



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:33 pm BST

PDB ID : 3SV1
Title : Crystal structure of APP peptide bound rat Mint2 PARM
Authors : Shen, Y.; Long, J.; Yan, X.; Xie, X.
Deposited on : 2011-07-12
Resolution : 3.30 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 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	:	2.11
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)	:	2.11

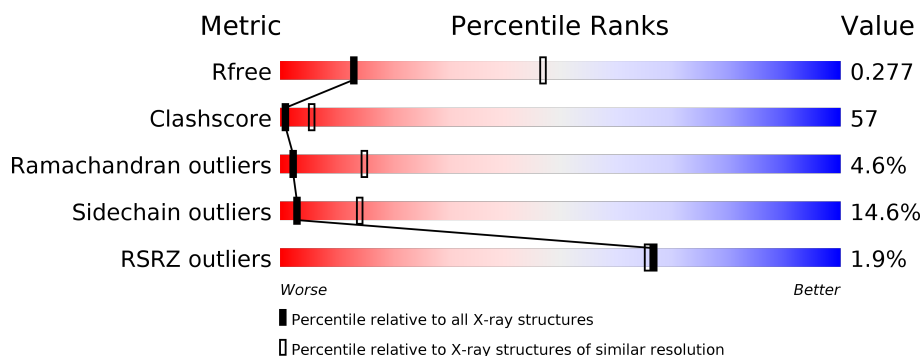
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	190	<div> <div>28%</div> <div>48%</div> <div>8%</div> <div>14%</div> </div>
1	B	190	<div>3%</div> <div>26%</div> <div>41%</div> <div>8%</div> <div>25%</div>
1	C	190	<div>2%</div> <div>24%</div> <div>45%</div> <div>10%</div> <div>21%</div>
2	D	14	<div>7%</div> <div>14%</div> <div>71%</div> <div>7%</div> <div>7%</div>
2	E	14	<div>43%</div> <div>36%</div> <div>21%</div>
2	F	14	<div>7%</div> <div>14%</div> <div>79%</div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3732 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 Amyloid beta A4 precursor protein-binding family A member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1236	769	214	245	8			
1	B	143	Total	C	N	O	S	0	0	0
			1094	684	192	210	8			
1	C	150	Total	C	N	O	S	0	0	0
			1130	705	199	218	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	363	GLY	-	EXPRESSION TAG	UNP O35431
A	364	SER	-	EXPRESSION TAG	UNP O35431
B	363	GLY	-	EXPRESSION TAG	UNP O35431
B	364	SER	-	EXPRESSION TAG	UNP O35431
C	363	GLY	-	EXPRESSION TAG	UNP O35431
C	364	SER	-	EXPRESSION TAG	UNP O35431

- Molecule 2 is a protein called Amyloid beta A4 protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	14	Total	C	N	O	0	0	0
			126	81	19	26			
2	E	11	Total	C	N	O	0	0	0
			87	60	12	15			
2	F	3	Total	C	N	O	0	0	0
			14	8	3	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		

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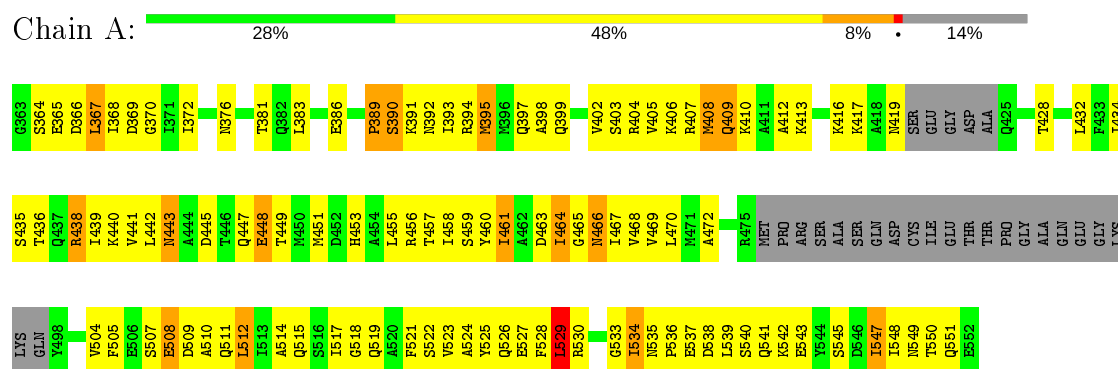
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	17	Total	O	0	0
			17	17		
3	C	10	Total	O	0	0
			10	10		

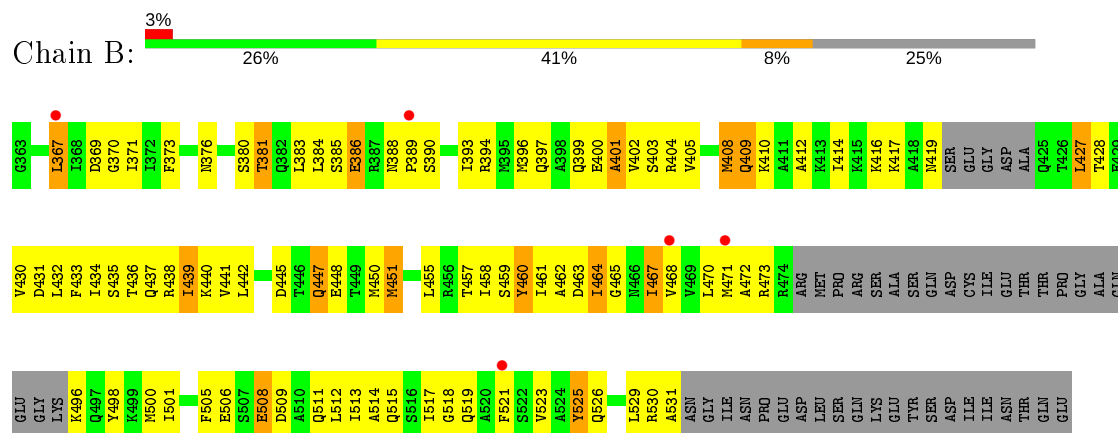
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

