Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:15 pm BST

PDB ID	:	1OVL
Title	:	Crystal Structure of Nurr1 LBD
Authors	:	Wang, Z.; Liu, J.; Walker, N.
Deposited on	:	2003-03-26
Resolution	:	2.20 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:

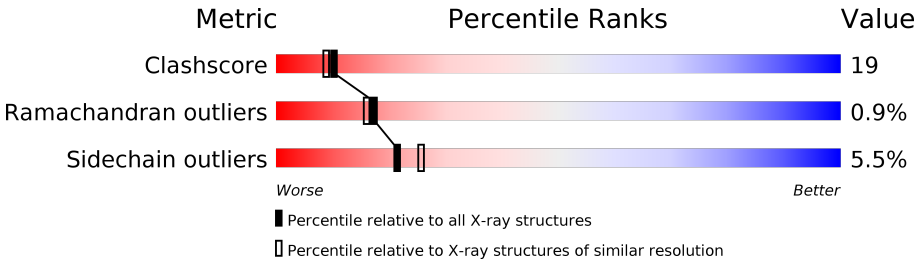
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	271	59% 23% • 16%
1	D	271	52% 30% • 15%
2	B	271	63% 22% • 13%
2	C	271	52% 28% • 17%
2	E	271	58% 30% • 8%
2	F	271	55% 26% • 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BR	E	815	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11703 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 Orphan nuclear receptor NURR1 (MSE 414, 496, 511).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	Se	0	0	0
			1819	1169	310	331	7	2			
1	D	230	Total	C	N	O	S	Se	0	0	0
			1834	1178	312	335	7	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
A	511	MSE	MET	MODIFIED RESIDUE	UNP P43354
D	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
D	511	MSE	MET	MODIFIED RESIDUE	UNP P43354

- Molecule 2 is a protein called Orphan nuclear receptor NURR1 (MSE 496, 511).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	Se	0	0	0
			1881	1206	319	346	7	3			
2	C	226	Total	C	N	O	S	Se	0	0	0
			1803	1160	304	330	6	3			
2	E	250	Total	C	N	O	S	Se	0	0	0
			1992	1271	346	365	7	3			
2	F	223	Total	C	N	O	S	Se	0	0	0
			1784	1149	301	325	6	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	414	MSE	MET	MODIFIED RESIDUE	UNP P43354
B	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
B	511	MSE	MET	MODIFIED RESIDUE	UNP P43354
C	414	MSE	MET	MODIFIED RESIDUE	UNP P43354

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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
C	511	MSE	MET	MODIFIED RESIDUE	UNP P43354
E	414	MSE	MET	MODIFIED RESIDUE	UNP P43354
E	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
E	511	MSE	MET	MODIFIED RESIDUE	UNP P43354
F	414	MSE	MET	MODIFIED RESIDUE	UNP P43354
F	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
F	511	MSE	MET	MODIFIED RESIDUE	UNP P43354

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total K 3 3	0	0
3	A	1	Total K 1 1	0	0
3	D	2	Total K 2 2	0	0
3	F	1	Total K 1 1	0	0
3	E	1	Total K 1 1	0	0

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	4	Total Br 4 4	0	0
4	E	7	Total Br 7 7	0	0
4	B	1	Total Br 1 1	0	0
4	C	1	Total Br 1 1	0	0
4	A	4	Total Br 4 4	0	0
4	F	2	Total Br 2 2	0	0

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total I 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	88	Total O 88 88	0	0
6	B	100	Total O 100 100	0	0
6	C	68	Total O 68 68	0	0
6	D	107	Total O 107 107	0	0
6	E	114	Total O 114 114	0	0
6	F	85	Total O 85 85	0	0

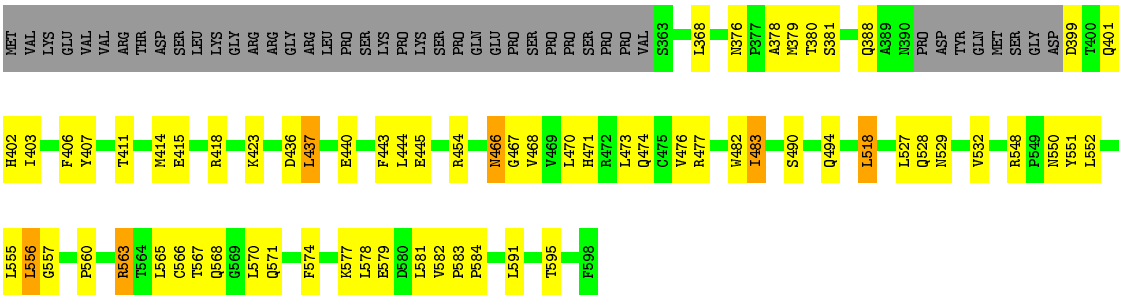
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

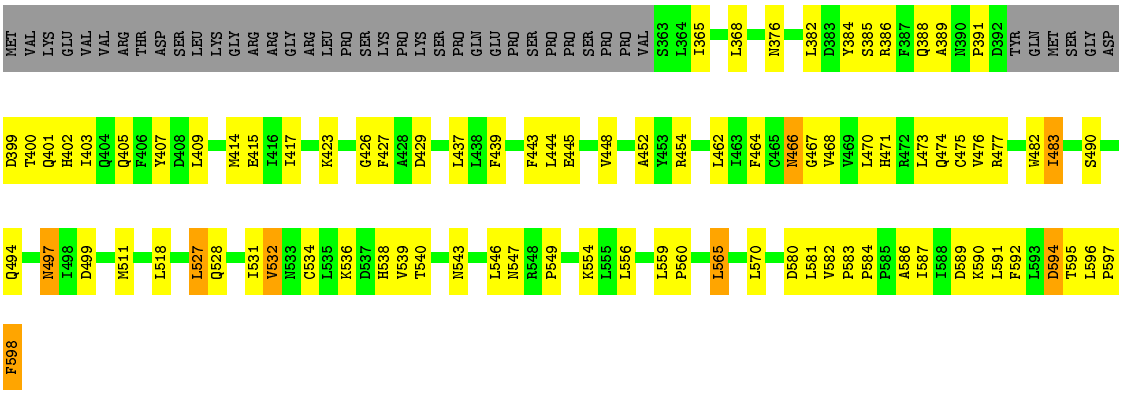
- Molecule 1: Orphan nuclear receptor NURR1 (MSE 414, 496, 511)

Chain A:



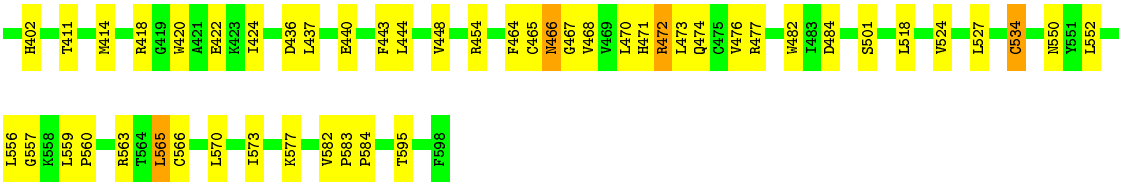
- Molecule 1: Orphan nuclear receptor NURR1 (MSE 414, 496, 511)

Chain D:



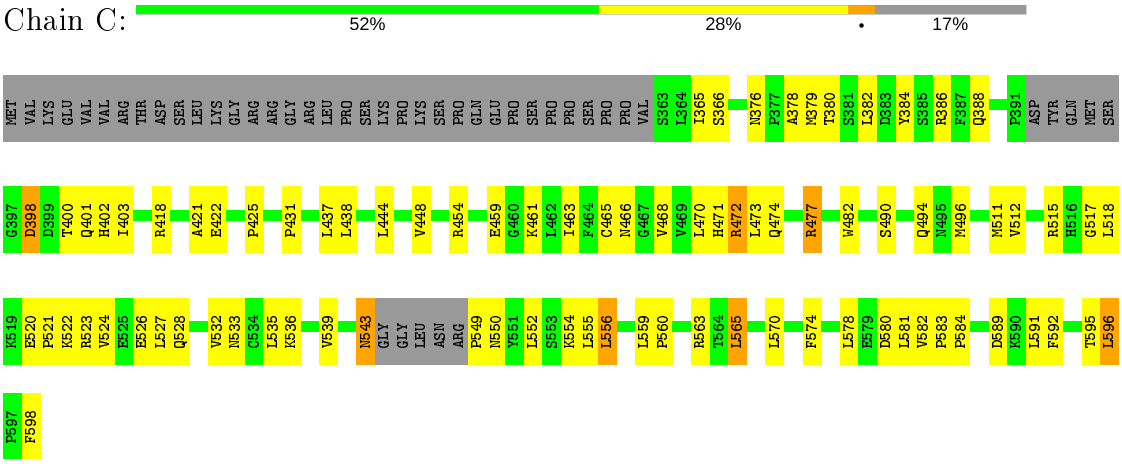
- Molecule 2: Orphan nuclear receptor NURR1 (MSE 496, 511)

Chain B:



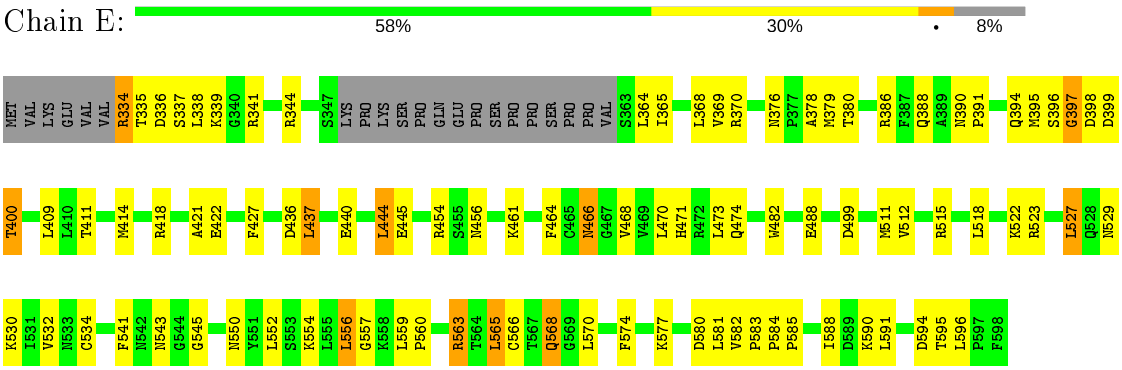
• Molecule 2: Orphan nuclear receptor NURR1 (MSE 496, 511)

Chain C:



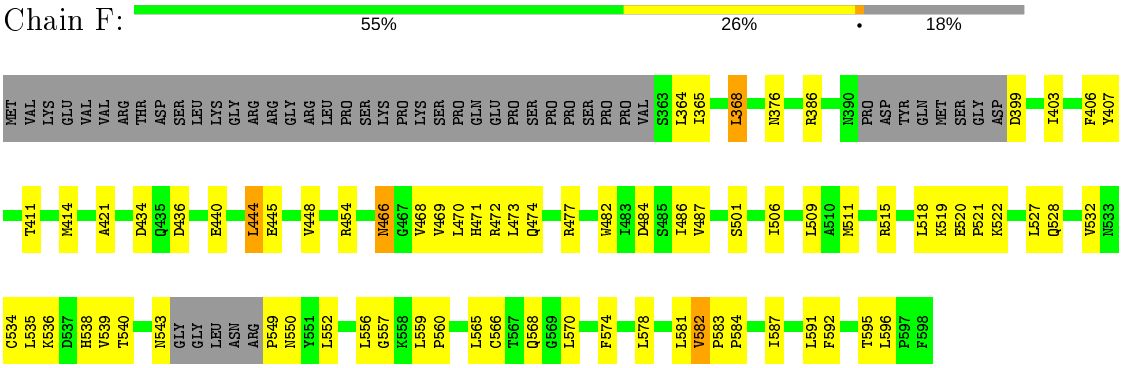
• Molecule 2: Orphan nuclear receptor NURR1 (MSE 496, 511)

Chain E:



• Molecule 2: Orphan nuclear receptor NURR1 (MSE 496, 511)

Chain F:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	80.38Å 80.38Å 227.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	500.00 – 2.20	Depositor
% Data completeness (in resolution range)	98.7 (500.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.217 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11703	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, IOD, BR

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	0.35	0/1854	0.54	0/2505
1	D	0.34	0/1870	0.56	0/2528
2	B	0.36	0/1918	0.56	0/2592
2	C	0.34	1/1837 (0.1%)	0.53	0/2480
2	E	0.35	0/2029	0.55	0/2737
2	F	0.33	0/1817	0.51	0/2452
All	All	0.35	1/11325 (0.0%)	0.54	0/15294

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	465	CYS	CB-SG	5.29	1.91	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1819	0	1837	70	0
1	D	1834	0	1848	80	0
2	B	1881	0	1887	57	0
2	C	1803	0	1815	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1992	0	2007	82	0
2	F	1784	0	1801	61	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	4	0	0	1	0
4	E	7	0	0	2	0
4	F	2	0	0	0	0
5	B	1	0	0	1	0
6	A	88	0	0	11	0
6	B	100	0	0	4	0
6	C	68	0	0	2	0
6	D	107	0	0	4	0
6	E	114	0	0	4	0
6	F	85	0	0	5	0
All	All	11703	0	11195	420	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 19.

