68%	19%	12%
1	С	336	68%	19%	12%
1	D	336	% 71%	18%	11%
1	Е	336	8%	18%	• 12%



Mol	Chain	Length	Quality of chain		
1	F	336	65%	22%	12%
1	G	336	3% 69%	18%	12%
1	Н	336	6% 67%	21%	• 12%



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 35246 atoms, of which 17506 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.

Mol	Chain	Residues		Atoms						AltConf	Trace
1	Р	204	Total	С	Η	Ν	0	S	0	0	0
	D	294	4370	1399	2170	379	412	10	0		0
1	Δ	208	Total	С	Н	Ν	0	S	0	0	0
	A	290	4456	1427	2217	384	418	10	0	0	0
1	С	204	Total	С	Η	Ν	0	S	0	0	0
	U	294	4323	1390	2139	375	409	10	0	0	0
1	Л	208	Total	С	Η	Ν	0	S	0	0	0
	D	290	4523	1440	2260	390	423	10	0	0	0
1	1 5	206	Total	С	Η	Ν	0	S	0	0	0
	Ľ	290	4387	1407	2179	379	412	10	0	0	
1	Б	204	Total	С	Η	Ν	0	S	0	0	0
		294	4382	1405	2169	380	418	10	0	0	0
1	C	205	Total	С	Η	Ν	0	S	0	0	0
	G	295	4423	1411	2202	386	414	10	0	0	0
1	ц	206	Total	С	Н	Ν	0	S	0	0	0
	п	Н 296	4382	1407	2170	380	415	10		U	U

• Molecule 1 is a protein called M-phase phosphoprotein 8.

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	525	MET	-	initiating methionine	UNP Q99549
В	526	GLY	-	expression tag	UNP Q99549
В	527	SER	-	expression tag	UNP Q99549
В	528	SER	-	expression tag	UNP Q99549
В	529	HIS	-	expression tag	UNP Q99549
В	530	HIS	-	expression tag	UNP Q99549
В	531	HIS	-	expression tag	UNP Q99549
В	532	HIS	-	expression tag	UNP Q99549
В	533	HIS	-	expression tag	UNP Q99549
В	534	HIS	-	expression tag	UNP Q99549
В	535	SER	-	expression tag	UNP Q99549
В	536	SER	-	expression tag	UNP Q99549
В	537	GLY	-	expression tag	UNP Q99549



Chain	Residue	Modelled	Actual Comment		Reference
В	538	LEU	-	expression tag	UNP Q99549
В	539	VAL	-	expression tag	UNP Q99549
В	540	PRO	-	expression tag	UNP Q99549
В	541	ARG	-	expression tag	UNP Q99549
В	542	GLY	-	expression tag	UNP Q99549
В	543	SER	-	expression tag	UNP Q99549
В	544	HIS	_	expression tag	UNP Q99549
В	545	MET	-	expression tag	UNP Q99549
А	525	MET	-	initiating methionine	UNP Q99549
А	526	GLY	-	expression tag	UNP Q99549
А	527	SER	-	expression tag	UNP Q99549
А	528	SER	-	expression tag	UNP Q99549
А	529	HIS	-	expression tag	UNP Q99549
А	530	HIS	-	expression tag	UNP Q99549
А	531	HIS	-	expression tag	UNP Q99549
А	532	HIS	-	expression tag	UNP Q99549
А	533	HIS	-	expression tag	UNP Q99549
А	534	HIS	-	expression tag	UNP Q99549
А	535	SER	-	expression tag	UNP Q99549
А	536	SER	-	expression tag	UNP Q99549
А	537	GLY	-	expression tag	UNP Q99549
А	538	LEU	-	expression tag	UNP Q99549
А	539	VAL	-	expression tag	UNP Q99549
А	540	PRO	-	expression tag	UNP Q99549
А	541	ARG	-	expression tag	UNP Q99549
А	542	GLY	-	expression tag	UNP Q99549
А	543	SER	-	expression tag	UNP Q99549
А	544	HIS	-	expression tag	UNP Q99549
А	545	MET	-	expression tag	UNP Q99549
С	525	MET	-	initiating methionine	UNP Q99549
С	526	GLY	-	expression tag	UNP Q99549
С	527	SER	-	expression tag	UNP Q99549
С	528	SER	-	expression tag	UNP Q99549
С	529	HIS	-	expression tag	UNP Q99549
С	530	HIS	-	expression tag	UNP Q99549
С	531	HIS	-	expression tag	UNP Q99549
С	532	HIS	-	expression tag	UNP Q99549
С	533	HIS	-	expression tag	UNP Q99549
С	534	HIS	-	expression tag	UNP Q99549
С	535	SER	-	expression tag	UNP Q99549
С	536	SER	-	expression tag	UNP Q99549
С	537	GLY	-	expression tag	UNP Q99549



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Chain	Residue	Modelled	Actual	Comment	Reference
С	538	LEU	-	expression tag	UNP Q99549
С	539	VAL	-	expression tag	UNP Q99549
С	540	PRO	-	expression tag	UNP Q99549
С	541	ARG	-	expression tag	UNP Q99549
С	542	GLY	-	expression tag	UNP Q99549
С	543	SER	-	expression tag	UNP Q99549
С	544	HIS	-	expression tag	UNP Q99549
С	545	MET	-	expression tag	UNP Q99549
D	525	MET	-	initiating methionine	UNP Q99549
D	526	GLY	-	expression tag	UNP Q99549
D	527	SER	-	expression tag	UNP Q99549
D	528	SER	-	expression tag	UNP Q99549
D	529	HIS	-	expression tag	UNP Q99549
D	530	HIS	-	expression tag	UNP Q99549
D	531	HIS	-	expression tag	UNP Q99549
D	532	HIS	-	expression tag	UNP Q99549
D	533	HIS	-	expression tag	UNP Q99549
D	534	HIS	-	expression tag	UNP Q99549
D	535	SER	-	expression tag	UNP Q99549
D	536	SER	-	expression tag	UNP Q99549
D	537	GLY	-	expression tag	UNP Q99549
D	538	LEU	-	expression tag	UNP Q99549
D	539	VAL	-	expression tag	UNP Q99549
D	540	PRO	-	expression tag	UNP Q99549
D	541	ARG	-	expression tag	UNP Q99549
D	542	GLY	-	expression tag	UNP Q99549
D	543	SER	-	expression tag	UNP Q99549
D	544	HIS	-	expression tag	UNP Q99549
D	545	MET	-	expression tag	UNP Q99549
E	525	MET	-	initiating methionine	UNP Q99549
E	526	GLY	-	expression tag	UNP Q99549
E	527	SER	-	expression tag	UNP Q99549
E	528	SER	-	expression tag	UNP Q99549
Ε	529	HIS	-	expression tag	UNP Q99549
E	530	HIS	-	expression tag	UNP Q99549
E	531	HIS	-	expression tag	UNP Q99549
E	532	HIS	-	expression tag	UNP Q99549
E	533	HIS	-	expression tag	UNP Q99549
E	534	HIS	-	expression tag	UNP Q99549
E	535	SER	-	expression tag	UNP Q99549
E	536	SER	-	expression tag	UNP Q99549
E	537	GLY	-	expression tag	UNP Q99549



Comment	Reference
xpression tag	UNP Q99549
ating methionine	UNP Q99549
	TIND COOF 10

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Chain | Residue | Modelled | Actual |