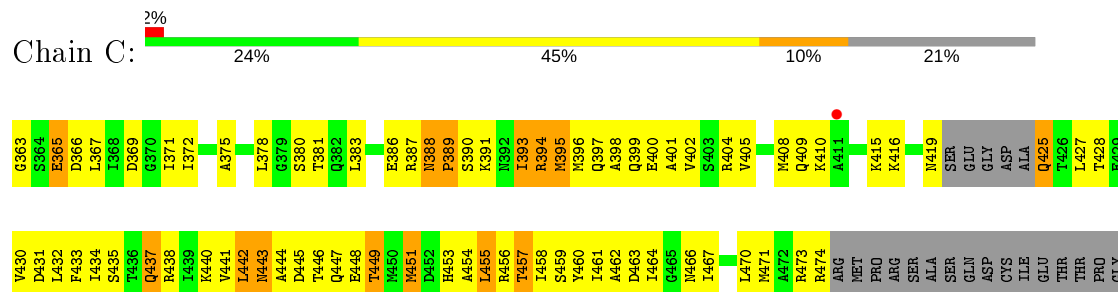
- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 2

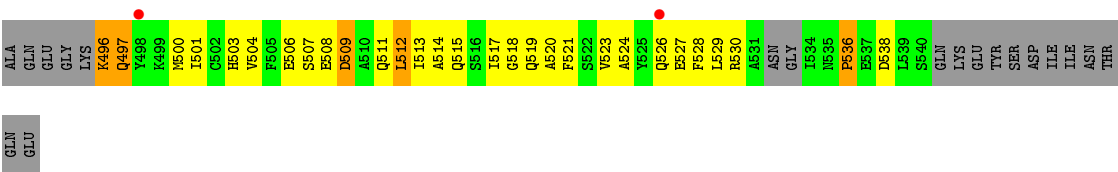


- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 2



- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 2





• Molecule 2: Amyloid beta A4 protein



• Molecule 2: Amyloid beta A4 protein



• Molecule 2: Amyloid beta A4 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.12Å 52.09Å 121.28Å 90.00° 127.80° 90.00°	Depositor
Resolution (Å)	40.70 – 3.30 40.70 – 3.28	Depositor EDS
% Data completeness (in resolution range)	94.5 (40.70-3.30) 99.6 (40.70-3.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 3.25Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.243 , 0.301 0.251 , 0.277	Depositor DCC
R_{free} test set	555 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	102.5	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 128.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3732	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/1246	0.69	1/1677 (0.1%)
1	B	0.38	0/1102	0.66	0/1481
1	C	0.40	0/1136	0.65	1/1525 (0.1%)
2	D	0.48	0/130	0.53	0/173
2	E	0.45	0/91	0.52	0/124
2	F	0.83	0/13	0.69	0/16
All	All	0.40	0/3718	0.66	2/4996 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	536	PRO	N-CA-CB	5.63	110.05	103.30
1	A	529	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1236	0	1198	157	0
1	B	1094	0	1090	124	0
1	C	1130	0	1117	128	0
2	D	126	0	105	24	0
2	E	87	0	64	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	14	0	6	2	0
3	A	18	0	0	1	0
3	B	17	0	0	3	0
3	C	10	0	0	0	0
All	All	3732	0	3580	412	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 57.