All (420) 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)
2:F:471:HIS:H	2:F:474:GLN:HE21	0.98	0.95
2:E:365:ILE:HG13	2:E:534:CYS:SG	2.10	0.91
2:B:388:GLN:HE21	2:B:390:ASN:H	1.21	0.89
2:C:472:ARG:HH11	2:C:472:ARG:HG3	1.40	0.87
2:E:563:ARG:HH11	2:E:563:ARG:HB2	1.38	0.87
2:C:522:LYS:H	2:C:522:LYS:HD3	1.40	0.86
2:B:471:HIS:H	2:B:474:GLN:HE21	1.24	0.84
2:F:471:HIS:H	2:F:474:GLN:NE2	1.77	0.82
2:E:437:LEU:HD13	2:E:518:LEU:HD12	1.62	0.82
2:B:472:ARG:HH11	2:B:472:ARG:HG3	1.45	0.81
2:B:518:LEU:HD21	2:B:524:VAL:HG21	1.61	0.81
1:D:365:ILE:HB	1:D:534:CYS:SG	2.23	0.79
2:F:522:LYS:H	2:F:522:LYS:HD3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:581:LEU:HD12	2:E:582:VAL:HG23	1.67	0.76
1:A:466:ASN:ND2	1:A:468:VAL:H	1.82	0.75
2:B:471:HIS:H	2:B:474:GLN:NE2	1.84	0.75
4:E:815:BR:BR	6:E:923:HOH:O	2.60	0.74
2:C:528:GLN:O	2:C:532:VAL:HG23	1.86	0.74
2:E:334:ARG:HB3	2:E:334:ARG:NH1	2.03	0.74
2:B:466:ASN:ND2	2:B:468:VAL:H	1.85	0.74
2:C:471:HIS:H	2:C:474:GLN:HE21	1.36	0.73
2:B:365:ILE:HD11	2:B:501:SER:HB3	1.69	0.73
1:D:471:HIS:HD2	1:D:473:LEU:H	1.37	0.73
2:E:563:ARG:NH1	2:E:563:ARG:HB2	2.02	0.73
1:D:570:LEU:HD21	1:D:595:THR:HB	1.71	0.72
2:B:395:MET:HE1	2:B:477:ARG:HD3	1.71	0.72
2:F:581:LEU:HD22	2:F:582:VAL:HG12	1.71	0.72
2:C:532:VAL:HG12	2:C:536:LYS:HE3	1.72	0.71
2:C:386:ARG:HH22	2:C:468:VAL:HG21	1.54	0.71
1:D:448:VAL:HG11	1:D:565:LEU:HD13	1.73	0.71
2:C:518:LEU:HD23	2:C:524:VAL:HG21	1.73	0.70
2:C:552:LEU:O	2:C:556:LEU:HD13	1.92	0.70
1:D:559:LEU:HB2	1:D:560:PRO:HD3	1.72	0.70
2:F:472:ARG:NH2	2:F:487:VAL:HG11	2.07	0.69
2:F:471:HIS:N	2:F:474:GLN:HE21	1.83	0.69
1:A:378:ALA:C	1:A:380:THR:H	1.95	0.69
2:E:529:ASN:HA	2:E:532:VAL:HG22	1.75	0.69
1:A:466:ASN:HD22	1:A:466:ASN:C	1.95	0.68
2:B:376:ASN:HD22	2:B:454:ARG:HE	1.42	0.68
1:A:376:ASN:ND2	1:A:454:ARG:HH21	1.92	0.68
2:C:388:GLN:H	2:C:474:GLN:NE2	1.93	0.67
2:C:559:LEU:HB2	2:C:560:PRO:HD3	1.76	0.67
1:D:554:LYS:NZ	4:D:805:BR:BR	2.76	0.67
2:F:515:ARG:O	2:F:518:LEU:HD23	1.94	0.67
2:E:334:ARG:HH11	2:E:335:THR:N	1.93	0.66
1:A:388:GLN:H	1:A:474:GLN:NE2	1.94	0.66
2:E:376:ASN:HD22	2:E:454:ARG:HE	1.44	0.65
1:A:473:LEU:O	1:A:476:VAL:HG12	1.96	0.65
2:C:490:SER:O	2:C:494:GLN:HG3	1.95	0.65
2:B:418:ARG:O	2:B:422:GLU:HG3	1.97	0.65
1:D:471:HIS:CD2	1:D:473:LEU:H	2.15	0.64
2:C:468:VAL:HG12	2:C:470:LEU:HD13	1.80	0.64
2:C:471:HIS:H	2:C:474:GLN:NE2	1.95	0.64
2:E:471:HIS:H	2:E:474:GLN:NE2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:GLN:O	1:D:389:ALA:HB3	1.97	0.64
1:D:376:ASN:ND2	1:D:454:ARG:HH21	1.96	0.64
1:D:466:ASN:ND2	1:D:468:VAL:H	1.94	0.64
2:E:334:ARG:NH1	2:E:335:THR:N	2.45	0.64
2:E:364:LEU:O	2:E:368:LEU:HD13	1.98	0.63
2:F:522:LYS:N	2:F:522:LYS:HD3	2.13	0.63
1:A:570:LEU:HD21	1:A:595:THR:HB	1.79	0.63
2:B:395:MET:CE	2:B:477:ARG:HD3	2.29	0.63
2:B:466:ASN:ND2	2:B:468:VAL:HG23	2.13	0.63
2:C:520:GLU:HA	2:C:522:LYS:NZ	2.14	0.62
2:E:334:ARG:HB3	2:E:334:ARG:HH11	1.63	0.62
2:E:418:ARG:O	2:E:422:GLU:HG3	1.98	0.62
2:B:482:TRP:HE1	2:B:565:LEU:HD22	1.64	0.62
1:D:591:LEU:HD23	1:D:591:LEU:O	1.98	0.62
2:C:522:LYS:CD	2:C:522:LYS:H	2.12	0.62
2:E:334:ARG:NH1	2:E:335:THR:H	1.98	0.62
2:C:398:ASP:HB3	2:C:400:THR:HG22	1.81	0.61
2:F:414:MSE:HE1	6:F:853:HOH:O	2.01	0.61
2:E:552:LEU:HD13	2:E:556:LEU:HD22	1.81	0.61
2:F:552:LEU:HD13	2:F:552:LEU:O	2.00	0.61
2:E:334:ARG:HH11	2:E:335:THR:H	1.47	0.61
2:C:471:HIS:CD2	2:C:473:LEU:H	2.17	0.61
2:C:388:GLN:H	2:C:474:GLN:HE22	1.45	0.61
2:E:436:ASP:O	2:E:440:GLU:HG3	2.00	0.61
2:B:444:LEU:HD12	2:B:566:CYS:HB3	1.83	0.60
2:C:459:GLU:CB	2:C:461:LYS:HE2	2.31	0.60
2:F:557:GLY:O	2:F:560:PRO:HD2	2.00	0.60
2:B:471:HIS:CD2	2:B:473:LEU:H	2.18	0.60
1:D:547:ASN:HD22	2:E:543:ASN:ND2	2.00	0.60
2:E:398:ASP:OD1	2:E:400:THR:HG23	2.02	0.60
2:B:550:ASN:HB2	5:B:900:IOD:I	2.72	0.59
2:B:436:ASP:O	2:B:440:GLU:HG3	2.02	0.59
2:C:535:LEU:O	2:C:539:VAL:HG23	2.01	0.59
2:E:482:TRP:HE1	2:E:565:LEU:HD22	1.66	0.59
2:F:535:LEU:O	2:F:539:VAL:HG23	2.03	0.59
2:B:472:ARG:HD3	2:B:484:ASP:OD1	2.03	0.59
1:A:399:ASP:HB2	1:A:477:ARG:HH21	1.68	0.59
2:F:421:ALA:HB1	2:F:511:MSE:HE1	1.84	0.59
1:A:466:ASN:ND2	1:A:468:VAL:HG23	2.18	0.59
2:B:471:HIS:HD2	2:B:473:LEU:H	1.48	0.59
2:E:376:ASN:ND2	2:E:454:ARG:HH21	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:HD22	1:A:454:ARG:HE	1.49	0.59
2:C:570:LEU:HD21	2:C:595:THR:HB	1.83	0.59
2:B:570:LEU:HD21	2:B:595:THR:HB	1.85	0.58
2:B:388:GLN:H	2:B:474:GLN:NE2	2.00	0.58
1:D:482:TRP:HE1	1:D:565:LEU:HD22	1.67	0.58
1:A:376:ASN:HD21	1:A:454:ARG:HH21	1.51	0.58
1:A:490:SER:O	1:A:494:GLN:HG3	2.03	0.58
1:A:388:GLN:H	1:A:474:GLN:HE22	1.50	0.58
2:C:496:MSE:CE	2:C:554:LYS:HG3	2.34	0.58
1:A:401:GLN:HG3	1:A:402:HIS:ND1	2.19	0.58
