Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:37 PM GMT

PDB ID	:	4FLN
Title	:	Crystal structure of plant protease Deg2
Authors	:	Gong, W.; Liu, L.; Sun, R.; Gao, F.
Deposited on	:	2012-06-15
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

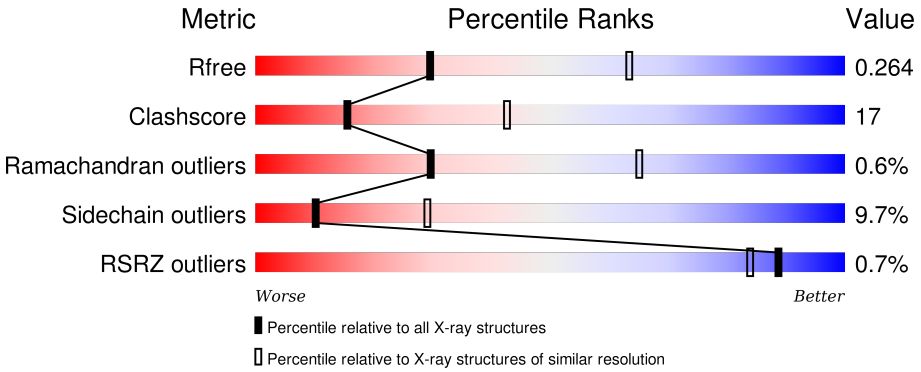
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	539	% 55% 27% · 14%
1	B	539	58% 26% · 14%
1	C	539	% 53% 30% · 14%
2	D	4	100%
2	F	4	100%

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Mol	Chain	Length	Quality of chain
3	E	20	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10921 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 Protease Do-like 2, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	8	4	0
			3553	2262	613	666	12			
1	B	464	Total	C	N	O	S	0	0	0
			3517	2240	604	661	12			
1	C	463	Total	C	N	O	S	0	2	0
			3506	2236	603	655	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	ASN	-	EXPRESSION TAG	UNP O82261
A	70	ALA	-	EXPRESSION TAG	UNP O82261
B	69	ASN	-	EXPRESSION TAG	UNP O82261
B	70	ALA	-	EXPRESSION TAG	UNP O82261
C	69	ASN	-	EXPRESSION TAG	UNP O82261
C	70	ALA	-	EXPRESSION TAG	UNP O82261

- Molecule 2 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			29	20	5	4			
2	F	4	Total	C	N	O	0	0	0
			29	20	5	4			

- Molecule 3 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	20	Total	C	N	O	0	0	0
			109	66	21	22			

- Molecule 4 is water.

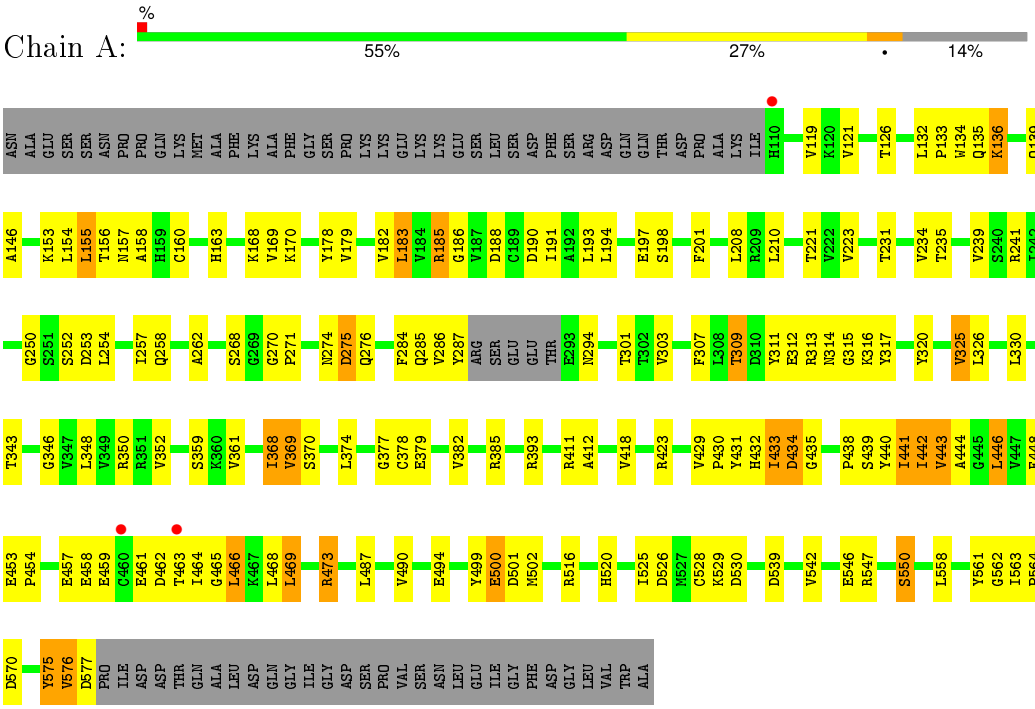
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	75	Total O 75 75	0	0
4	B	61	Total O 61 61	0	0
4	C	42	Total O 42 42	0	0