All (412) 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:A:464:ILE:HG22	2:D:754:GLN:HA	1.45	0.97
1:C:512:LEU:HD22	1:C:512:LEU:H	1.31	0.93
1:A:536:PRO:HA	1:A:539:LEU:HG	1.49	0.93
1:C:529:LEU:HG	1:C:530:ARG:H	1.31	0.91
1:C:496:LYS:HD3	1:C:497:GLN:H	1.36	0.89
1:B:440:LYS:HE3	1:B:442:LEU:HD21	1.56	0.88
1:B:512:LEU:HD22	1:B:512:LEU:H	1.39	0.86
1:B:438:ARG:HD3	1:B:440:LYS:HG3	1.58	0.85
1:B:509:ASP:O	1:B:513:ILE:HG13	1.76	0.84
1:A:394:ARG:HE	2:D:763:LYS:NZ	1.75	0.83
1:A:512:LEU:HD22	1:A:512:LEU:H	1.42	0.82
1:A:526:GLN:O	1:A:529:LEU:HB3	1.81	0.80
1:A:410:LYS:NZ	1:B:369:ASP:HB3	1.97	0.80
2:D:762:TYR:O	2:D:764:PHE:N	2.15	0.80
1:A:527:GLU:C	1:A:529:LEU:H	1.84	0.79
1:B:389:PRO:HB2	1:B:393:ILE:HG21	1.65	0.79
1:C:443:ASN:HD22	1:C:444:ALA:N	1.79	0.78
1:A:522:SER:HA	1:A:525:TYR:HB3	1.66	0.78
1:A:394:ARG:HE	2:D:763:LYS:HZ1	1.29	0.77
1:C:518:GLY:HA2	1:C:521:PHE:HD2	1.49	0.77
2:D:762:TYR:C	2:D:764:PHE:H	1.86	0.77
1:B:367:LEU:HD22	1:B:367:LEU:H	1.50	0.76
1:A:461:ILE:HG21	1:A:517:ILE:HG21	1.68	0.76
1:A:408:MET:HB2	3:B:34:HOH:O	1.85	0.75
1:A:438:ARG:NH2	1:A:438:ARG:HB3	2.02	0.75
1:C:513:ILE:O	1:C:517:ILE:HG13	1.85	0.75
1:C:518:GLY:HA2	1:C:521:PHE:CD2	2.22	0.74
1:C:442:LEU:H	1:C:442:LEU:HD12	1.52	0.74
1:A:381:THR:OG1	1:A:404:ARG:HG2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:VAL:HG12	1:A:469:VAL:HG21	1.70	0.74
1:A:543:GLU:O	1:A:547:ILE:HB	1.86	0.74
1:C:509:ASP:O	1:C:513:ILE:HG13	1.88	0.74
1:A:519:GLN:O	1:A:523:VAL:HG23	1.89	0.73
1:A:441:VAL:C	1:A:442:LEU:HD12	2.09	0.72
1:C:443:ASN:ND2	1:C:445:ASP:H	1.87	0.72
2:D:762:TYR:CZ	2:D:766:GLU:HG2	2.23	0.72
1:A:399:GLN:O	1:A:402:VAL:HG22	1.89	0.72
1:B:459:SER:O	1:B:460:TYR:HB2	1.88	0.72
1:A:536:PRO:HB3	1:A:539:LEU:HB2	1.69	0.72
1:A:542:LYS:O	1:A:542:LYS:HD3	1.90	0.71
1:A:372:ILE:HA	1:A:432:LEU:O	1.91	0.71
1:A:365:GLU:O	1:A:368:ILE:HG13	1.91	0.70
1:C:388:ASN:HD22	1:C:388:ASN:N	1.89	0.70
1:B:470:LEU:HD23	1:B:471:MET:N	2.05	0.70
1:B:389:PRO:HB2	1:B:393:ILE:CG2	2.22	0.70
1:A:405:VAL:HA	1:A:408:MET:HG2	1.73	0.70
1:C:391:LYS:HA	1:C:394:ARG:HB2	1.74	0.70
1:C:529:LEU:CG	1:C:530:ARG:H	2.02	0.69
1:B:460:TYR:HA	2:E:757:TYR:O	1.93	0.69
1:B:410:LYS:HB2	1:C:371:ILE:HG22	1.75	0.69
1:C:454:ALA:O	1:C:457:THR:HG23	1.93	0.69
1:C:394:ARG:HA	1:C:397:GLN:OE1	1.93	0.68
1:C:473:ARG:HA	1:C:500:MET:SD	2.33	0.68
1:B:402:VAL:HG13	1:B:403:SER:N	2.09	0.68
1:C:470:LEU:HD21	1:C:503:HIS:HB2	1.75	0.68
1:B:427:LEU:HD23	1:B:427:LEU:H	1.57	0.68
1:C:372:ILE:CG2	1:C:431:ASP:HB3	2.24	0.68
1:B:512:LEU:HD22	1:B:512:LEU:N	2.09	0.68
1:A:467:ILE:HD12	1:A:467:ILE:N	2.09	0.67
1:C:427:LEU:HD12	1:C:427:LEU:O	1.94	0.67
1:B:512:LEU:CD2	1:B:512:LEU:H	2.06	0.67
1:C:395:MET:SD	1:C:396:MET:N	2.67	0.67
1:C:470:LEU:CD2	1:C:503:HIS:HB2	2.24	0.66
1:B:461:ILE:HG21	1:B:517:ILE:HG21	1.77	0.66
1:C:380:SER:HG	1:C:503:HIS:HD1	1.40	0.66
1:A:405:VAL:HG11	1:A:504:VAL:HG21	1.78	0.66
1:A:410:LYS:HZ3	1:B:369:ASP:HB3	1.58	0.66
1:B:461:ILE:HD11	2:E:757:TYR:CD2	2.31	0.66
1:A:518:GLY:O	1:A:521:PHE:HB2	1.96	0.66
1:B:530:ARG:HH11	1:B:530:ARG:HG3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:SER:HA	1:A:406:LYS:HE3	1.77	0.65
1:C:453:HIS:HB3	1:C:458:ILE:HD11	1.79	0.65
1:C:458:ILE:HD12	1:C:458:ILE:N	2.13	0.64
1:C:437:GLN:H	1:C:437:GLN:NE2	1.94	0.64
1:A:381:THR:CB	1:A:404:ARG:HG2	2.28	0.63
1:B:462:ALA:HB1	1:B:464:ILE:HG23	1.80	0.63
1:C:463:ASP:HB2	1:C:511:GLN:NE2	2.13	0.63
1:A:535:ASN:HB2	1:A:536:PRO:HD3	1.80	0.63
1:C:390:SER:HB3	1:C:393:ILE:HG23	1.81	0.63
1:C:460:TYR:HB3	1:C:471:MET:HG2	1.79	0.63
1:A:530:ARG:HG3	1:A:535:ASN:HA	1.79	0.63
1:A:536:PRO:O	1:A:540:SER:N	2.28	0.63
1:C:529:LEU:HG	1:C:530:ARG:N	2.09	0.63
1:B:463:ASP:HB3	1:B:514:ALA:CB	2.28	0.63
1:A:394:ARG:HG2	1:A:397:GLN:OE1	1.99	0.62
1:A:512:LEU:CD2	1:A:512:LEU:H	2.11	0.62
1:A:527:GLU:O	1:A:529:LEU:N	2.28	0.62
1:A:402:VAL:O	1:A:406:LYS:HG3	1.99	0.62
1:C:471:MET:HA	1:C:501:ILE:O	2.00	0.62
1:B:473:ARG:HA	1:B:500:MET:SD	2.40	0.61
1:B:394:ARG:HD3	1:B:397:GLN:OE1	2.00	0.61
1:B:463:ASP:HB3	1:B:514:ALA:HB3	1.83	0.61
1:A:368:ILE:HA	1:A:436:THR:HG23	1.82	0.60
1:C:453:HIS:CB	1:C:458:ILE:HD11	2.30	0.60
1:B:525:TYR:CE2	1:B:529:LEU:HD21	2.36	0.60
1:B:526:GLN:O	1:B:530:ARG:HG2	2.02	0.60
1:A:367:LEU:CD2	1:A:367:LEU:H	2.14	0.60
1:C:496:LYS:O	1:C:497:GLN:HB2	2.01	0.60
1:B:381:THR:OG1	1:B:404:ARG:HG2	2.02	0.60
1:C:509:ASP:CB	1:C:512:LEU:HD23	2.32	0.60
1:C:496:LYS:HD3	1:C:497:GLN:N	2.13	0.59
1:B:370:GLY:HA3	1:B:433:PHE:CE1	2.37	0.59
1:C:527:GLU:HG2	1:C:527:GLU:O	2.03	0.59
1:B:511:GLN:HG3	1:B:515:GLN:HE21	1.67	0.59