1:D:471:HIS:H	1:D:474:GLN:HE21	1.51	0.57
2:E:574:PHE:O	2:E:577:LYS:HG2	2.04	0.57
1:D:591:LEU:HD23	1:D:591:LEU:C	2.25	0.57
1:D:580:ASP:OD1	1:D:583:PRO:HG3	2.04	0.57
2:C:471:HIS:HD2	2:C:473:LEU:H	1.50	0.57
1:A:468:VAL:HG12	1:A:470:LEU:HD22	1.86	0.57
2:C:403:ILE:HG21	2:C:582:VAL:HG13	1.86	0.57
2:C:459:GLU:HB2	2:C:461:LYS:HE2	1.87	0.57
2:E:386:ARG:HG3	2:E:386:ARG:HH11	1.69	0.57
2:E:437:LEU:HD13	2:E:518:LEU:CD1	2.35	0.57
2:F:466:ASN:ND2	2:F:468:VAL:H	2.03	0.57
2:F:448:VAL:HG11	2:F:565:LEU:HD12	1.87	0.57
2:E:378:ALA:C	2:E:380:THR:H	2.08	0.57
2:B:390:ASN:O	2:B:394:GLN:HG2	2.05	0.56
1:A:399:ASP:HB2	1:A:477:ARG:NH2	2.21	0.56
1:D:581:LEU:HD23	1:D:581:LEU:O	2.04	0.56
1:D:423:LYS:HE2	6:D:839:HOH:O	2.03	0.56
2:B:466:ASN:HD22	2:B:466:ASN:C	2.09	0.56
1:D:437:LEU:O	1:D:437:LEU:HD23	2.05	0.56
1:D:475:CYS:HB3	1:D:483:ILE:HG13	1.87	0.56
2:E:411:THR:HA	2:E:414:MSE:HE3	1.88	0.56
2:F:520:GLU:HA	2:F:522:LYS:NZ	2.20	0.56
2:F:592:PHE:O	2:F:596:LEU:HD13	2.06	0.56
1:A:414:MET:HG2	1:A:443:PHE:CZ	2.41	0.55
2:E:334:ARG:HH11	2:E:334:ARG:CB	2.20	0.55
1:D:547:ASN:HD22	2:E:543:ASN:HD21	1.55	0.55
1:D:437:LEU:HD23	1:D:437:LEU:C	2.27	0.55
2:E:581:LEU:CD1	2:E:582:VAL:HG23	2.36	0.55
2:B:378:ALA:C	2:B:380:THR:H	2.09	0.55
2:C:522:LYS:N	2:C:522:LYS:HD3	2.16	0.55
2:B:472:ARG:CG	2:B:472:ARG:HH11	2.16	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:425:PRO:O	2:C:527:LEU:HD21	2.08	0.54
2:F:522:LYS:H	2:F:522:LYS:CD	2.17	0.54
2:B:573:ILE:O	2:B:577:LYS:HG3	2.06	0.54
2:E:337:SER:O	2:E:341:ARG:HG3	2.07	0.54
2:C:386:ARG:NH2	2:C:468:VAL:HG21	2.20	0.54
1:A:581:LEU:O	1:A:581:LEU:HD23	2.07	0.54
2:C:543:ASN:OD1	2:C:549:PRO:HG2	2.08	0.54
2:C:379:MET:HE3	2:C:382:LEU:HD11	1.88	0.54
1:D:490:SER:O	1:D:494:GLN:HG3	2.08	0.54
1:D:596:LEU:C	1:D:598:PHE:H	2.11	0.54
1:A:403:ILE:HG21	1:A:582:VAL:CG1	2.38	0.54
1:A:579:GLU:HG2	1:A:581:LEU:HB2	1.90	0.53
2:E:341:ARG:O	2:E:344:ARG:HD3	2.08	0.53
2:F:365:ILE:HD11	2:F:501:SER:HB3	1.89	0.53
2:F:559:LEU:HB2	2:F:560:PRO:HD3	1.89	0.53
2:E:427:PHE:CE1	2:E:511:MSE:HE3	2.44	0.53
2:E:391:PRO:O	2:E:394:GLN:HG2	2.09	0.53
1:A:466:ASN:C	1:A:466:ASN:ND2	2.61	0.53
1:D:382:LEU:HB2	1:D:384:TYR:CE1	2.43	0.53
1:A:563:ARG:HD2	6:A:836:HOH:O	2.09	0.53
1:A:591:LEU:O	1:A:591:LEU:HD23	2.09	0.53
2:C:472:ARG:HG3	2:C:472:ARG:NH1	2.15	0.53
1:D:475:CYS:CB	1:D:483:ILE:HG13	2.38	0.53
1:D:452:ALA:HB1	1:D:490:SER:HA	1.91	0.52
2:F:421:ALA:CB	2:F:511:MSE:HE1	2.39	0.52
2:C:472:ARG:HH11	2:C:472:ARG:CG	2.15	0.52
2:E:388:GLN:H	2:E:474:GLN:NE2	2.08	0.52
2:E:444:LEU:HD13	2:E:566:CYS:HB3	1.92	0.52
2:F:445:GLU:HG3	6:F:811:HOH:O	2.08	0.52
2:B:363:SER:HB3	6:B:938:HOH:O	2.10	0.52
2:C:496:MSE:HE3	2:C:554:LYS:HG3	1.91	0.52
2:E:570:LEU:HD21	2:E:595:THR:HB	1.90	0.52
2:B:444:LEU:O	2:B:448:VAL:HG23	2.09	0.52
2:C:418:ARG:O	2:C:422:GLU:HG3	2.10	0.52
1:D:536:LYS:O	1:D:540:THR:HG23	2.10	0.52
1:A:407:TYR:OH	1:A:584:PRO:HG3	2.09	0.52
2:C:596:LEU:O	2:E:339:LYS:HE2	2.10	0.52
2:E:559:LEU:HB2	2:E:560:PRO:HD3	1.92	0.52
2:F:399:ASP:N	2:F:477:ARG:HH11	2.09	0.51
2:B:464:PHE:C	2:B:466:ASN:H	2.14	0.51
1:D:399:ASP:HB3	1:D:401:GLN:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:GLN:O	1:D:389:ALA:CB	2.58	0.51
1:D:539:VAL:HA	1:D:543:ASN:HB2	1.91	0.51
2:E:482:TRP:CD1	2:E:568:GLN:HB3	2.45	0.51
2:F:376:ASN:ND2	2:F:454:ARG:HH21	2.07	0.51
1:A:436:ASP:O	1:A:440:GLU:HG3	2.11	0.51
1:D:382:LEU:HB2	1:D:384:TYR:HE1	1.75	0.51
1:D:466:ASN:HD21	1:D:468:VAL:HB	1.75	0.51
2:F:506:ILE:HD13	2:F:509:LEU:HD12	1.93	0.51
1:A:471:HIS:CD2	1:A:473:LEU:H	2.28	0.51
2:C:398:ASP:HB3	2:C:400:THR:CG2	2.41	0.51
2:F:570:LEU:HD21	2:F:595:THR:HB	1.92	0.51
1:A:378:ALA:C	1:A:380:THR:N	2.63	0.51
2:C:520:GLU:HA	2:C:522:LYS:HZ1	1.76	0.51
2:B:559:LEU:HB2	2:B:560:PRO:HD3	1.92	0.51
1:A:466:ASN:HD22	1:A:468:VAL:H	1.54	0.51
1:D:468:VAL:HG12	1:D:470:LEU:HD22	1.92	0.51
1:A:468:VAL:HG12	1:A:470:LEU:CD2	2.40	0.51
2:E:515:ARG:O	2:E:518:LEU:HD13	2.11	0.51
2:F:471:HIS:CD2	2:F:473:LEU:H	2.29	0.51
2:F:471:HIS:HD2	2:F:473:LEU:HB2	1.76	0.50
2:C:580:ASP:OD1	2:C:583:PRO:HG3	2.11	0.50
1:D:528:GLN:O	1:D:532:VAL:HG13	2.11	0.50
2:E:550:ASN:HB2	4:E:815:BR:BR	2.67	0.50
2:F:414:MSE:HE2	6:F:826:HOH:O	2.12	0.50
1:A:528:GLN:O	1:A:532:VAL:HG13	2.12	0.50
2:C:512:VAL:HG11	2:C:527:LEU:HB3	1.93	0.50
1:D:445:GLU:HG3	6:D:819:HOH:O	2.11	0.50
1:D:386:ARG:HD2	1:D:470:LEU:HD11	1.94	0.50
2:B:557:GLY:O	2:B:560:PRO:HD2	2.12	0.50
2:F:403:ILE:HG21	2:F:582:VAL:HG13	1.93	0.50
2:C:472:ARG:CG	2:C:472:ARG:NH1	2.75	0.49
1:A:557:GLY:O	1:A:560:PRO:HD2	2.11	0.49
2:B:466:ASN:HD21	2:B:468:VAL:HG23	1.78	0.49
2:E:488:GLU:HA	6:E:874:HOH:O	2.12	0.49
2:F:574:PHE:CE1	2:F:578:LEU:HD11	2.48	0.49
2:C:402:HIS:CD2	2:C:477:ARG:HB3	2.48	0.49