Chan	itesidae	mouellea	ricual	Comment	iterenee
Е	538	LEU	-	expression tag	UNP Q99549
Е	539	VAL	-	expression tag	UNP Q99549
Е	540	PRO	-	expression tag	UNP Q99549
Е	541	ARG	-	expression tag	UNP Q99549
Е	542	GLY	-	expression tag	UNP Q99549
Е	543	SER	-	expression tag	UNP Q99549
Е	544	HIS	-	expression tag	UNP Q99549
Е	545	MET	-	expression tag	UNP Q99549
F	525	MET	-	initiating methionine	UNP Q99549
F	526	GLY	-	expression tag	UNP Q99549
F	527	SER	-	expression tag	UNP Q99549
F	528	SER	-	expression tag	UNP Q99549
F	529	HIS	-	expression tag	UNP Q99549
F	530	HIS	-	expression tag	UNP Q99549
F	531	HIS	-	expression tag	UNP Q99549
F	532	HIS	-	expression tag	UNP Q99549
F	533	HIS	-	expression tag	UNP Q99549
F	534	HIS	-	expression tag	UNP Q99549
F	535	SER	-	expression tag	UNP Q99549
F	536	SER	-	expression tag	UNP Q99549
F	537	GLY	-	expression tag	UNP Q99549
F	538	LEU	-	expression tag	UNP Q99549
F	539	VAL	-	expression tag	UNP Q99549
F	540	PRO	-	expression tag	UNP Q99549
F	541	ARG	-	expression tag	UNP Q99549
F	542	GLY	-	expression tag	UNP Q99549
F	543	SER	-	expression tag	UNP Q99549
F	544	HIS	-	expression tag	UNP Q99549
F	545	MET	-	expression tag	UNP Q99549
G	525	MET	-	initiating methionine	UNP Q99549
G	526	GLY	-	expression tag	UNP Q99549
G	527	SER	-	expression tag	UNP Q99549
G	528	SER	-	expression tag	UNP Q99549
G	529	HIS	-	expression tag	UNP Q99549
G	530	HIS	-	expression tag	UNP Q99549
G	531	HIS	-	expression tag	UNP Q99549
G	532	HIS	-	expression tag	UNP Q99549
G	533	HIS	-	expression tag	UNP Q99549
G	534	HIS	-	expression tag	UNP Q99549
G	535	SER	-	expression tag	UNP Q99549
G	536	SER	-	expression tag	UNP Q99549
G	537	GLY	-	expression tag	UNP Q99549



Chain	Residue	Modelled	Actual	Comment	Reference
G	538	LEU	-	expression tag	UNP Q99549
G	539	VAL	-	expression tag	UNP Q99549
G	540	PRO	-	expression tag	UNP Q99549
G	541	ARG	-	expression tag	UNP Q99549
G	542	GLY	-	expression tag	UNP Q99549
G	543	SER	-	expression tag	UNP Q99549
G	544	HIS	-	expression tag	UNP Q99549
G	545	MET	-	expression tag	UNP Q99549
Н	525	MET	-	initiating methionine	UNP Q99549
Н	526	GLY	-	expression tag	UNP Q99549
Н	527	SER	-	expression tag	UNP Q99549
Н	528	SER	-	expression tag	UNP Q99549
Н	529	HIS	-	expression tag	UNP Q99549
Н	530	HIS	-	expression tag	UNP Q99549
Н	531	HIS	-	expression tag	UNP Q99549
Н	532	HIS	-	expression tag	UNP Q99549
Н	533	HIS	-	expression tag	UNP Q99549
Н	534	HIS	-	expression tag	UNP Q99549
Н	535	SER	-	expression tag	UNP Q99549
Н	536	SER	-	expression tag	UNP Q99549
Н	537	GLY	-	expression tag	UNP Q99549
Н	538	LEU	-	expression tag	UNP Q99549
Н	539	VAL	-	expression tag	UNP Q99549
Н	540	PRO	-	expression tag	UNP Q99549
H	541	ARG	-	expression tag	UNP Q99549
Н	542	GLY	-	expression tag	UNP Q99549
Н	543	SER	-	expression tag	UNP Q99549
Н	544	HIS	-	expression tag	UNP Q99549
H	545	MET	-	expression tag	UNP Q99549



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: M-phase phosphoprotein 8



M602 T603 T603 M604 W605 M006 L616 L616 L617 L621 1629 1649 T649 1652 L653 L653 L653 L653	A670 L671 6678 6678 V683 V683 V683 1687 1687 1687 1687 1685 1685 1685 1685 1685 1685 1685 1685	L704 L704 N712 V715 V715 L723 L726 L726 L726 L728 F738 F738 F738
IN 44 IN 44 IN 44 IN 44 IN 76 IN	6902 8903 8903 8903 1806 1819 1819 1819 1823 1823 1823 1823 1823 1823 1836	1838 1841 1841 1841 1842 1842 1457 1986 1859
• Molecule 1: M-phase phosp	phoprotein 8	
Chain D:	71%	18% 11%
MET GLY SER SER HIS HIS HIS HIS SER RIS CLU VAL LEU VAL ARG ARG SER SER SER ARG CLY MET	ASP ASP ASP ASP ASP ALN ALN ALA ALA ALA ALA ALA ALA ALA ALA	P566 7579 1580 1580 1581 7581 7581 7682 8600 8601 8601 8601 8601 8601 8601 8601
D615 1616 1617 1621 1621 1632 1633 1633 1633 1633 1653 1653 1653 1653	R677 R677 V683 C689 C689 A691 C709 H709 H715 H722 H722 H722	1734 1734 1734 1734 1744 1744 1774 1774
V808 1809 1809 1809 1809 1805 1815 1815 1836 1837 1836 1837 1838 1837 1838 1839 1837 1838 1837 1841 1841 1841 1841 1841 1841 1841 184	7855 7 066 0	
• Molecule 1: M-phase phosp	phoprotein 8	
Chain E:	70%	18% <mark>•</mark> 12%
MET ALY SER SER SER HIS HIS HIS HIS HIS SER HIS SER CLY VAL CLZ VAL CLY CLZ VAL PRO CLY SER RES SER MIS SER MIS SER MIS SER MIS SER MIS SER SER SER SER SER SER SER SER SER SE	ASP ASP CLU CLN CLN CLN CLN CLN LLS ASP CLU CLU ALA ALA ALA ASP CLU ALA ASP CLU ASP ASP CLU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	RE 71 U574 0578 1580 1580 1580 1583 1584 1584 1584 0595 0595 0595 0595 0595
M606 L607 D614 L617 L617 L621 1635 1635 1635 L646 L647 L647 L649 L649 L649	1652 L653 L653 R660 A672 R672 R672 L685 C689 C689 C689 C689 C689	1695 H995 4700 4700 4700 8710 8710 8711 8711 8721 H721 H721 H721 1722
V729 Y737 F738 F738 F739 A740 A743 A743 L744 F749 F749 F749 F749 T774 T774 L781 L781	F789 L790 E793 E793 E793 F795 F801 F801 F803 S803 S803 S803 S803 S803 F803 F813 F813	D820 F827 F827 F836 F836 F836 F837 F837 F837 F836 F836 F836 F836 F836 F856 F856 F856 F856 F856 F856 F856 F85
• Molecule 1: M-phase phosp	phoprotein 8	
Chain F:	65%	22% 12%
MET CLY SER SER SER HIS HIS HIS HIS SER HIS SER RIS SER RIS SER RIS PRO CLY VAL PRO CLY SER RIS SER MET	ASP ASP CIJA CJAN CJAN CJAN CJAN CJAN ALA ALA ALA ALA ALA ALA ALA	PR0 5567 5671 V574 V579 V579 V582 5 590 1 596 1 594 1 594 1 594
6597 6698 8599 8599 8599 8599 8612 8612 8613 8614 8625 8645 8645 8645 8645 8645 8645 8645 8645 8645 86555 86555 85555 85555 85555 85555 85555 85555 85555 85555 85555 85555 85555 85555 85555 85555555 855555 85555555 855555 855555555	6629 8630 1635 1635 1635 1635 1639 1644 1644 1643 1653 1653 1653 1653 1653 1653 1653	668 1671 1669 4670 4677 1667 1667 1667 1667 1728 1728 1728 1728 1728
R728 1734 1734 1734 1737 1737 1744 1744 1744	F789 L790 G791 K793 K793 C799 C799 C799 C799 C799 C799 C799 C	B820 B20 F823 F823 F827 F827 F827 F827 F827 F827 F836 F837 F836 F836 F844 F843 F844 F843 F845 F845 F845