1:C:512:LEU:HD22	1:C:512:LEU:N	2.11	0.59
1:A:536:PRO:HB3	1:A:539:LEU:HD12	1.85	0.59
1:B:416:LYS:O	1:B:419:ASN:HB3	2.03	0.59
1:B:438:ARG:CD	1:B:440:LYS:HG3	2.32	0.59
1:A:392:ASN:O	1:A:395:MET:HG3	2.03	0.58
1:A:466:ASN:N	1:A:467:ILE:HD12	2.19	0.58
1:A:536:PRO:HG2	3:A:45:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ILE:H	1:B:458:ILE:HD12	1.67	0.58
1:B:381:THR:CB	1:B:404:ARG:HG2	2.33	0.58
1:C:393:ILE:HD12	1:C:393:ILE:O	2.02	0.58
1:C:378:LEU:HD13	1:C:504:VAL:HG12	1.85	0.58
1:C:375:ALA:CB	1:C:507:SER:HB2	2.34	0.58
2:D:762:TYR:C	2:D:764:PHE:N	2.56	0.58
1:B:370:GLY:HA3	1:B:433:PHE:HE1	1.68	0.58
1:C:443:ASN:ND2	1:C:444:ALA:N	2.49	0.58
1:C:437:GLN:NE2	1:C:437:GLN:N	2.52	0.58
1:B:400:GLU:O	1:B:403:SER:N	2.37	0.58
1:B:427:LEU:H	1:B:427:LEU:CD2	2.15	0.58
1:B:464:ILE:HD12	1:B:465:GLY:N	2.18	0.57
1:C:430:VAL:HA	1:C:444:ALA:H	1.68	0.57
1:C:430:VAL:HG12	1:C:443:ASN:HA	1.86	0.57
1:A:405:VAL:O	1:A:408:MET:HG2	2.04	0.57
1:A:464:ILE:HG12	1:A:464:ILE:O	2.05	0.57
1:A:527:GLU:C	1:A:529:LEU:N	2.53	0.57
1:A:530:ARG:HB2	1:A:537:GLU:OE1	2.04	0.57
1:A:441:VAL:O	1:A:442:LEU:HD12	2.04	0.57
1:A:525:TYR:CD1	2:D:760:PRO:HB2	2.40	0.57
1:A:463:ASP:HB3	1:A:514:ALA:HB2	1.85	0.57
1:C:416:LYS:O	1:C:419:ASN:HB3	2.03	0.57
1:B:448:GLU:OE2	1:B:448:GLU:HA	2.05	0.56
1:B:463:ASP:HB2	1:B:511:GLN:NE2	2.20	0.56
1:C:388:ASN:ND2	1:C:388:ASN:N	2.48	0.56
1:C:464:ILE:O	1:C:464:ILE:HG13	2.05	0.56
1:C:386:GLU:OE2	1:C:386:GLU:N	2.38	0.56
2:D:762:TYR:CE1	2:D:767:GLN:HG3	2.41	0.56
1:A:511:GLN:HB3	1:A:512:LEU:HD22	1.86	0.56
1:C:443:ASN:ND2	1:C:443:ASN:C	2.58	0.56
1:A:527:GLU:OE2	1:A:527:GLU:HA	2.04	0.56
1:C:459:SER:HA	2:F:757:TYR:CB	2.37	0.55
1:A:455:LEU:HD23	1:A:524:ALA:CB	2.36	0.55
1:B:390:SER:O	1:B:393:ILE:HG22	2.06	0.55
1:B:467:ILE:HG23	1:B:468:VAL:N	2.21	0.55
1:A:390:SER:HB3	1:A:393:ILE:HG22	1.89	0.55
1:A:512:LEU:HD22	1:A:512:LEU:N	2.19	0.55
1:C:455:LEU:HA	1:C:458:ILE:HD13	1.89	0.55
1:B:410:LYS:NZ	1:C:366:ASP:HA	2.22	0.55
1:C:518:GLY:O	1:C:521:PHE:HB2	2.06	0.55
1:A:442:LEU:HG	1:A:449:THR:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:VAL:CA	1:A:408:MET:HG2	2.37	0.54
1:A:549:ASN:C	1:A:551:GLN:H	2.11	0.54
1:A:507:SER:C	1:A:509:ASP:H	2.10	0.54
1:A:370:GLY:HA2	1:A:434:ILE:O	2.07	0.54
1:A:461:ILE:HG22	1:A:470:LEU:HB2	1.89	0.54
1:B:461:ILE:HG12	2:E:757:TYR:HB2	1.88	0.54
1:C:446:THR:O	1:C:447:GLN:HB2	2.08	0.54
1:C:471:MET:CE	1:C:500:MET:HG3	2.38	0.54
1:A:535:ASN:N	1:A:536:PRO:CD	2.70	0.54
1:A:403:SER:HB3	1:A:407:ARG:NH1	2.23	0.54
1:B:381:THR:C	1:B:501:ILE:HD12	2.28	0.54
1:B:462:ALA:HB1	1:B:464:ILE:CG2	2.38	0.54
1:B:509:ASP:HA	1:B:512:LEU:HD23	1.90	0.54
1:B:511:GLN:HE21	1:B:511:GLN:HA	1.72	0.53
1:A:381:THR:HB	1:A:404:ARG:HG2	1.89	0.53
2:E:758:GLU:O	2:E:760:PRO:HD3	2.08	0.53
1:A:438:ARG:HB3	1:A:438:ARG:CZ	2.39	0.53
1:A:461:ILE:HD11	2:D:757:TYR:HD2	1.74	0.53
1:B:511:GLN:NE2	1:B:511:GLN:HA	2.23	0.53
1:C:431:ASP:HB2	1:C:442:LEU:HD13	1.89	0.53
1:A:534:ILE:O	1:A:537:GLU:N	2.42	0.53
1:B:467:ILE:HG13	1:B:505:PHE:O	2.08	0.53
1:A:367:LEU:HD23	1:A:367:LEU:H	1.73	0.53
1:B:386:GLU:OE1	1:B:386:GLU:N	2.41	0.53
1:B:436:THR:HG21	1:B:523:VAL:HB	1.91	0.53
1:C:383:LEU:HD12	1:C:383:LEU:C	2.29	0.53
2:D:760:PRO:O	2:D:764:PHE:HB2	2.10	0.53
1:B:496:LYS:O	1:B:498:TYR:HD1	1.90	0.52
1:A:409:GLN:O	1:A:412:ALA:HB3	2.09	0.52
1:C:380:SER:HB3	1:C:501:ILE:HD11	1.91	0.52
1:B:381:THR:HB	1:B:404:ARG:HG2	1.90	0.52
1:A:394:ARG:NH1	1:A:397:GLN:OE1	2.42	0.52
1:A:525:TYR:O	1:A:529:LEU:HB2	2.09	0.52
1:C:463:ASP:CG	1:C:511:GLN:HE22	2.13	0.52
1:C:512:LEU:CD2	1:C:512:LEU:H	2.09	0.52
1:C:458:ILE:HD12	1:C:458:ILE:H	1.75	0.52
1:B:436:THR:CG2	1:B:523:VAL:HB	2.40	0.52
1:B:458:ILE:HA	1:B:472:ALA:HB2	1.92	0.52
1:C:461:ILE:O	1:C:461:ILE:HD12	2.10	0.52
1:B:402:VAL:CG1	1:B:403:SER:N	2.72	0.51
1:C:443:ASN:HD22	1:C:443:ASN:C	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ARG:HB2	2:D:765:PHE:HE2	1.75	0.51
1:A:511:GLN:O	1:A:515:GLN:HG3	2.10	0.51
1:C:441:VAL:HB	1:C:451:MET:HB2	1.91	0.51
1:C:511:GLN:O	1:C:515:GLN:HG3	2.10	0.51
1:C:529:LEU:CG	1:C:530:ARG:N	2.72	0.51
1:C:433:PHE:HB3	1:C:440:LYS:HB2	1.93	0.51
1:B:408:MET:SD	1:B:409:GLN:HG2	2.51	0.51
1:C:427:LEU:C	1:C:427:LEU:HD12	2.31	0.51
1:C:430:VAL:HA	1:C:444:ALA:N	2.26	0.51
1:A:390:SER:C	1:A:392:ASN:H	2.12	0.51
1:A:439:ILE:HB	1:A:458:ILE:HD11	1.93	0.51
1:C:466:ASN:O	1:C:506:GLU:HA	2.10	0.51
1:A:410:LYS:HZ1	1:B:369:ASP:HB3	1.76	0.51
1:A:438:ARG:HB2	1:A:453:HIS:O	2.11	0.51
1:C:509:ASP:HB2	1:C:512:LEU:HD23	1.91	0.51
1:B:441:VAL:O	1:B:441:VAL:HG12	2.10	0.50