2:B:466:ASN:ND2	2:B:466:ASN:C	2.65	0.49
2:C:518:LEU:CD2	2:C:524:VAL:HG21	2.41	0.49
2:C:589:ASP:O	2:C:592:PHE:HB3	2.13	0.49
1:D:399:ASP:N	1:D:477:ARG:HH21	2.10	0.49
1:A:378:ALA:HB3	1:A:381:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:407:TYR:OH	2:F:584:PRO:HG3	2.13	0.49
2:F:587:ILE:HG13	6:F:853:HOH:O	2.12	0.49
1:D:482:TRP:HE1	1:D:565:LEU:CD2	2.25	0.49
1:D:586:ALA:O	1:D:590:LYS:HB2	2.12	0.49
1:A:378:ALA:O	1:A:380:THR:N	2.45	0.49
2:C:403:ILE:HG21	2:C:582:VAL:CG1	2.43	0.49
2:E:466:ASN:HD22	2:E:466:ASN:C	2.15	0.49
1:D:596:LEU:O	1:D:598:PHE:N	2.45	0.49
2:E:421:ALA:HB1	2:E:511:MSE:HE1	1.94	0.49
2:F:468:VAL:HG12	2:F:470:LEU:HD22	1.93	0.49
2:F:520:GLU:HA	2:F:522:LYS:HZ3	1.77	0.49
1:A:591:LEU:HD23	1:A:591:LEU:C	2.33	0.49
2:C:471:HIS:HB3	2:C:474:GLN:HG3	1.95	0.49
1:D:401:GLN:HG3	1:D:402:HIS:ND1	2.28	0.49
1:D:414:MET:HG2	1:D:443:PHE:CE1	2.48	0.49
2:F:528:GLN:O	2:F:532:VAL:HG23	2.13	0.49
2:B:472:ARG:CG	2:B:472:ARG:NH1	2.76	0.48
1:D:389:ALA:HA	1:D:471:HIS:CG	2.48	0.48
2:E:523:ARG:HG3	2:E:523:ARG:HH11	1.77	0.48
1:D:538:HIS:HD2	6:D:872:HOH:O	1.95	0.48
2:B:386:ARG:HH21	2:B:468:VAL:HG11	1.78	0.48
1:D:386:ARG:HH11	1:D:405:GLN:HE21	1.61	0.48
2:E:529:ASN:HA	2:E:532:VAL:CG2	2.43	0.48
2:F:376:ASN:HD22	2:F:454:ARG:HE	1.62	0.48
1:A:466:ASN:HD22	1:A:467:GLY:N	2.10	0.48
2:E:466:ASN:ND2	2:E:468:VAL:H	2.12	0.48
2:B:466:ASN:HD22	2:B:467:GLY:N	2.11	0.48
2:C:421:ALA:HB1	2:C:511:MSE:HE1	1.94	0.48
2:E:557:GLY:O	2:E:560:PRO:HD2	2.14	0.48
1:A:552:LEU:C	1:A:552:LEU:HD13	2.34	0.48
2:C:574:PHE:CE1	2:C:578:LEU:HD11	2.48	0.48
1:A:376:ASN:HB3	6:A:895:HOH:O	2.12	0.48
1:D:587:ILE:O	1:D:590:LYS:HB3	2.14	0.48
2:C:549:PRO:O	2:C:550:ASN:HB2	2.14	0.47
1:D:399:ASP:HB2	1:D:477:ARG:NH2	2.29	0.47
1:D:399:ASP:OD2	1:D:400:THR:N	2.46	0.47
2:F:581:LEU:HD23	2:F:581:LEU:C	2.35	0.47
2:F:407:TYR:O	2:F:411:THR:HG23	2.13	0.47
2:C:591:LEU:HD13	2:C:591:LEU:C	2.35	0.47
1:D:399:ASP:HB2	1:D:477:ARG:HH22	1.78	0.47
2:C:382:LEU:HB2	2:C:384:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:532:VAL:CG1	2:C:536:LYS:HE3	2.44	0.47
2:B:472:ARG:HG3	2:B:472:ARG:NH1	2.22	0.47
2:B:464:PHE:O	2:B:466:ASN:N	2.47	0.47
2:E:456:ASN:HB3	2:E:461:LYS:HB2	1.97	0.47
1:D:376:ASN:HD22	1:D:454:ARG:HE	1.61	0.47
1:A:414:MET:HA	1:A:443:PHE:CE1	2.50	0.47
1:A:445:GLU:HG3	6:A:819:HOH:O	2.13	0.47
1:D:444:LEU:HD12	1:D:595:THR:HG21	1.97	0.47
2:E:397:GLY:O	2:E:398:ASP:HB3	2.16	0.46
2:C:496:MSE:HE1	2:C:555:LEU:HD12	1.96	0.46
1:D:589:ASP:O	1:D:592:PHE:HB3	2.15	0.46
1:A:403:ILE:HG21	1:A:582:VAL:HG11	1.97	0.46
2:E:580:ASP:OD1	2:E:583:PRO:HG3	2.16	0.46
2:C:421:ALA:CB	2:C:511:MSE:HE1	2.46	0.46
1:D:546:LEU:HB2	2:E:336:ASP:OD1	2.15	0.46
1:A:414:MET:HB3	6:A:877:HOH:O	2.15	0.46
1:A:423:LYS:HE2	6:A:892:HOH:O	2.16	0.46
1:A:411:THR:HA	1:A:414:MET:HG3	1.98	0.46
1:A:445:GLU:HA	1:A:566:CYS:SG	2.55	0.46
1:A:532:VAL:HG21	6:A:901:HOH:O	2.16	0.46
2:B:468:VAL:HG12	2:B:470:LEU:HD22	1.97	0.46
2:C:520:GLU:HA	2:C:522:LYS:HZ3	1.81	0.45
2:E:529:ASN:O	2:E:532:VAL:HG22	2.16	0.45
2:F:472:ARG:HH22	2:F:487:VAL:HG11	1.77	0.45
2:E:529:ASN:CA	2:E:532:VAL:HG22	2.44	0.45
1:A:529:ASN:O	1:A:532:VAL:HG22	2.17	0.45
2:C:378:ALA:C	2:C:380:THR:H	2.19	0.45
1:D:407:TYR:OH	1:D:584:PRO:HG3	2.16	0.45
2:E:471:HIS:CD2	2:E:473:LEU:H	2.34	0.45
2:F:386:ARG:HH22	2:F:468:VAL:HG21	1.81	0.45
1:D:386:ARG:HD3	1:D:405:GLN:NE2	2.30	0.45
1:D:409:LEU:HD13	1:D:464:PHE:CE2	2.52	0.45
2:E:338:LEU:HD21	2:F:596:LEU:CD2	2.46	0.45
2:F:538:HIS:HD2	6:F:876:HOH:O	1.99	0.45
1:A:407:TYR:O	1:A:411:THR:HG23	2.16	0.45
2:C:448:VAL:HG11	2:C:565:LEU:HD13	1.97	0.45
1:A:401:GLN:HG2	1:A:401:GLN:H	1.61	0.45
2:C:386:ARG:HD3	6:C:864:HOH:O	2.17	0.45
2:B:464:PHE:C	2:B:466:ASN:N	2.70	0.45
2:B:583:PRO:HA	2:B:584:PRO:HD3	1.83	0.44
1:D:596:LEU:C	1:D:598:PHE:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:434:ASP:OD1	2:F:519:LYS:HB2	2.17	0.44
2:E:583:PRO:HA	2:E:584:PRO:HD3	1.90	0.44
2:F:364:LEU:HD23	2:F:534:CYS:HB2	1.99	0.44
2:B:365:ILE:HB	2:B:534:CYS:SG	2.57	0.44
2:C:556:LEU:CD1	2:C:556:LEU:N	2.80	0.44
1:D:527:LEU:O	1:D:531:ILE:HG13	2.17	0.44
1:A:552:LEU:HD13	1:A:556:LEU:HD22	1.99	0.44
2:F:364:LEU:HG	2:F:368:LEU:HD22	1.99	0.44
2:C:365:ILE:HG23	2:C:366:SER:N	2.32	0.44
1:D:598:PHE:N	1:D:598:PHE:CD1	2.84	0.44
2:E:522:LYS:O	2:E:522:LYS:HD3	2.17	0.44
1:A:471:HIS:CD2	1:A:473:LEU:HG	2.53	0.44
2:F:549:PRO:O	2:F:550:ASN:HB2	2.18	0.44
1:A:550:ASN:HA	6:A:822:HOH:O	2.17	0.44
2:B:414:MSE:HA	2:B:443:PHE:CE1	2.53	0.44
1:A:403:ILE:O	1:A:406:PHE:HB3	2.18	0.44
1:A:466:ASN:HD21	1:A:468:VAL:HB	1.83	0.44
2:B:376:ASN:ND2	2:B:454:ARG:HE	2.11	0.44
2:C:533:ASN:HD22	2:C:536:LYS:HD2	1.83	0.44
1:D:427:PHE:CE1	1:D:511:MSE:HE3	2.53	0.44
2:B:363:SER:HB2	6:B:979:HOH:O	2.18	0.43