• Molecule 1: M-phase phosphoprotein 8





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	102.56Å 179.53Å 228.08Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	93.54 - 3.04	Depositor
Resolution (A)	93.54 - 3.04	EDS
% Data completeness	98.8 (93.54-3.04)	Depositor
(in resolution range)	98.8 (93.54 - 3.04)	EDS
R_{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.88 (at 3.01 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.256 , 0.295	Depositor
n, n_{free}	0.258 , 0.295	DCC
R_{free} test set	4189 reflections (5.12%)	wwPDB-VP
Wilson B-factor $(Å^2)$	100.7	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 78.0	EDS
L-test for $twinning^2$	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35246	wwPDB-VP
Average B, all atoms $(Å^2)$	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	Bond lengths		angles
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.34	0/2279	0.60	0/3101
1	В	0.31	0/2238	0.57	0/3044
1	С	0.30	0/2222	0.56	0/3026
1	D	0.35	0/2303	0.61	0/3129
1	Е	0.33	0/2246	0.59	0/3056
1	F	0.32	0/2252	0.59	0/3065
1	G	0.30	0/2260	0.58	0/3073
1	Н	0.31	0/2251	0.57	0/3065
All	All	0.32	0/18051	0.58	0/24559

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	А	2239	2217	2217	65	0
1	В	2200	2170	2170	46	0
1	С	2184	2139	2139	50	0
1	D	2263	2260	2260	52	0
1	Е	2208	2179	2179	47	0
1	F	2213	2169	2169	68	2
1	G	2221	2202	2202	56	0
1	Н	2212	2170	2170	53	2



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17740	17506	17506	416	2

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 12.

All (416) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:645:ASN:OD1	1:D:677:ARG:NE	2.01	0.91
1:H:778:SER:OG	1:H:858:GLN:OE1	1.94	0.84
1:D:617:LEU:HD23	1:D:652:ILE:HD11	1.59	0.83
1:C:738:PHE:CD2	1:C:742:LEU:HD22	2.14	0.82
1:G:745:LEU:HD23	1:G:746:GLU:HG2	1.65	0.79
1:B:645:ASN:OD1	1:B:677:ARG:NE	2.17	0.78
1:C:697:SER:OG	1:C:701:ASN:OD1	2.02	0.77
1:A:704:LEU:HD11	1:A:716:TYR:HD1	1.50	0.76
1:A:704:LEU:HD11	1:A:716:TYR:CD1	2.21	0.76
1:G:795:ILE:HD11	1:H:795:ILE:HD11	1.67	0.75
1:G:795:ILE:CD1	1:H:795:ILE:HD11	2.17	0.75
1:E:790:LEU:CB	1:F:790:LEU:HD13	2.16	0.75
1:F:768:TYR:OH	1:F:856:ARG:NH2	2.19	0.74
1:A:617:LEU:HD13	1:A:652:ILE:HD11	1.70	0.74
1:F:571:ARG:HD3	1:F:604:LEU:HD21	1.68	0.73
1:D:566:PRO:HD3	1:F:837:PHE:CE2	2.23	0.73
1:C:596:GLN:N	1:C:596:GLN:OE1	2.22	0.73
1:H:617:LEU:HD13	1:H:652:ILE:HD11	1.70	0.73
1:H:819:LEU:HD13	1:H:819:LEU:O	1.87	0.73
1:A:697:SER:OG	1:A:701:ASN:OD1	2.06	0.73
1:F:645:ASN:OD1	1:F:677:ARG:NH2	2.21	0.73
1:H:768:TYR:OH	1:H:856:ARG:NH2	2.22	0.71
1:B:671:LEU:HD23	1:B:686:VAL:CG2	2.21	0.71
1:B:790:LEU:HB3	1:A:790:LEU:HD22	1.73	0.71
1:F:614:ASP:OD1	1:F:649:THR:HG22	1.89	0.71
1:D:614:ASP:OD1	1:D:649:THR:HG22	1.91	0.71
1:A:768:TYR:OH	1:A:856:ARG:NH2	2.24	0.70
1:B:819:LEU:HD13	1:B:819:LEU:O	1.91	0.70
1:B:795:ILE:HD11	1:A:795:ILE:CD1	2.21	0.69
1:G:744:LEU:HD22	1:G:855:TYR:HD2	1.54	0.69
1:C:738:PHE:HD2	1:C:742:LEU:HD22	1.57	0.69
1:D:734:ILE:HD12	1:D:744:LEU:HD11	1.74	0.69
1:E:742:LEU:HD21	1:E:857:VAL:HG21	1.74	0.68



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:582:VAL:O	1:B:586:LEU:HD13	1.92	0.68	
1:B:768:TYR:OH	1:B:856:ARG:NH2	2.26	0.67	
1:G:768:TYR:OH	1:G:856:ARG:NH2	2.27	0.67	
1:B:596:GLN:N	1:B:596:GLN:OE1	2.28	0.67	
1:H:602:MET:SD	1:H:602:MET:N	2.68	0.67	
1:H:617:LEU:CD1	1:H:652:ILE:HD11	2.24	0.67	
1:F:742:LEU:HD21	1:F:857:VAL:HG21	1.75	0.66	
1:A:614:ASP:OD1	1:A:649:THR:HG22	1.94	0.66	
1:C:671:LEU:HD23	1:C:686:VAL:CG2	2.25	0.66	
1:G:793:GLU:OE1	1:H:790:LEU:HD21	1.96	0.66	
1:E:578:ASP:OD2	1:E:581:THR:OG1	2.12	0.66	
1:B:808:VAL:HG22	1:B:813:PHE:CD1	2.31	0.65	
1:B:795:ILE:HD11	1:A:795:ILE:HD12	1.78	0.65	
1:C:639:ILE:HD13	1:C:670:ALA:HB2	1.78	0.65	
1:A:639:ILE:HD13	1:A:670:ALA:HB2	1.78	0.65	
1:E:639:ILE:HD13	1:E:670:ALA:HB2	1.79	0.65	
1:G:565:ILE:O	1:G:592:TYR:OH	2.15	0.65	
1:A:617:LEU:CD1	1:A:652:ILE:HD11	2.26	0.64	
1:A:742:LEU:HD21	1:A:857:VAL:HG21	1.79	0.64	
1:C:819:LEU:HD13	1:C:819:LEU:O	1.98	0.64	
1:A:734:ILE:HG21	1:A:744:LEU:HD11	1.80	0.64	
1:G:639:ILE:HD13	1:G:670:ALA:HB2	1.79	0.64	
1:G:745:LEU:CD2	1:G:746:GLU:HG2	2.28	0.64	
1:H:570:LEU:HD21	1:H:585:ALA:HB1	1.80	0.64	
1:C:693:CYS:HB2	1:C:723:LEU:HD21	1.79	0.63	
1:H:614:ASP:OD1	1:H:649:THR:HG22	1.99	0.63	
1:A:734:ILE:HG21	1:A:744:LEU:CD1	2.28	0.63	
1:E:738:PHE:HD2	1:E:742:LEU:HD22	1.64	0.63	
1:F:586:LEU:HD22	1:F:623:LYS:HD2	1.80	0.63	
1:F:594:LEU:HD23	1:F:623:LYS:HD3	1.79	0.63	
1:C:569:VAL:HG23	1:C:570:LEU:HD12	1.80	0.63	
1:B:671:LEU:HD23	1:B:686:VAL:HG21	1.82	0.62	
1:D:639:ILE:HD13	1:D:670:ALA:HB2	1.82	0.62	
1:B:681:ASP:O	1:B:685:LEU:HD23	2.00	0.62	
1:A:671:LEU:HD23	1:A:686:VAL:CG2	2.29	0.62	
1:E:669:THR:HG22	1:E:670:ALA:N	2.14	0.61	
1:E:692:ASP:OD2	1:E:695:ILE:HD11	2.00	0.61	
1:B:639:ILE:HD13	1:B:670:ALA:HB2	1.82	0.61	
1:A:778:SER:OG	1:A:858:GLN:OE1	2.18	0.61	
1:C:790:LEU:HD13	1:D:790:LEU:O	1.99	0.61	
1:F:836:LEU:HD23	1:F:837:PHE:N	2.15	0.61	