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 errors 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.

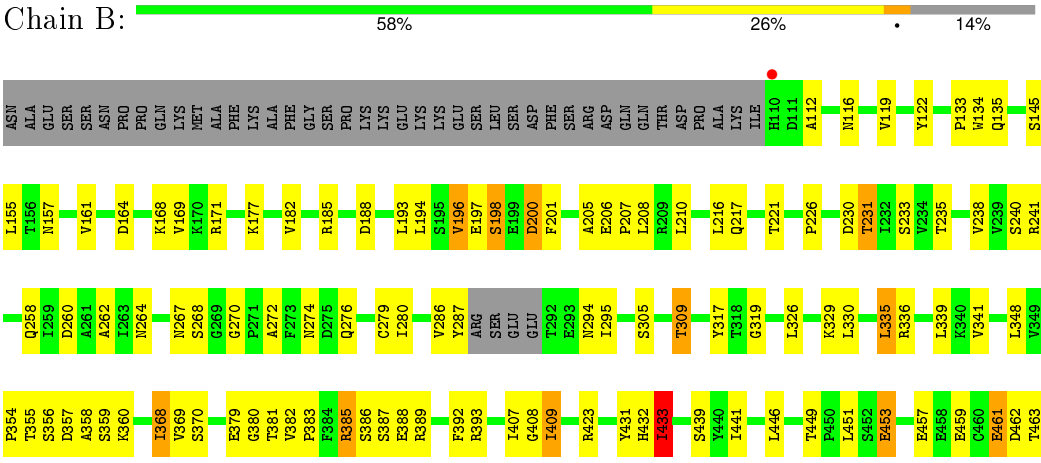
- Molecule 1: Protease Do-like 2, chloroplastic

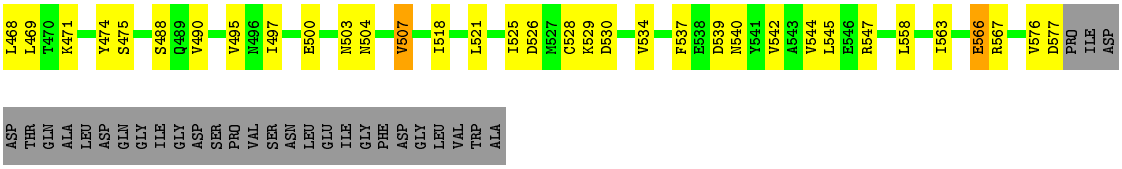
Chain A:



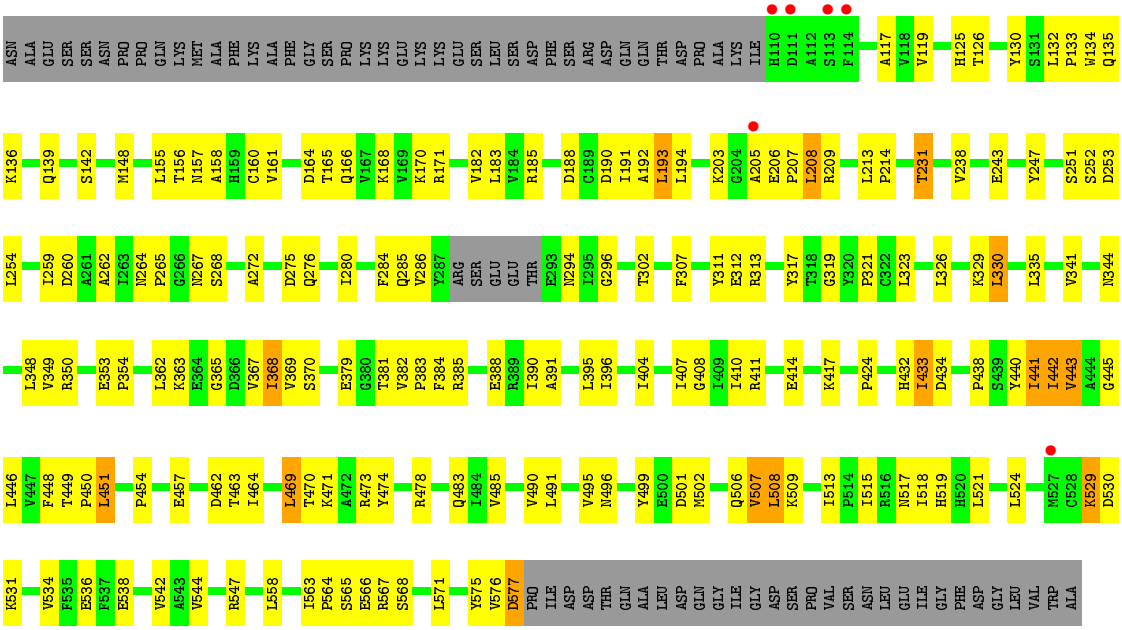
- Molecule 1: Protease Do-like 2, chloroplastic

Chain B:





• Molecule 1: Protease Do-like 2, chloroplastic



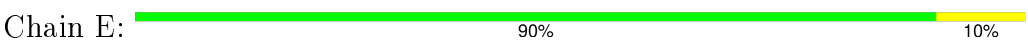
• Molecule 2: Unknown peptide

There are no outlier residues recorded for this chain.

• Molecule 2: Unknown peptide

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown peptide



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	125.40Å 188.16Å 166.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 2.80 39.63 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.74-2.80) 95.6 (39.63-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	4.43 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.203 , 0.274 0.193 , 0.264	Depositor DCC
R_{free} test set	2336 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	62.2	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 48432 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10921	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.38	0/3634	0.65	1/4941 (0.0%)
1	B	0.35	0/3585	0.58	0/4878
1	C	0.31	0/3581	0.55	0/4874
2	D	0.44	0/15	0.44	0/20
2	F	0.33	0/15	0.34	0/20
3	E	0.33	0/22	0.34	0/28
All	All	0.35	0/10852	0.59	1/14761 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	458	GLU	N-CA-C	-5.15	97.10	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	GLY	Peptide
1	A	575	TYR	Peptide
1	C	251	SER	Peptide
1	C	501	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	C	507	VAL	Peptide