2:B:392:ASP:C	2:B:394:GLN:H	2.21	0.43
1:A:583:PRO:HA	1:A:584:PRO:HD3	1.85	0.43
1:D:399:ASP:OD2	1:D:400:THR:HG22	2.16	0.43
1:D:403:ILE:HG21	1:D:582:VAL:HG13	1.99	0.43
2:F:436:ASP:HB3	2:F:440:GLU:OE2	2.18	0.43
1:A:482:TRP:CD1	1:A:568:GLN:HB2	2.53	0.43
2:C:459:GLU:HB3	2:C:461:LYS:HE2	2.00	0.43
1:D:466:ASN:HD22	1:D:467:GLY:N	2.16	0.43
1:D:540:THR:HG23	6:D:887:HOH:O	2.18	0.43
2:F:386:ARG:NH2	2:F:468:VAL:HG21	2.33	0.43
2:E:409:LEU:HD13	2:E:464:PHE:CE2	2.54	0.43
2:F:486:ILE:HG12	2:F:565:LEU:HD11	1.99	0.43
2:C:583:PRO:HA	2:C:584:PRO:HD3	1.84	0.43
2:E:378:ALA:C	2:E:380:THR:N	2.71	0.43
2:F:444:LEU:HD13	2:F:566:CYS:HB3	1.99	0.43
2:C:518:LEU:O	2:C:521:PRO:HD3	2.18	0.43
2:C:581:LEU:HD23	2:C:581:LEU:O	2.18	0.43
1:D:462:LEU:HD22	1:D:462:LEU:N	2.33	0.43
1:D:591:LEU:HA	1:D:594:ASP:HB2	2.00	0.43
2:E:590:LYS:HG2	2:E:594:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:471:HIS:N	2:B:474:GLN:HE21	2.04	0.43
2:C:582:VAL:HG22	2:C:582:VAL:O	2.18	0.43
2:B:577:LYS:HG2	2:B:584:PRO:HG2	2.01	0.43
2:C:482:TRP:HE1	2:C:565:LEU:HD22	1.84	0.43
1:D:384:TYR:C	1:D:386:ARG:H	2.22	0.43
2:E:585:PRO:HG2	2:E:588:ILE:HG12	2.00	0.43
2:F:536:LYS:O	2:F:540:THR:HG23	2.19	0.43
1:A:415:GLU:HG2	6:A:878:HOH:O	2.18	0.43
2:C:437:LEU:O	2:C:437:LEU:HD13	2.19	0.43
1:A:466:ASN:HD21	1:A:468:VAL:CB	2.32	0.42
2:B:582:VAL:HG22	6:B:965:HOH:O	2.19	0.42
2:C:523:ARG:HG3	2:C:523:ARG:HH11	1.84	0.42
2:C:563:ARG:HB2	2:C:563:ARG:HE	1.58	0.42
2:C:543:ASN:HD22	2:C:543:ASN:C	2.22	0.42
1:D:466:ASN:C	1:D:466:ASN:HD22	2.22	0.42
1:D:403:ILE:HG21	1:D:582:VAL:CG1	2.49	0.42
2:C:552:LEU:HD13	2:C:552:LEU:C	2.40	0.42
1:D:426:GLY:HA2	1:D:429:ASP:OD2	2.20	0.42
1:D:499:ASP:OD2	1:D:538:HIS:HE1	2.02	0.42
1:A:471:HIS:CB	1:A:474:GLN:HE21	2.31	0.42
2:C:496:MSE:CE	2:C:555:LEU:HD12	2.49	0.42
2:E:388:GLN:HE21	2:E:390:ASN:H	1.65	0.42
1:A:483:ILE:HD13	1:A:483:ILE:O	2.19	0.42
1:A:567:THR:O	1:A:571:GLN:HG3	2.20	0.42
2:B:411:THR:HA	2:B:414:MSE:HG3	2.01	0.42
2:E:512:VAL:HG11	2:E:527:LEU:HB3	2.01	0.42
1:D:546:LEU:O	1:D:549:PRO:HD3	2.19	0.42
2:F:466:ASN:HD21	2:F:468:VAL:HB	1.84	0.42
2:F:518:LEU:HB2	2:F:521:PRO:HG3	2.02	0.42
2:F:583:PRO:HA	2:F:584:PRO:HD3	1.92	0.42
1:A:574:PHE:CZ	1:A:578:LEU:HD11	2.55	0.42
1:A:577:LYS:HG3	6:A:905:HOH:O	2.19	0.42
2:C:376:ASN:HD22	2:C:454:ARG:HE	1.68	0.42
2:F:448:VAL:HG11	2:F:565:LEU:CD1	2.49	0.42
2:F:472:ARG:NH1	2:F:484:ASP:OD1	2.52	0.42
1:A:376:ASN:ND2	1:A:454:ARG:HE	2.17	0.42
1:A:471:HIS:H	1:A:474:GLN:NE2	2.17	0.42
1:A:548:ARG:HB2	1:A:551:TYR:HB2	2.02	0.42
2:B:394:GLN:HA	2:B:394:GLN:OE1	2.20	0.42
2:E:365:ILE:O	2:E:369:VAL:HG23	2.19	0.42
1:A:418:ARG:NH1	6:A:878:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ASN:HD21	1:A:468:VAL:HG23	1.83	0.41
2:F:403:ILE:O	2:F:406:PHE:HB3	2.20	0.41
2:E:471:HIS:H	2:E:474:GLN:HE21	1.65	0.41
2:E:471:HIS:HD2	2:E:473:LEU:H	1.68	0.41
2:B:378:ALA:O	2:B:380:THR:N	2.53	0.41
2:B:559:LEU:HD12	6:B:950:HOH:O	2.19	0.41
2:E:530:LYS:HB2	2:E:530:LYS:HE3	1.84	0.41
1:A:466:ASN:HD21	1:A:468:VAL:CG2	2.33	0.41
1:D:547:ASN:OD1	2:E:341:ARG:HD3	2.21	0.41
2:E:445:GLU:OE1	2:E:563:ARG:NH1	2.52	0.41
1:D:546:LEU:H	2:E:336:ASP:CG	2.24	0.41
2:B:473:LEU:O	2:B:476:VAL:HG12	2.20	0.41
2:C:533:ASN:HA	2:C:536:LYS:HD2	2.02	0.41
2:E:445:GLU:HG3	6:E:821:HOH:O	2.21	0.41
2:B:399:ASP:O	2:B:402:HIS:N	2.53	0.41
2:B:420:TRP:CZ2	2:B:424:ILE:HD11	2.56	0.41
2:C:431:PRO:HD3	2:C:520:GLU:OE1	2.21	0.41
2:C:379:MET:HE3	2:C:463:ILE:HD13	2.03	0.41
1:D:417:ILE:HG22	1:D:439:PHE:HE1	1.85	0.41
2:C:517:GLY:HA2	2:E:554:LYS:NZ	2.36	0.41
1:A:437:LEU:HD13	1:A:518:LEU:HD13	2.02	0.41
2:C:472:ARG:NH1	6:C:843:HOH:O	2.53	0.41
2:F:469:VAL:O	2:F:470:LEU:HD13	2.21	0.41
2:C:400:THR:HG23	2:C:401:GLN:N	2.36	0.41
2:B:466:ASN:HD21	2:B:468:VAL:CG2	2.34	0.41
1:D:497:ASN:HB3	2:E:541:PHE:CE2	2.55	0.41
2:E:388:GLN:H	2:E:474:GLN:HE22	1.67	0.41
2:F:482:TRP:CD1	2:F:568:GLN:HB3	2.56	0.41
1:A:411:THR:HG21	6:A:848:HOH:O	2.21	0.40
1:D:476:VAL:O	1:D:476:VAL:HG22	2.21	0.40
2:C:438:LEU:HD23	2:C:515:ARG:HG3	2.02	0.40
1:D:546:LEU:HD13	2:E:336:ASP:OD2	2.21	0.40
2:C:365:ILE:CG2	2:C:366:SER:N	2.84	0.40
1:D:376:ASN:O	2:E:370:ARG:NH2	2.55	0.40
2:E:557:GLY:C	2:E:560:PRO:HD2	2.42	0.40
2:E:338:LEU:HD21	2:F:596:LEU:HD23	2.04	0.40
2:E:466:ASN:ND2	2:E:466:ASN:C	2.75	0.40
2:E:545:GLY:HA2	6:E:854:HOH:O	2.22	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	224/271 (83%)	216 (96%)	7 (3%)	1 (0%)	34 37
1	D	226/271 (83%)	215 (95%)	8 (4%)	3 (1%)	12 9
2	B	234/271 (86%)	225 (96%)	5 (2%)	4 (2%)	9 6
2	C	220/271 (81%)	209 (95%)	11 (5%)	0	100 100
2	E	246/271 (91%)	236 (96%)	6 (2%)	4 (2%)	9 7
2	F	217/271 (80%)	209 (96%)	8 (4%)	0	100 100
All	All	1367/1626 (84%)	1310 (96%)	45 (3%)	12 (1%)	17 16