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:639:ILE:HD13	1:F:670:ALA:HB2	1.83	0.61
1:D:669:THR:HG22	1:D:670:ALA:N	2.16	0.61
1:F:594:LEU:HD22	1:F:625:ALA:HB2	1.82	0.61
1:A:565:ILE:HD11	1:A:569:VAL:HG11	1.83	0.60
1:G:742:LEU:HD11	1:G:857:VAL:HG21	1.83	0.60
1:G:790:LEU:HD22	1:H:790:LEU:HB2	1.84	0.60
1:H:704:LEU:HD11	1:H:716:TYR:CE1	2.37	0.60
1:D:742:LEU:HD11	1:D:857:VAL:HG11	1.84	0.60
1:F:734:ILE:HD13	1:F:744:LEU:HD11	1.83	0.59
1:H:569:VAL:HG23	1:H:570:LEU:HD12	1.84	0.59
1:G:742:LEU:HD21	1:G:857:VAL:HG21	1.85	0.59
1:B:616:LEU:O	1:B:620:LEU:HD13	2.03	0.59
1:A:809:LEU:HD12	1:A:827:PHE:CE1	2.37	0.59
1:C:802:CYS:HB2	1:C:823:PHE:HE1	1.68	0.59
1:D:582:VAL:HG21	1:D:616:LEU:HD22	1.85	0.59
1:A:582:VAL:O	1:A:586:LEU:HD13	2.02	0.59
1:C:809:LEU:HD12	1:C:827:PHE:CE1	2.37	0.59
1:G:777:GLY:O	1:G:859:LEU:HD13	2.03	0.59
1:D:581:THR:O	1:D:584:VAL:HG12	2.03	0.58
1:C:774:ILE:HD12	1:C:774:ILE:O	2.03	0.58
1:D:809:LEU:HD12	1:D:827:PHE:CE1	2.37	0.58
1:F:582:VAL:O	1:F:586:LEU:HG	2.04	0.58
1:F:789:PHE:CD2	1:F:794:VAL:HG12	2.38	0.58
1:B:713:VAL:HG13	1:B:714:LEU:HD22	1.85	0.58
1:D:704:LEU:HD11	1:D:716:TYR:CE1	2.38	0.58
1:E:645:ASN:OD1	1:E:677:ARG:NH2	2.37	0.58
1:B:742:LEU:HD21	1:B:857:VAL:HG21	1.86	0.57
1:E:808:VAL:HG22	1:E:813:PHE:CD1	2.39	0.57
1:H:742:LEU:HD21	1:H:857:VAL:HG21	1.87	0.57
1:C:798:LEU:HA	1:C:823:PHE:HD2	1.70	0.57
1:B:809:LEU:HD12	1:B:827:PHE:CE1	2.40	0.57
1:B:789:PHE:CD2	1:B:794:VAL:HG12	2.39	0.57
1:C:582:VAL:O	1:C:586:LEU:HD13	2.03	0.57
1:H:568:ASN:OD1	1:H:569:VAL:N	2.38	0.57
1:E:614:ASP:OD1	1:E:649:THR:HG22	2.05	0.57
1:E:859:LEU:O	1:E:860:GLN:HG3	2.04	0.56
1:H:639:ILE:HD13	1:H:670:ALA:HB2	1.86	0.56
1:A:789:PHE:CD1	1:A:794:VAL:HG12	2.41	0.56
1:B:726:LEU:O	1:B:729:VAL:HG12	2.05	0.56
1:A:617:LEU:O	1:A:621:ILE:HG12	2.06	0.56
1:A:774:ILE:HD12	1:A:774:ILE:O	2.06	0.56



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:F:579:TYR:O	1:F:582:VAL:HG22	2.05	0.56
1:H:809:LEU:HD12	1:H:827:PHE:CE1	2.40	0.56
1:B:704:LEU:HD11	1:B:716:TYR:CE1	2.40	0.56
1:B:778:SER:OG	1:B:858:GLN:OE1	2.24	0.55
1:A:628:ASN:HD21	1:A:659:PHE:H	1.54	0.55
1:E:738:PHE:CD2	1:E:742:LEU:HD22	2.41	0.55
1:E:809:LEU:HD12	1:E:827:PHE:CE1	2.41	0.55
1:G:671:LEU:HD23	1:G:686:VAL:CG2	2.36	0.55
1:F:623:LYS:O	1:F:623:LYS:HG2	2.06	0.55
1:F:809:LEU:HD12	1:F:827:PHE:CE1	2.41	0.55
1:C:762:PHE:O	1:C:837:PHE:HD1	1.90	0.55
1:C:616:LEU:O	1:C:620:LEU:HD13	2.07	0.55
1:C:742:LEU:HD21	1:C:857:VAL:HG21	1.89	0.55
1:H:571:ARG:HD3	1:H:604:LEU:HD21	1.89	0.55
1:B:738:PHE:HD2	1:B:742:LEU:HD22	1.72	0.54
1:G:681:ASP:O	1:G:685:LEU:HD23	2.06	0.54
1:H:704:LEU:HD11	1:H:716:TYR:CD1	2.42	0.54
1:A:671:LEU:HD23	1:A:686:VAL:HG21	1.89	0.54
1:D:638:LEU:HD11	1:D:654:LEU:HD11	1.89	0.54
1:E:647:LEU:HD11	1:E:685:LEU:HD12	1.89	0.54
1:G:744:LEU:HD22	1:G:855:TYR:CD2	2.40	0.53
1:B:795:ILE:HD11	1:A:795:ILE:HD11	1.89	0.53
1:D:744:LEU:HD22	1:D:855:TYR:HD2	1.73	0.53
1:E:741:ARG:O	1:E:741:ARG:HG2	2.05	0.53
1:A:744:LEU:HD23	1:A:855:TYR:HD2	1.73	0.53
1:H:594:LEU:HD12	1:H:624:GLY:O	2.09	0.53
1:E:774:ILE:O	1:E:774:ILE:HD12	2.07	0.53
1:H:789:PHE:CD1	1:H:794:VAL:HG12	2.42	0.53
1:G:693:CYS:HB2	1:G:723:LEU:HD21	1.90	0.53
1:A:777:GLY:O	1:A:859:LEU:HD13	2.09	0.53
1:A:713:VAL:HG13	1:A:714:LEU:HD22	1.91	0.53
1:G:790:LEU:HB2	1:H:790:LEU:HD22	1.90	0.53
1:E:859:LEU:O	1:E:860:GLN:CG	2.57	0.52
1:B:774:ILE:HD12	1:B:774:ILE:O	2.09	0.52
1:G:614:ASP:OD1	1:G:649:THR:HG22	2.09	0.52
1:H:808:VAL:HG22	1:H:813:PHE:CD1	2.44	0.52
1:F:744:LEU:CD2	1:F:855:TYR:HD2	2.23	0.52
1:D:744:LEU:HD23	1:D:857:VAL:HG22	1.91	0.51
1:A:744:LEU:HD23	1:A:855:TYR:CD2	2.44	0.51
1:C:692:ASP:OD2	1:C:695:ILE:HD11	2.09	0.51
1:E:756:LEU:HD13	1:E:756:LEU:O	2.10	0.51