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	3553	0	3516	135	1
1	B	3517	0	3457	99	0
1	C	3506	0	3427	136	0
2	D	29	0	15	0	0
2	F	29	0	15	0	0
3	E	109	0	34	2	0
4	A	75	0	0	3	0
4	B	61	0	0	3	0
4	C	42	0	0	4	0
All	All	10921	0	10464	364	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (364) 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:C:341:VAL:HG12	1:C:410:ILE:HD12	1.51	0.91
1:A:526:ASP:OD1	1:A:567:ARG:NH2	2.04	0.89
1:A:461:GLU:HA	1:A:464:ILE:HD11	1.56	0.86
1:A:443:VAL:HG21	1:A:525:ILE:HD13	1.58	0.86
1:C:238:VAL:H	1:C:260:ASP:HB2	1.45	0.82
1:B:576:VAL:HG13	1:B:577:ASP:H	1.46	0.81
1:C:433:ILE:HG12	1:C:454:PRO:HG2	1.62	0.80
1:A:432:HIS:O	1:A:433:ILE:HG13	1.84	0.78
1:C:384:PHE:HD2	1:C:388:GLU:HG2	1.47	0.77
1:B:197:GLU:HA	1:B:198:SER:OG	1.84	0.77
1:A:439:SER:O	1:A:449:THR:HG22	1.85	0.76
1:C:133:PRO:HG2	1:C:440:TYR:HB3	1.68	0.75
1:A:516:ARG:HG3	1:A:520:HIS:ND1	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:TYR:HB2	1:C:252:SER:HB3	1.68	0.75
1:C:135:GLN:NE2	4:C:736:HOH:O	2.20	0.75
1:A:119:VAL:HG11	1:A:169:VAL:HB	1.68	0.73
1:C:384:PHE:CD2	1:C:388:GLU:HG2	2.24	0.73
1:C:294:ASN:ND2	4:C:709:HOH:O	2.22	0.72
1:B:439:SER:O	1:B:449:THR:HG22	1.89	0.72
1:B:185:ARG:HD3	4:B:723:HOH:O	1.89	0.72
1:C:350:ARG:HA	1:C:350:ARG:HE	1.55	0.72
1:B:330:LEU:HD21	1:B:348:LEU:HB2	1.70	0.71
1:A:188:ASP:OD1	1:A:317:TYR:OH	2.05	0.71
1:C:509:LYS:HB2	1:C:536:GLU:HB2	1.72	0.71
1:C:529:LYS:O	1:C:547:ARG:NH1	2.24	0.70
1:A:526:ASP:CG	1:A:567:ARG:HH22	1.93	0.70
1:A:433:ILE:HD12	1:A:435:GLY:H	1.56	0.70
1:C:157:ASN:OD1	1:C:268:SER:HB2	1.91	0.70
1:C:262:ALA:HB2	1:C:294:ASN:HA	1.74	0.69
1:C:350:ARG:HA	1:C:350:ARG:NE	2.07	0.69
1:A:132:LEU:HD22	1:A:134:TRP:CH2	2.28	0.69
1:B:530:ASP:O	1:B:547:ARG:HD3	1.93	0.68
1:C:275:ASP:OD1	1:C:276:GLN:NE2	2.26	0.67
1:B:566:GLU:OE1	1:B:567:ARG:NE	2.28	0.67
1:C:390:ILE:HG13	1:C:391:ALA:H	1.60	0.67
1:C:576:VAL:HG13	1:C:577:ASP:H	1.59	0.67
1:B:241:ARG:HB3	1:B:258:GLN:HB2	1.75	0.67
1:C:381:THR:O	1:C:382:VAL:HG23	1.95	0.66
1:C:276:GLN:OE1	4:C:724:HOH:O	2.13	0.66
1:C:382:VAL:HG11	1:C:395:LEU:HD11	1.76	0.66
1:C:132:LEU:HB3	1:C:134:TRP:CZ2	2.30	0.66
1:A:155:LEU:HD12	1:A:156:THR:N	2.11	0.66
1:A:221:THR:HG21	1:B:217:GLN:NE2	2.11	0.66
1:A:243:GLU:OE1	1:C:231:THR:HB	1.96	0.66
1:A:453:GLU:OE2	1:A:473[B]:ARG:NH2	2.28	0.66