1:B:459:SER:O	1:B:460:TYR:CB	2.58	0.50
1:C:383:LEU:HD12	1:C:383:LEU:O	2.11	0.50
1:A:466:ASN:N	1:A:466:ASN:HD22	2.07	0.50
1:A:533:GLY:C	1:A:535:ASN:H	2.14	0.50
1:B:441:VAL:HB	1:B:451:MET:HB2	1.93	0.50
1:B:414:ILE:O	1:B:417:LYS:HB3	2.11	0.50
1:C:448:GLU:OE1	1:C:449:THR:N	2.42	0.50
1:B:408:MET:CG	3:B:40:HOH:O	2.58	0.50
1:C:460:TYR:HE1	1:C:462:ALA:HB2	1.76	0.50
1:C:375:ALA:HB1	1:C:506:GLU:O	2.11	0.50
1:A:455:LEU:HD12	1:A:458:ILE:HD12	1.94	0.50
1:B:461:ILE:HG21	1:B:517:ILE:CG2	2.41	0.50
1:C:521:PHE:O	1:C:524:ALA:HB3	2.11	0.50
1:C:431:ASP:HB2	1:C:442:LEU:CD1	2.42	0.50
2:E:761:THR:C	2:E:763:LYS:H	2.13	0.50
1:A:368:ILE:HD12	1:A:369:ASP:N	2.26	0.49
2:D:762:TYR:CE1	2:D:766:GLU:HG2	2.46	0.49
1:B:473:ARG:CA	1:B:500:MET:SD	3.01	0.49
1:B:402:VAL:HG13	1:B:403:SER:H	1.74	0.49
1:C:372:ILE:HG21	1:C:431:ASP:HB3	1.94	0.49
1:A:536:PRO:CA	1:A:539:LEU:HG	2.34	0.49
1:A:541:GLN:C	1:A:543:GLU:H	2.15	0.49
1:A:547:ILE:O	1:A:547:ILE:HG23	2.12	0.49
1:A:390:SER:O	1:A:392:ASN:N	2.45	0.49
1:B:433:PHE:O	1:B:439:ILE:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:PRO:HB3	1:A:539:LEU:CB	2.42	0.49
1:B:410:LYS:HZ1	1:C:366:ASP:HA	1.78	0.49
1:C:375:ALA:HB2	1:C:507:SER:HB2	1.95	0.49
1:A:438:ARG:HA	1:A:455:LEU:H	1.78	0.49
1:A:525:TYR:CG	2:D:760:PRO:HB2	2.47	0.49
1:B:457:THR:OG1	1:B:458:ILE:HD12	2.13	0.49
1:B:511:GLN:HB3	1:B:512:LEU:HD22	1.95	0.49
1:A:466:ASN:C	1:A:467:ILE:HD12	2.33	0.48
1:C:449:THR:HG22	1:C:451:MET:O	2.13	0.48
1:C:383:LEU:CD1	1:C:500:MET:HB2	2.43	0.48
1:A:440:LYS:HG3	1:A:442:LEU:CD1	2.42	0.48
1:A:545:SER:C	1:A:547:ILE:H	2.16	0.48
1:B:402:VAL:CG1	1:B:403:SER:H	2.27	0.48
1:B:515:GLN:O	1:B:518:GLY:N	2.45	0.48
1:C:409:GLN:O	1:C:410:LYS:C	2.51	0.48
1:B:410:LYS:CB	1:C:371:ILE:HG22	2.40	0.48
1:C:375:ALA:HB1	1:C:507:SER:HB2	1.95	0.48
1:A:549:ASN:OD1	1:A:550:THR:N	2.47	0.48
1:C:467:ILE:N	1:C:467:ILE:HD12	2.28	0.48
1:A:435:SER:O	1:A:455:LEU:HD22	2.14	0.48
1:A:509:ASP:O	1:A:510:ALA:C	2.51	0.48
1:A:537:GLU:HG3	1:A:538:ASP:N	2.28	0.48
1:B:367:LEU:CD2	1:B:367:LEU:H	2.22	0.48
1:B:508:GLU:CD	1:B:508:GLU:N	2.67	0.48
2:D:764:PHE:CD2	2:D:765:PHE:N	2.81	0.48
1:B:390:SER:O	1:B:393:ILE:CG2	2.62	0.48
1:A:439:ILE:HB	1:A:458:ILE:CD1	2.44	0.48
1:C:443:ASN:HD22	1:C:444:ALA:H	1.61	0.48
1:A:394:ARG:HA	1:A:397:GLN:HG2	1.96	0.47
1:C:453:HIS:HB3	1:C:458:ILE:CD1	2.44	0.47
1:A:534:ILE:C	1:A:536:PRO:N	2.63	0.47
1:B:431:ASP:O	1:B:432:LEU:HD23	2.14	0.47
1:B:436:THR:HG21	1:B:523:VAL:CG1	2.45	0.47
1:A:389:PRO:O	1:A:390:SER:HB2	2.14	0.47
1:A:398:ALA:O	1:A:402:VAL:HG13	2.14	0.47
1:B:464:ILE:HD12	1:B:464:ILE:C	2.35	0.47
2:D:762:TYR:HE1	2:D:767:GLN:HG3	1.77	0.47
1:A:394:ARG:NH1	1:A:394:ARG:HG2	2.30	0.47
1:B:438:ARG:HH21	1:B:438:ARG:HG2	1.79	0.47
1:A:390:SER:C	1:A:392:ASN:N	2.68	0.47
1:A:464:ILE:CG1	1:A:464:ILE:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:GLN:O	1:B:402:VAL:HG12	2.15	0.47
1:C:405:VAL:HG21	1:C:504:VAL:CG2	2.45	0.47
1:A:405:VAL:CG1	1:A:504:VAL:HG21	2.44	0.47
1:C:381:THR:OG1	1:C:404:ARG:HG2	2.15	0.47
1:B:530:ARG:NH1	1:B:530:ARG:HG3	2.28	0.47
1:C:454:ALA:O	1:C:456:ARG:N	2.48	0.47
1:A:466:ASN:HA	1:A:510:ALA:CB	2.45	0.47
1:B:371:ILE:HD12	1:B:373:PHE:HE2	1.80	0.47
1:B:409:GLN:O	1:B:412:ALA:HB3	2.14	0.47
1:C:526:GLN:C	1:C:528:PHE:H	2.19	0.47
1:B:394:ARG:NH1	1:B:459:SER:O	2.42	0.46
1:A:394:ARG:HG2	1:A:394:ARG:HH11	1.80	0.46
1:A:539:LEU:N	1:A:539:LEU:HD23	2.29	0.46
1:B:458:ILE:HD12	1:B:458:ILE:N	2.30	0.46
1:B:393:ILE:HA	1:B:396:MET:HB3	1.97	0.46
1:C:398:ALA:O	1:C:401:ALA:HB3	2.15	0.46
1:C:399:GLN:O	1:C:402:VAL:HG22	2.15	0.46
1:B:438:ARG:HA	1:B:455:LEU:N	2.29	0.46
1:C:380:SER:O	1:C:405:VAL:HG22	2.16	0.46
1:C:383:LEU:HD12	1:C:500:MET:HB2	1.96	0.46
2:F:757:TYR:O	2:F:758:GLU:C	2.53	0.46
1:B:371:ILE:HD12	1:B:373:PHE:CE2	2.51	0.46
1:A:394:ARG:NE	2:D:763:LYS:NZ	2.56	0.46
1:A:459:SER:HB3	2:D:762:TYR:CD2	2.50	0.46
1:A:383:LEU:HD12	1:A:383:LEU:C	2.36	0.46
1:A:410:LYS:NZ	1:B:369:ASP:OD2	2.49	0.46
1:B:529:LEU:C	1:B:531:ALA:H	2.19	0.46
1:A:417:LYS:C	1:A:419:ASN:H	2.20	0.45
1:B:384:LEU:HG	1:C:446:THR:HB	1.98	0.45
2:D:765:PHE:CG	2:D:766:GLU:N	2.84	0.45
1:A:470:LEU:HD23	1:A:470:LEU:H	1.80	0.45
1:B:438:ARG:O	1:B:439:ILE:HG13	2.17	0.45
1:C:463:ASP:HB3	1:C:514:ALA:HB3	1.99	0.45
1:B:381:THR:CG2	1:B:401:ALA:HB1	2.47	0.45
1:C:454:ALA:HB3	1:C:457:THR:HG23	1.97	0.45
1:A:522:SER:O	1:A:526:GLN:N	2.30	0.45
1:B:380:SER:O	1:B:381:THR:HB	2.17	0.45
1:B:439:ILE:HG22	1:B:439:ILE:O	2.16	0.45
1:C:432:LEU:HD13	1:C:441:VAL:HG22	1.97	0.45
1:A:392:ASN:O	1:A:395:MET:SD	2.74	0.45