	to de pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:774:ILE:HD12	1:D:774:ILE:O	2.11	0.51
1:B:617:LEU:O	1:B:621:ILE:HG12	2.10	0.51
1:C:836:LEU:HD23	1:C:837:PHE:N	2.25	0.51
1:D:839:ARG:NH1	1:D:840:LEU:O	2.44	0.51
1:D:808:VAL:HG22	1:D:813:PHE:CD1	2.45	0.51
1:H:683:VAL:HG21	1:H:715:VAL:HG13	1.93	0.51
1:D:738:PHE:CD2	1:D:742:LEU:HD13	2.45	0.51
1:G:809:LEU:HD12	1:G:827:PHE:CE1	2.46	0.51
1:A:636:THR:CG2	1:A:639:ILE:HG12	2.42	0.50
1:C:802:CYS:CB	1:C:823:PHE:HE1	2.24	0.50
1:A:628:ASN:ND2	1:A:659:PHE:H	2.09	0.50
1:D:565:ILE:HG22	1:D:566:PRO:HD2	1.93	0.50
1:E:737:TYR:CE1	1:F:801:PRO:HD3	2.46	0.50
1:F:808:VAL:HG22	1:F:813:PHE:CD1	2.47	0.50
1:G:617:LEU:O	1:G:621:ILE:HG12	2.12	0.50
1:H:738:PHE:HD2	1:H:742:LEU:HD22	1.76	0.50
1:C:671:LEU:HD23	1:C:686:VAL:HG21	1.93	0.50
1:C:798:LEU:C	1:C:823:PHE:CD2	2.85	0.50
1:B:602:MET:HA	1:B:606:MET:SD	2.52	0.50
1:G:738:PHE:CE2	1:G:742:LEU:HD13	2.46	0.50
1:H:726:LEU:O	1:H:729:VAL:HG12	2.12	0.50
1:F:734:ILE:HD12	1:F:744:LEU:HD21	1.93	0.49
1:A:616:LEU:O	1:A:620:LEU:HD13	2.11	0.49
1:H:617:LEU:O	1:H:621:ILE:HG12	2.13	0.49
1:A:570:LEU:HD23	1:A:570:LEU:O	2.12	0.49
1:A:586:LEU:HB3	1:A:623:LYS:HE3	1.92	0.49
1:D:638:LEU:HD11	1:D:654:LEU:CD1	2.43	0.49
1:H:725:THR:HA	1:H:728:ARG:HG2	1.94	0.49
1:F:742:LEU:HG	1:F:857:VAL:HG22	1.94	0.49
1:D:738:PHE:O	1:D:741:ARG:HG2	2.13	0.49
1:C:602:MET:HA	1:C:606:MET:SD	2.53	0.49
1:E:749:PHE:HE1	1:E:854:ALA:HB3	1.76	0.49
1:E:836:LEU:HD23	1:E:837:PHE:N	2.28	0.49
1:D:816:PRO:HB2	1:D:818:PHE:O	2.13	0.48
1:E:742:LEU:CD2	1:E:857:VAL:HG21	2.43	0.48
1:F:809:LEU:HD23	1:F:810:ASN:ND2	2.28	0.48
1:H:774:ILE:HD12	1:H:774:ILE:O	2.13	0.48
1:F:762:PHE:O	1:F:837:PHE:CD1	2.66	0.48
1:G:692:ASP:OD2	1:G:695:ILE:HD11	2.14	0.48
1:C:617:LEU:O	1:C:621:ILE:HG12	2.13	0.48
1:E:660:VAL:HG11	1:E:691:ALA:HB2	1.94	0.48