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	MET
2	B	465	CYS
2	E	395	MET
2	E	396	SER
2	B	379	MET
2	B	398	ASP
1	D	385	SER
1	D	597	PRO
2	E	379	MET
2	B	393	TYR
1	D	391	PRO
2	E	397	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/240 (84%)	191 (95%)	11 (5%)	22	26
1	D	204/240 (85%)	192 (94%)	12 (6%)	19	23
2	B	209/239 (87%)	198 (95%)	11 (5%)	22	27
2	C	201/239 (84%)	190 (94%)	11 (6%)	21	26
2	E	221/239 (92%)	206 (93%)	15 (7%)	16	17
2	F	199/239 (83%)	191 (96%)	8 (4%)	31	40
All	All	1236/1436 (86%)	1168 (94%)	68 (6%)	21	26

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	LEU
1	A	437	LEU
1	A	444	LEU
1	A	466	ASN
1	A	483	ILE
1	A	518	LEU
1	A	527	LEU
1	A	555	LEU
1	A	556	LEU
1	A	563	ARG
1	A	565	LEU
2	B	368	LEU
2	B	395	MET
2	B	437	LEU
2	B	466	ASN
2	B	472	ARG
2	B	527	LEU
2	B	534	CYS
2	B	552	LEU
2	B	556	LEU
2	B	563	ARG
2	B	565	LEU
2	C	398	ASP
2	C	444	LEU
2	C	466	ASN
2	C	472	ARG
2	C	477	ARG
2	C	526	GLU