1:A:460:TYR:CZ	2:D:756:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ILE:HD13	1:B:517:ILE:CD1	2.47	0.45
1:B:470:LEU:C	1:B:470:LEU:HD23	2.37	0.45
1:B:518:GLY:O	1:B:521:PHE:HB2	2.17	0.45
1:A:443:ASN:HB2	1:A:448:GLU:H	1.82	0.44
1:A:466:ASN:ND2	1:A:466:ASN:H	2.15	0.44
1:B:435:SER:HB2	1:B:437:GLN:OE1	2.16	0.44
1:C:386:GLU:CD	1:C:386:GLU:N	2.71	0.44
1:C:459:SER:O	1:C:460:TYR:HB2	2.17	0.44
1:B:396:MET:SD	1:B:396:MET:C	2.95	0.44
1:B:376:ASN:HB2	1:B:506:GLU:HB3	1.99	0.44
1:A:438:ARG:HB3	1:A:438:ARG:HH21	1.76	0.44
1:B:380:SER:O	1:B:405:VAL:CG2	2.66	0.44
1:A:534:ILE:O	1:A:535:ASN:C	2.56	0.44
1:B:410:LYS:HE2	1:C:366:ASP:HB3	2.00	0.44
1:B:432:LEU:CD2	1:B:441:VAL:HG22	2.47	0.44
1:A:460:TYR:HA	2:D:757:TYR:O	2.18	0.44
1:C:463:ASP:HB2	1:C:511:GLN:HA	2.00	0.44
1:C:425:GLN:OE1	1:C:425:GLN:N	2.50	0.44
1:A:465:GLY:C	1:A:467:ILE:HD12	2.38	0.44
1:A:466:ASN:N	1:A:466:ASN:ND2	2.65	0.44
1:C:466:ASN:C	1:C:467:ILE:HD12	2.37	0.44
1:A:368:ILE:C	1:A:368:ILE:HD12	2.38	0.44
1:A:440:LYS:HG3	1:A:442:LEU:HD11	1.98	0.44
1:A:455:LEU:HD23	1:A:524:ALA:HB2	2.00	0.44
1:A:409:GLN:O	1:A:412:ALA:N	2.51	0.44
1:C:397:GLN:O	1:C:401:ALA:HB2	2.18	0.44
1:C:367:LEU:HD22	1:C:367:LEU:N	2.33	0.43
1:A:456:ARG:HB2	2:D:765:PHE:CE2	2.52	0.43
1:A:441:VAL:HB	1:A:451:MET:HG2	2.01	0.43
1:B:380:SER:HB3	1:B:501:ILE:HD11	1.99	0.43
1:C:408:MET:CE	1:C:409:GLN:HE21	2.31	0.43
1:A:521:PHE:CZ	2:D:759:ASN:HB2	2.53	0.43
1:A:443:ASN:HB3	1:A:447:GLN:H	1.83	0.43
1:B:430:VAL:HG11	1:B:450:MET:CE	2.49	0.43
1:A:461:ILE:HG22	1:A:470:LEU:CB	2.49	0.43
1:B:455:LEU:HD11	1:B:521:PHE:CE1	2.53	0.43
1:A:368:ILE:HG22	1:A:436:THR:HG21	2.01	0.43
1:A:507:SER:C	1:A:509:ASP:N	2.72	0.43
1:A:405:VAL:HG11	1:A:504:VAL:CG2	2.47	0.43
1:A:409:GLN:O	1:A:413:LYS:HG2	2.19	0.43
1:B:381:THR:O	1:B:501:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:ILE:O	1:B:501:ILE:HG23	2.19	0.43
1:C:434:ILE:HG22	1:C:435:SER:N	2.34	0.43
1:C:458:ILE:CD1	1:C:458:ILE:N	2.82	0.43
1:C:511:GLN:NE2	1:C:511:GLN:HA	2.34	0.43
1:A:441:VAL:HG21	1:A:505:PHE:CZ	2.54	0.42
1:C:415:LYS:HE3	1:C:415:LYS:HB2	1.67	0.42
1:A:439:ILE:HD12	1:A:458:ILE:HD13	1.99	0.42
1:A:536:PRO:O	1:A:540:SER:HB2	2.18	0.42
1:A:537:GLU:CG	1:A:538:ASP:N	2.82	0.42
1:B:448:GLU:OE2	1:B:448:GLU:CA	2.67	0.42
1:B:385:SER:O	1:B:498:TYR:HB2	2.18	0.42
1:B:437:GLN:NE2	3:B:17:HOH:O	2.52	0.42
1:C:396:MET:C	1:C:396:MET:SD	2.97	0.42
1:C:470:LEU:HD23	1:C:503:HIS:HB2	1.98	0.42
1:A:368:ILE:HA	1:A:436:THR:CG2	2.48	0.42
1:A:367:LEU:HD23	1:A:367:LEU:N	2.33	0.42
1:A:464:ILE:O	1:A:467:ILE:HD13	2.20	0.42
1:A:416:LYS:O	1:A:419:ASN:HB3	2.20	0.42
1:C:473:ARG:O	1:C:474:ARG:C	2.58	0.42
1:A:457:THR:O	1:A:472:ALA:HB1	2.20	0.42
1:B:394:ARG:HG3	1:B:394:ARG:HH11	1.84	0.42
1:A:438:ARG:HA	1:A:455:LEU:N	2.35	0.42
1:A:540:SER:HA	1:A:543:GLU:HB3	2.02	0.42
1:B:431:ASP:OD2	1:B:447:GLN:NE2	2.53	0.42
1:C:461:ILE:HG21	1:C:517:ILE:HG21	2.02	0.42
1:A:402:VAL:CG1	1:A:469:VAL:HG21	2.43	0.41
1:A:508:GLU:OE1	1:A:508:GLU:N	2.53	0.41
1:A:521:PHE:O	1:A:525:TYR:HB2	2.20	0.41
1:B:471:MET:HG3	1:B:471:MET:O	2.19	0.41
1:B:434:ILE:HD13	1:B:517:ILE:HG13	2.03	0.41
1:C:453:HIS:HB2	1:C:458:ILE:HD11	2.00	0.41
1:A:381:THR:O	1:A:381:THR:HG23	2.20	0.41
1:A:394:ARG:HA	1:A:397:GLN:OE1	2.20	0.41
1:A:403:SER:O	1:A:407:ARG:HG3	2.21	0.41
1:A:453:HIS:CD2	1:A:472:ALA:HB3	2.56	0.41
1:C:386:GLU:O	1:C:387:ARG:C	2.59	0.41
1:C:405:VAL:HG21	1:C:504:VAL:HG21	2.03	0.41
1:B:393:ILE:O	1:B:397:GLN:HG3	2.20	0.41
1:B:430:VAL:HG11	1:B:450:MET:HE2	2.01	0.41
1:C:438:ARG:HA	1:C:455:LEU:H	1.86	0.41
1:C:367:LEU:H	1:C:367:LEU:CD2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:LYS:O	1:C:497:GLN:CB	2.68	0.41
1:B:458:ILE:H	1:B:458:ILE:CD1	2.34	0.41
1:C:363:GLY:N	1:C:365:GLU:OE2	2.54	0.41
1:C:520:ALA:O	1:C:524:ALA:HB2	2.21	0.41
1:B:461:ILE:HD12	1:B:514:ALA:HA	2.02	0.41
1:C:431:ASP:O	1:C:442:LEU:HD12	2.19	0.40
1:A:455:LEU:HA	1:A:458:ILE:HD12	2.02	0.40
1:A:522:SER:O	1:A:523:VAL:C	2.58	0.40
1:C:367:LEU:HD22	1:C:367:LEU:H	1.86	0.40
1:A:460:TYR:OH	2:D:756:GLY:HA3	2.21	0.40
1:A:470:LEU:HD23	1:A:470:LEU:N	2.36	0.40
1:B:394:ARG:NH1	1:B:394:ARG:HG3	2.36	0.40
1:B:417:LYS:O	1:B:417:LYS:HD2	2.21	0.40
1:C:519:GLN:O	1:C:523:VAL:HG23	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	157/190 (83%)	127 (81%)	24 (15%)	6 (4%)	3	19
1	B	137/190 (72%)	105 (77%)	24 (18%)	8 (6%)	1	11
1	C	142/190 (75%)	118 (83%)	19 (13%)	5 (4%)	3	21
2	D	12/14 (86%)	8 (67%)	2 (17%)	2 (17%)	0	1
2	E	9/14 (64%)	5 (56%)	4 (44%)	0	100	100
2	F	1/14 (7%)	1 (100%)	0	0	100	100
All	All	458/612 (75%)	364 (80%)	73 (16%)	21 (5%)	2	15