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:630:ARG:HG2	1:F:634:GLY:HA2	1.94	0.48
1:H:645:ASN:OD1	1:H:677:ARG:NE	2.40	0.48
1:G:605:VAL:HG22	1:G:620:LEU:HD23	1.96	0.48
1:A:734:ILE:HD13	1:A:744:LEU:HD11	1.96	0.48
1:D:836:LEU:HD23	1:D:837:PHE:N	2.29	0.48
1:G:683:VAL:HG21	1:G:715:VAL:HG13	1.95	0.48
1:A:726:LEU:O	1:A:729:VAL:HG12	2.14	0.48
1:D:605:VAL:HG13	1:D:617:LEU:HD11	1.96	0.48
1:G:742:LEU:HG	1:G:857:VAL:HG22	1.96	0.48
1:A:580:ILE:HG13	1:A:581:THR:N	2.29	0.48
1:F:837:PHE:HD1	1:F:838:ILE:N	2.11	0.48
1:G:795:ILE:HD12	1:H:795:ILE:HD11	1.92	0.48
1:E:593:ASN:O	1:E:596:GLN:OE1	2.31	0.47
1:E:710:SER:O	1:E:711:ASN:OD1	2.31	0.47
1:B:675:CYS:SG	1:B:719:LEU:HD11	2.54	0.47
1:D:566:PRO:HD3	1:F:837:PHE:CD2	2.49	0.47
1:F:617:LEU:O	1:F:621:ILE:HG12	2.14	0.47
1:F:800:GLY:O	1:F:823:PHE:HZ	1.97	0.47
1:G:605:VAL:CG2	1:G:625:ALA:HB1	2.45	0.47
1:G:742:LEU:HD21	1:G:857:VAL:CG2	2.43	0.47
1:G:809:LEU:HD23	1:G:810:ASN:OD1	2.14	0.47
1:B:579:TYR:O	1:B:582:VAL:HG22	2.15	0.47
1:B:678:GLY:O	1:B:712:ASN:ND2	2.48	0.47
1:A:638:LEU:HD11	1:A:654:LEU:HD11	1.97	0.47
1:A:668:GLU:HA	1:A:672:MET:SD	2.54	0.47
1:A:738:PHE:CD2	1:A:742:LEU:HD22	2.49	0.47
1:C:734:ILE:HG21	1:C:744:LEU:HD11	1.97	0.47
1:G:704:LEU:HD11	1:G:716:TYR:CD1	2.50	0.47
1:E:859:LEU:O	1:E:860:GLN:CB	2.63	0.47
1:G:745:LEU:HD23	1:G:746:GLU:CG	2.39	0.47
1:G:808:VAL:HG22	1:G:813:PHE:CD1	2.50	0.47
1:E:669:THR:CG2	1:E:670:ALA:N	2.78	0.47
1:F:744:LEU:HD23	1:F:855:TYR:CD2	2.50	0.47
1:G:594:LEU:HD13	1:G:625:ALA:HA	1.96	0.47
1:C:815:LEU:N	1:C:815:LEU:HD12	2.30	0.47
1:D:579:TYR:CZ	1:D:583:LYS:HE2	2.50	0.47
1:G:789:PHE:CD1	1:G:794:VAL:HG12	2.49	0.47
1:H:603:THR:H	1:H:606:MET:HE3	1.81	0.46
1:A:744:LEU:CD2	1:A:855:TYR:HD2	2.28	0.46
1:A:809:LEU:HD23	1:A:810:ASN:ND2	2.30	0.46
1:D:683:VAL:HG21	1:D:715:VAL:HG13	1.96	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:789:PHE:C	1:G:790:LEU:HD12	2.35	0.46
1:B:578:ASP:HB3	1:B:581:THR:HB	1.98	0.46
1:A:650:VAL:O	1:A:654:LEU:HD13	2.15	0.46
1:C:726:LEU:O	1:C:729:VAL:HG12	2.16	0.46
1:E:594:LEU:H	1:E:594:LEU:HD12	1.81	0.46
1:C:756:LEU:HD13	1:C:756:LEU:O	2.16	0.46
1:H:612:GLY:HA2	1:H:649:THR:HG21	1.96	0.46
1:B:568:ASN:OD1	1:B:569:VAL:N	2.48	0.46
1:D:565:ILE:HA	1:F:837:PHE:HE2	1.80	0.46
1:D:612:GLY:HA2	1:D:649:THR:HG21	1.98	0.46
1:G:790:LEU:HD12	1:G:790:LEU:N	2.30	0.46
1:H:578:ASP:HB3	1:H:581:THR:HG22	1.97	0.46
1:H:744:LEU:CD2	1:H:855:TYR:HD2	2.29	0.46
1:H:756:LEU:HD13	1:H:756:LEU:O	2.16	0.46
1:B:734:ILE:HD13	1:B:744:LEU:HD11	1.98	0.46
1:A:636:THR:HG22	1:A:639:ILE:HG12	1.98	0.46
1:D:617:LEU:O	1:D:621:ILE:HG12	2.16	0.46
1:E:617:LEU:O	1:E:621:ILE:HG12	2.16	0.46
1:B:683:VAL:HG21	1:B:715:VAL:HG13	1.99	0.45
1:F:762:PHE:O	1:F:837:PHE:HD1	1.99	0.45
1:H:734:ILE:HD13	1:H:744:LEU:HD11	1.97	0.45
1:C:704:LEU:HD11	1:C:716:TYR:CE1	2.51	0.45
1:G:836:LEU:HD23	1:G:837:PHE:N	2.31	0.45
1:H:628:ASN:ND2	1:H:659:PHE:H	2.14	0.45
1:B:756:LEU:HD13	1:B:756:LEU:O	2.16	0.45
1:D:615:ASP:N	1:D:615:ASP:OD1	2.49	0.45
1:E:726:LEU:O	1:E:729:VAL:HG12	2.16	0.45
1:E:859:LEU:HD12	1:E:859:LEU:N	2.31	0.45
1:A:582:VAL:HG21	1:A:616:LEU:HD22	1.97	0.45
1:G:647:LEU:C	1:G:647:LEU:HD23	2.37	0.45
1:G:738:PHE:CD2	1:G:742:LEU:HD22	2.51	0.45
1:G:756:LEU:HD13	1:G:756:LEU:O	2.16	0.45
1:C:738:PHE:CE2	1:C:742:LEU:HD22	2.49	0.45
1:E:669:THR:HG22	1:E:670:ALA:H	1.82	0.45
1:F:744:LEU:HD23	1:F:855:TYR:HD2	1.82	0.45
1:H:638:LEU:HD11	1:H:654:LEU:HD11	1.98	0.45
1:C:678:GLY:O	1:C:712:ASN:ND2	2.50	0.45
1:D:649:THR:HA	1:D:652:ILE:HG12	1.99	0.45
1:F:639:ILE:HG21	1:F:664:GLN:HE21	1.81	0.45
1:D:669:THR:CG2	1:D:670:ALA:N	2.80	0.45
1:F:841:THR:HG22	1:F:842:GLU:N	2.32	0.45



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:726:LEU:O	1:G:729:VAL:HG12	2.16	0.45
1:H:748:VAL:HB	1:H:854:ALA:O	2.17	0.45
1:E:602:MET:HA	1:E:606:MET:SD	2.56	0.45
1:E:801:PRO:HD3	1:F:737:TYR:CE1	2.52	0.45
1:F:836:LEU:HD21	1:F:838:ILE:HG13	1.99	0.44
1:B:808:VAL:HG22	1:B:813:PHE:HD1	1.80	0.44
1:B:836:LEU:HD23	1:B:837:PHE:N	2.33	0.44
1:A:734:ILE:HD12	1:A:744:LEU:HD21	1.99	0.44
1:F:636:THR:HG22	1:F:639:ILE:HG12	1.98	0.44
1:C:761:ASP:OD1	1:C:837:PHE:CE1	2.71	0.44
1:D:704:LEU:HD11	1:D:716:TYR:CD1	2.52	0.44
1:E:649:THR:HA	1:E:652:ILE:HG12	1.99	0.44
1:A:762:PHE:O	1:A:837:PHE:HD1	2.00	0.44
1:A:816:PRO:HB3	1:A:825:TYR:CE1	2.53	0.44
1:E:627:VAL:HG13	1:E:653:LEU:HD22	2.00	0.44
1:F:808:VAL:HG22	1:F:813:PHE:HD1	1.82	0.44
1:G:790:LEU:CD2	1:H:790:LEU:HB2	2.48	0.44
1:E:571:ARG:HD3	1:E:596:GLN:HE21	1.81	0.44
1:F:668:GLU:HA	1:F:672:MET:SD	2.57	0.44
1:G:738:PHE:O	1:G:741:ARG:HG2	2.18	0.44
1:A:568:ASN:OD1	1:A:569:VAL:N	2.51	0.44
1:C:798:LEU:CA	1:C:823:PHE:HD2	2.30	0.44
1:D:738:PHE:CE2	1:D:742:LEU:HD13	2.53	0.44
1:F:725:THR:HA	1:F:728:ARG:HG2	1.99	0.44
1:G:841:THR:HG22	1:G:842:GLU:N	2.33	0.44
1:D:803:SER:O	1:D:840:LEU:HA	2.17	0.44
1:F:704:LEU:HD11	1:F:716:TYR:CD1	2.53	0.44
1:C:823:PHE:CD1	1:C:823:PHE:N	2.85	0.44
1:F:771:PRO:HD2	1:F:856:ARG:NH2	2.32	0.44
1:A:699:HIS:ND1	1:F:845:SER:HB3	2.33	0.43
1:E:722:HIS:HE1	1:E:789:PHE:HE2	1.66	0.43
1:F:586:LEU:CD2	1:F:623:LYS:HD2	2.47	0.43
1:C:807:VAL:HG22	1:C:838:ILE:HG12	2.01	0.43
1:F:671:LEU:HD13	1:F:686:VAL:CG2	2.48	0.43
1:F:737:TYR:CD2	1:F:798:LEU:HB2	2.53	0.43
1:G:649:THR:HA	1:G:652:ILE:HG12	1.99	0.43
1:D:605:VAL:HG13	1:D:617:LEU:CD1	2.48	0.43
1:G:738:PHE:HD2	1:G:742:LEU:HB3	1.82	0.43
1:B:742:LEU:HG	1:B:857:VAL:HG22	2.00	0.43
1:A:638:LEU:HD11	1:A:654:LEU:CD1	2.48	0.43
1:A:737:TYR:CD2	1:A:798:LEU:HB2	2.53	0.43