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Mol	Chain	Res	Type
2	C	543	ASN
2	C	556	LEU
2	C	565	LEU
2	C	596	LEU
2	C	598	PHE
1	D	368	LEU
1	D	415	GLU
1	D	466	ASN
1	D	483	ILE
1	D	497	ASN
1	D	518	LEU
1	D	527	LEU
1	D	532	VAL
1	D	556	LEU
1	D	565	LEU
1	D	594	ASP
1	D	598	PHE
2	E	334	ARG
2	E	399	ASP
2	E	400	THR
2	E	437	LEU
2	E	444	LEU
2	E	466	ASN
2	E	470	LEU
2	E	499	ASP
2	E	527	LEU
2	E	556	LEU
2	E	563	ARG
2	E	565	LEU
2	E	568	GLN
2	E	591	LEU
2	E	596	LEU
2	F	368	LEU
2	F	444	LEU
2	F	466	ASN
2	F	527	LEU
2	F	543	ASN
2	F	556	LEU
2	F	582	VAL
2	F	591	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	401	GLN
1	A	466	ASN
1	A	471	HIS
1	A	474	GLN
1	A	528	GLN
1	A	529	ASN
1	A	533	ASN
1	A	547	ASN
1	A	568	GLN
1	A	571	GLN
2	B	376	ASN
2	B	388	GLN
2	B	401	GLN
2	B	466	ASN
2	B	471	HIS
2	B	474	GLN
2	B	497	ASN
2	B	529	ASN
2	B	533	ASN
2	B	543	ASN
2	B	571	GLN
2	C	376	ASN
2	C	402	HIS
2	C	466	ASN
2	C	471	HIS
2	C	474	GLN
2	C	529	ASN
2	C	533	ASN
2	C	542	ASN
2	C	543	ASN
2	C	550	ASN
2	C	571	GLN
1	D	376	ASN
1	D	388	GLN
1	D	401	GLN
1	D	404	GLN
1	D	405	GLN
1	D	456	ASN
1	D	466	ASN
1	D	471	HIS
1	D	474	GLN
1	D	529	ASN

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Mol	Chain	Res	Type
1	D	533	ASN
1	D	538	HIS
1	D	542	ASN
1	D	568	GLN
2	E	376	ASN
2	E	388	GLN
2	E	466	ASN
2	E	471	HIS
2	E	474	GLN
2	E	528	GLN
2	E	529	ASN
2	E	533	ASN
2	E	543	ASN
2	E	550	ASN
2	F	376	ASN
2	F	466	ASN
2	F	471	HIS
2	F	474	GLN
2	F	529	ASN
2	F	533	ASN
2	F	543	ASN
2	F	550	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 28 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.