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	PRO
1	B	439	ILE
2	D	763	LYS
1	A	528	PHE
1	C	455	LEU
1	A	391	LYS
1	B	381	THR
1	B	386	GLU
1	B	460	TYR
1	B	367	LEU
1	C	389	PRO
1	C	497	GLN
1	C	538	ASP
2	D	766	GLU
1	A	364	SER
1	A	390	SER
1	A	534	ILE
1	B	401	ALA
1	B	525	TYR
1	B	388	ASN
1	C	536	PRO

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	128/162 (79%)	107 (84%)	21 (16%)	2	10
1	B	114/162 (70%)	102 (90%)	12 (10%)	7	25
1	C	116/162 (72%)	96 (83%)	20 (17%)	2	9
2	D	13/13 (100%)	11 (85%)	2 (15%)	2	12
2	E	7/13 (54%)	7 (100%)	0	100	100
All	All	378/512 (74%)	323 (85%)	55 (15%)	3	14

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	366	ASP
1	A	367	LEU
1	A	376	ASN
1	A	386	GLU
1	A	395	MET
1	A	408	MET
1	A	409	GLN
1	A	428	THR
1	A	438	ARG
1	A	443	ASN
1	A	445	ASP
1	A	448	GLU
1	A	461	ILE
1	A	464	ILE
1	A	466	ASN
1	A	468	VAL
1	A	508	GLU
1	A	512	LEU
1	A	529	LEU
1	A	547	ILE
1	A	548	ILE
1	B	383	LEU
1	B	408	MET
1	B	409	GLN
1	B	427	LEU
1	B	428	THR
1	B	445	ASP
1	B	447	GLN
1	B	451	MET
1	B	464	ILE
1	B	467	ILE
1	B	508	GLU
1	B	519	GLN
1	C	365	GLU
1	C	369	ASP
1	C	388	ASN
1	C	389	PRO
1	C	393	ILE
1	C	394	ARG
1	C	395	MET
1	C	400	GLU
1	C	425	GLN
1	C	428	THR