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:738:PHE:CD2	1:A:742:LEU:HD13	2.54	0.43
1:A:836:LEU:HD23	1:A:837:PHE:N	2.34	0.43
1:E:749:PHE:HE1	1:E:854:ALA:CB	2.31	0.43
1:D:841:THR:HG22	1:D:842:GLU:N	2.34	0.43
1:H:678:GLY:O	1:H:712:ASN:OD1	2.37	0.43
1:C:802:CYS:SG	1:C:823:PHE:CE1	3.12	0.43
1:A:802:CYS:SG	1:A:823:PHE:CE2	3.12	0.43
1:C:638:LEU:HD11	1:C:654:LEU:HD11	2.00	0.43
1:B:738:PHE:CD2	1:B:742:LEU:HD13	2.54	0.42
1:D:602:MET:HE2	1:D:631:GLN:HE22	1.85	0.42
1:D:792:LYS:HG3	1:D:792:LYS:O	2.19	0.42
1:H:748:VAL:HG13	1:H:768:TYR:CD1	2.53	0.42
1:F:636:THR:CG2	1:F:639:ILE:HG12	2.49	0.42
1:B:636:THR:HG22	1:B:639:ILE:HG12	2.01	0.42
1:A:742:LEU:HG	1:A:857:VAL:HG22	2.00	0.42
1:E:647:LEU:HD11	1:E:685:LEU:CD1	2.48	0.42
1:H:571:ARG:HD3	1:H:604:LEU:CD2	2.49	0.42
1:D:726:LEU:O	1:D:729:VAL:HG12	2.19	0.42
1:F:836:LEU:HD23	1:F:836:LEU:C	2.40	0.42
1:H:708:LYS:HZ3	1:H:716:TYR:HE2	1.67	0.42
1:B:704:LEU:HD11	1:B:716:TYR:CD1	2.54	0.42
1:B:744:LEU:CD2	1:B:855:TYR:HD2	2.32	0.42
1:B:807:VAL:HG22	1:B:838:ILE:HG12	2.01	0.42
1:D:792:LYS:O	1:D:792:LYS:CG	2.67	0.42
1:E:704:LEU:HD11	1:E:716:TYR:CE1	2.54	0.42
1:A:704:LEU:HD12	1:A:704:LEU:HA	1.84	0.42
1:D:816:PRO:HB3	1:D:825:TYR:CE1	2.54	0.42
1:F:744:LEU:CD2	1:F:855:TYR:CD2	3.02	0.42
1:G:671:LEU:HD12	1:G:703:ALA:CB	2.50	0.42
1:G:671:LEU:CD1	1:G:703:ALA:HB1	2.50	0.42
1:D:602:MET:CG	1:D:606:MET:HG3	2.49	0.42
1:F:643:GLU:OE2	1:F:673:LYS:HD2	2.20	0.42
1:G:774:ILE:O	1:G:774:ILE:HG13	2.20	0.42
1:F:738:PHE:CD2	1:F:742:LEU:HD22	2.55	0.42
1:G:782:LEU:HD12	1:G:827:PHE:CE1	2.55	0.42
1:B:613:GLN:HB2	1:B:616:LEU:HD12	2.02	0.42
1:A:571:ARG:CD	1:A:604:LEU:HD21	2.49	0.42
1:C:590:GLU:OE1	1:C:592:TYR:OH	2.27	0.42
1:E:689:CYS:O	1:E:755:ARG:NH1	2.53	0.42
1:E:635:THR:HG23	1:E:639:ILE:HB	2.01	0.41
1:B:777:GLY:O	1:B:859:LEU:HD13	2.20	0.41



	, and pagetti	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:809:LEU:HD12	1:D:827:PHE:CD1	2.55	0.41
1:F:807:VAL:HG22	1:F:838:ILE:HG12	2.02	0.41
1:F:605:VAL:HG21	1:F:626:LYS:O	2.20	0.41
1:A:782:LEU:HD12	1:A:827:PHE:CE1	2.54	0.41
1:C:738:PHE:N	1:C:738:PHE:CD1	2.88	0.41
1:E:582:VAL:O	1:E:586:LEU:HD13	2.21	0.41
1:F:612:GLY:HA2	1:F:649:THR:HG21	2.02	0.41
1:F:639:ILE:HG21	1:F:664:GLN:NE2	2.36	0.41
1:F:652:ILE:HG13	1:F:653:LEU:N	2.34	0.41
1:H:575:LYS:HD3	1:H:607:LEU:HD22	2.01	0.41
1:B:782:LEU:HD23	1:B:782:LEU:C	2.41	0.41
1:C:569:VAL:HG23	1:C:570:LEU:N	2.36	0.41
1:H:713:VAL:HG13	1:H:714:LEU:HD22	2.02	0.41
1:A:747:PRO:HA	1:A:855:TYR:CD1	2.55	0.41
1:F:742:LEU:CD2	1:F:857:VAL:HG21	2.47	0.41
1:H:728:ARG:NH2	1:H:732:GLU:OE2	2.54	0.41
1:A:808:VAL:HG22	1:A:813:PHE:CD1	2.56	0.41
1:F:704:LEU:HD11	1:F:716:TYR:CE1	2.55	0.41
1:B:647:LEU:C	1:B:647:LEU:HD23	2.40	0.41
1:G:636:THR:HG22	1:G:639:ILE:HG12	2.03	0.41
1:G:737:TYR:CE1	1:H:801:PRO:HD3	2.56	0.41
1:C:649:THR:HA	1:C:652:ILE:HG12	2.03	0.41
1:C:683:VAL:HG21	1:C:715:VAL:HG13	2.01	0.41
1:C:795:ILE:HD12	1:C:795:ILE:C	2.41	0.41
1:D:600:SER:O	1:D:632:LYS:HG2	2.21	0.41
1:D:602:MET:HG3	1:D:631:GLN:HE21	1.85	0.41
1:D:722:HIS:HA	1:D:792:LYS:NZ	2.36	0.41
1:F:726:LEU:O	1:F:729:VAL:HG12	2.21	0.41
1:G:617:LEU:HB3	1:G:652:ILE:HD12	2.03	0.41
1:H:684:ARG:HA	1:H:687:ILE:HG12	2.03	0.41
1:A:602:MET:HA	1:A:606:MET:SD	2.61	0.41
1:C:579:TYR:O	1:C:582:VAL:HG22	2.21	0.41
1:C:803:SER:O	1:C:840:LEU:HA	2.20	0.41
1:F:782:LEU:C	1:F:782:LEU:HD23	2.41	0.41
1:A:677:ARG:O	1:A:677:ARG:HG2	2.21	0.40
1:D:579:TYR:HA	1:D:616:LEU:HD21	2.04	0.40
1:E:669:THR:H	1:E:672:MET:HG3	1.86	0.40
1:E:749:PHE:CE1	1:E:854:ALA:HB3	2.55	0.40
1:H:728:ARG:HG3	1:H:729:VAL:N	2.36	0.40
1:H:782:LEU:HD12	1:H:827:PHE:CE1	2.56	0.40
1:F:590:GLU:HG2	1:F:592:TYR:CZ	2.56	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:799:CYS:HA	1:F:823:PHE:CE2	2.56	0.40
1:A:738:PHE:HD2	1:A:742:LEU:HD22	1.86	0.40
1:C:568:ASN:O	1:C:568:ASN:ND2	2.49	0.40
1:C:841:THR:HG22	1:C:842:GLU:N	2.35	0.40
1:E:836:LEU:CD2	1:E:838:ILE:HG13	2.51	0.40
1:F:574:VAL:HG21	1:F:604:LEU:HD22	2.03	0.40
1:G:784:ILE:CD1	1:G:804:VAL:HG21	2.51	0.40
1:A:800:GLY:O	1:A:823:PHE:HZ	2.03	0.40
1:F:616:LEU:O	1:F:620:LEU:HD13	2.21	0.40
1:C:790:LEU:HD13	1:D:790:LEU:C	2.41	0.40
1:C:836:LEU:HD21	1:C:838:ILE:HG13	2.03	0.40
1:F:635:THR:HG23	1:F:639:ILE:HB	2.04	0.40
1:F:837:PHE:CD1	1:F:838:ILE:N	2.89	0.40
1:G:738:PHE:HE2	1:G:742:LEU:HD13	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:F:677:ARG:NH1	1:H:577:GLY:O[4_445]	2.12	0.08	
1:F:677:ARG:HH11	1:H:577:GLY:O[4_445]	1.57	0.03	

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	Perce	ntiles
1	А	296/336~(88%)	289~(98%)	7 (2%)	0	100	100
1	В	292/336~(87%)	284 (97%)	8 (3%)	0	100	100
1	С	292/336~(87%)	283 (97%)	9 (3%)	0	100	100
1	D	296/336~(88%)	293 (99%)	3 (1%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	Ε	294/336~(88%)	289~(98%)	5(2%)	0	100	100
1	F	292/336~(87%)	287~(98%)	5(2%)	0	100	100
1	G	293/336~(87%)	286~(98%)	7 (2%)	0	100	100
1	Н	294/336~(88%)	286~(97%)	8~(3%)	0	100	100
All	All	2349/2688~(87%)	2297~(98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	Perce	ntiles
1	А	237/283~(84%)	237 (100%)	0	100	100
1	В	232/283~(82%)	231 (100%)	1 (0%)	89	94
1	С	228/283~(81%)	225~(99%)	3 (1%)	65	83
1	D	243/283~(86%)	243 (100%)	0	100	100
1	Ε	231/283~(82%)	228~(99%)	3 (1%)	65	83
1	F	234/283~(83%)	233 (100%)	1 (0%)	89	94
1	G	236/283~(83%)	235~(100%)	1 (0%)	89	94
1	Н	232/283~(82%)	230 (99%)	2 (1%)	75	88
All	All	1873/2264 (83%)	1862 (99%)	11 (1%)	84	92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	837	PHE
1	С	568	ASN
1	С	741	ARG
1	С	797	ARG
1	Е	716	TYR
1	Е	720	LYS



Continued from previous page...

Mol	Chain	Res	Type
1	Е	837	PHE
1	F	837	PHE
1	G	837	PHE
1	Н	602	MET
1	Н	712	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	А	628	ASN
1	D	631	GLN
1	Е	722	HIS
1	F	705	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	А	298/336~(88%)	0.35	12 (4%) 43 25	62, 113, 186, 237	0
1	В	294/336~(87%)	0.33	8 (2%) 56 35	95, 143, 210, 243	0
1	С	294/336~(87%)	0.65	24 (8%) 19 10	97, 143, 216, 268	0
1	D	298/336~(88%)	0.14	3 (1%) 79 61	61, 111, 183, 262	0
1	Е	296/336~(88%)	0.69	28 (9%) 15 8	87, 145, 206, 266	0
1	F	294/336~(87%)	0.59	16 (5%) 32 18	81, 130, 208, 255	0
1	G	295/336~(87%)	0.39	11 (3%) 45 27	98, 146, 232, 297	0
1	Н	296/336~(88%)	0.65	20 (6%) 25 14	110, 159, 223, 311	0
All	All	2365/2688~(87%)	0.47	122 (5%) 34 19	61, 138, 213, 311	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	621	ILE	5.7
1	F	860	GLN	4.6
1	Е	739	GLU	4.4
1	F	845	SER	4.4
1	С	860	GLN	4.4
1	Ε	795	ILE	4.4
1	Н	773	ASN	4.3
1	Н	716	TYR	4.1
1	G	820	ASP	4.0
1	F	737	TYR	4.0
1	F	773	ASN	3.9
1	Ε	740	ALA	3.9
1	С	819	LEU	3.8
1	В	574	VAL	3.7
1	Е	574	VAL	3.6
1	А	820	ASP	3.5



Mol	Chain	Res	Type	RSRZ
1	G	582	VAL	3.5
1	С	820	ASP	3.4
1	G	742	LEU	3.4
1	Е	782	LEU	3.4
1	G	738	PHE	3.4
1	G	744	LEU	3.3
1	Е	806	ALA	3.3
1	В	773	ASN	3.3
1	С	582	VAL	3.1
1	В	744	LEU	3.1
1	Н	683	VAL	3.0
1	С	586	LEU	3.0
1	В	579	TYR	2.9
1	Е	845	SER	2.9
1	Е	808	VAL	2.9
1	Е	844	PRO	2.9
1	Н	693	CYS	2.8
1	Е	803	SER	2.8
1	F	629	GLY	2.8
1	Е	819	LEU	2.8
1	G	734	ILE	2.8
1	С	806	ALA	2.8
1	Е	607	LEU	2.8
1	Н	781	LEU	2.8
1	Е	580	ILE	2.8
1	Е	699	HIS	2.7
1	G	772	GLN	2.7
1	Н	737	TYR	2.7
1	Н	806	ALA	2.7
1	Н	819	LEU	2.7
1	Н	855	TYR	2.7
1	С	739	GLU	2.7
1	С	803	SER	2.6
1	Н	691	ALA	2.6
1	Н	703	ALA	2.6
1	Е	773	ASN	2.6
1	Е	671	LEU	2.6
1	Е	793	GLU	2.6
1	С	574	VAL	2.5
1	F	582	VAL	2.5
1	F	844	PRO	2.5
1	D	689	CYS	2.5



Mol	Chain	Res	Type	RSRZ
1	Н	847	LYS	2.5
1	А	748	VAL	2.5
1	А	854	ALA	2.4
1	Е	820	ASP	2.4
1	В	819	LEU	2.4
1	А	836	LEU	2.4
1	С	845	SER	2.4
1	Н	774	ILE	2.4
1	С	773	ASN	2.4
1	Е	827	PHE	2.4
1	F	837	PHE	2.4
1	Е	700	GLN	2.4
1	А	580	ILE	2.3
1	А	827	PHE	2.3
1	С	570	LEU	2.3
1	Е	850	LEU	2.3
1	С	621	ILE	2.3
1	D	691	ALA	2.3
1	Н	808	VAL	2.3
1	G	859	LEU	2.3
1	С	762	PHE	2.3
1	С	810	ASN	2.3
1	G	794	VAL	2.3
1	А	859	LEU	2.3
1	С	604	LEU	2.3
1	А	789	PHE	2.3
1	С	688	GLU	2.3
1	Е	691	ALA	2.3
1	Н	807	VAL	2.3
1	С	742	LEU	2.3
1	С	794	VAL	2.2
1	С	808	VAL	2.2
1	G	615	ASP	2.2
1	D	709	GLN	2.2
1	В	857	VAL	2.2
1	Е	744	LEU	2.2
1	Н	749	PHE	2.2
1	Η	750	PRO	2.2
1	A	860	GLN	2.2
1	Е	742	LEU	2.2
1	F	604	LEU	2.2
1	Н	744	LEU	2.2



Mol	Chain	Res	Type	RSRZ
1	F	670	ALA	2.2
1	F	597	GLU	2.2
1	F	792	LYS	2.2
1	А	807	VAL	2.2
1	Е	781	LEU	2.2
1	Н	813	PHE	2.1
1	F	744	LEU	2.1
1	В	860	GLN	2.1
1	F	820	ASP	2.1
1	А	742	LEU	2.1
1	С	591	GLU	2.1
1	С	740	ALA	2.1
1	А	626	LYS	2.1
1	С	859	LEU	2.1
1	Н	650	VAL	2.1
1	С	797	ARG	2.0
1	F	599	SER	2.0
1	Е	705	HIS	2.0
1	В	792	LYS	2.0
1	Е	741	ARG	2.0
1	Е	743	ALA	2.0
1	G	776	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