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Mol	Chain	Res	Type
1	C	437	GLN
1	C	442	LEU
1	C	443	ASN
1	C	449	THR
1	C	451	MET
1	C	457	THR
1	C	496	LYS
1	C	508	GLU
1	C	509	ASP
1	C	512	LEU
2	D	761	THR
2	D	763	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	399	GLN
1	A	409	GLN
1	A	453	HIS
1	A	466	ASN
1	A	511	GLN
1	A	515	GLN
1	A	526	GLN
1	B	376	ASN
1	B	382	GLN
1	B	409	GLN
1	B	447	GLN
1	B	497	GLN
1	B	511	GLN
1	B	515	GLN
1	C	376	ASN
1	C	382	GLN
1	C	388	ASN
1	C	399	GLN
1	C	409	GLN
1	C	437	GLN
1	C	443	ASN
1	C	511	GLN
1	C	526	GLN
2	D	754	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 carbohydrates 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	A	163/190 (85%)	-0.03	0 100 100	63, 101, 158, 189	0
1	B	143/190 (75%)	0.21	5 (3%) 44 42	76, 116, 177, 198	0
1	C	150/190 (78%)	0.14	3 (2%) 65 64	74, 114, 177, 198	0
2	D	14/14 (100%)	0.46	1 (7%) 16 16	68, 121, 160, 173	0
2	E	11/14 (78%)	0.64	0 100 100	126, 148, 198, 205	0
2	F	3/14 (21%)	1.15	0 100 100	108, 108, 131, 161	0
All	All	484/612 (79%)	0.13	9 (1%) 66 65	63, 111, 175, 205	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	498	TYR	2.9
1	B	521	PHE	2.6
1	C	526	GLN	2.5
2	D	757	TYR	2.3
1	B	367	LEU	2.2
1	B	471	MET	2.2
1	B	389	PRO	2.1
1	B	468	VAL	2.0
1	C	411	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.