1:C:119:VAL:HG23	1:C:171:ARG:HA	1.75	0.66
1:C:348:LEU:HD12	1:C:349:VAL:H	1.61	0.65
1:A:154:LEU:HB2	1:A:194:LEU:HB2	1.79	0.65
1:A:431:TYR:CD1	1:A:453:GLU:HG2	2.32	0.65
1:A:446:LEU:HB3	1:A:487:LEU:HD11	1.79	0.65
1:B:407:ILE:HG22	1:B:409:ILE:HD13	1.79	0.65
1:A:132:LEU:HD22	1:A:134:TRP:CZ2	2.32	0.65
1:A:575:TYR:CD1	1:A:576:VAL:HG12	2.32	0.64
1:C:161:VAL:HG11	1:C:194:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:OD2	1:A:393:ARG:NH1	2.32	0.63
1:C:442:ILE:O	1:C:446:LEU:O	2.17	0.63
1:B:197:GLU:HA	1:B:198:SER:CB	2.27	0.63
1:C:330:LEU:HB3	1:C:335:LEU:HD12	1.81	0.63
1:A:446:LEU:HB3	1:A:487:LEU:CD1	2.29	0.62
1:C:155:LEU:HD11	1:C:191:ILE:HG23	1.80	0.62
1:A:133:PRO:HG2	1:A:440:TYR:HD2	1.65	0.62
1:A:155:LEU:HD12	1:A:156:THR:H	1.62	0.62
1:B:253:ASP:H	3:E:119:UNK:C	2.13	0.62
1:B:133:PRO:HG3	1:B:449:THR:HG21	1.82	0.62
1:B:286:VAL:HG13	1:B:287:TYR:H	1.65	0.62
1:A:441:ILE:O	1:A:566:GLU:O	2.18	0.62
1:C:441:ILE:HB	1:C:448:PHE:HB2	1.81	0.61
1:A:155:LEU:HD11	1:A:191:ILE:HG23	1.81	0.61
1:A:241:ARG:HB3	1:A:258:GLN:HB2	1.82	0.61
1:A:500:GLU:O	1:A:501:ASP:HB2	2.00	0.61
1:B:462:ASP:O	1:B:463:THR:OG1	2.18	0.61
1:B:446:LEU:HD22	1:B:490:VAL:HG22	1.82	0.61
1:B:149:ILE:HG21	1:B:155:LEU:HD22	1.82	0.61
1:C:341:VAL:HG11	1:C:367:VAL:HG21	1.82	0.61
1:B:380:GLY:O	1:B:392:PHE:HB2	2.01	0.61
1:C:385:ARG:CB	1:C:388:GLU:HB2	2.31	0.61
1:A:462:ASP:C	1:A:464:ILE:H	2.04	0.61
1:B:245:THR:HG22	4:B:729:HOH:O	2.00	0.60
1:C:507:VAL:HG12	1:C:507:VAL:O	1.99	0.60
1:B:112:ALA:O	1:B:116:ASN:ND2	2.32	0.60
1:A:193:LEU:HD13	1:A:307:PHE:HE2	1.66	0.60
1:A:499:TYR:O	1:A:502:MET:HB2	2.01	0.60
1:C:513:ILE:HG21	1:C:524:LEU:HD11	1.84	0.60
1:A:145:SER:HB2	1:A:270:GLY:N	2.16	0.59
1:A:439:SER:O	1:A:449:THR:CG2	2.49	0.59
1:B:521:LEU:O	1:B:525:ILE:HD13	2.01	0.59
1:B:329:LYS:HD3	1:B:379:GLU:OE1	2.03	0.59
1:C:132:LEU:HD22	1:C:134:TRP:CH2	2.37	0.59
1:A:330:LEU:HD21	1:A:348:LEU:HB2	1.84	0.59
1:C:563:ILE:HG22	1:C:565:SER:H	1.68	0.59
1:C:519:HIS:HD2	1:C:575:TYR:HB2	1.68	0.59
1:B:317:TYR:CZ	1:B:319:GLY:HA2	2.38	0.59
1:B:461:GLU:HA	1:B:461:GLU:OE1	2.02	0.58
1:A:576:VAL:HG22	1:A:577:ASP:H	1.66	0.58
1:A:432:HIS:CE1	1:A:434:ASP:HA	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:HIS:ND1	1:B:432:HIS:O	2.37	0.58
1:A:461:GLU:HA	1:A:464:ILE:CD1	2.30	0.58
1:B:526:ASP:CG	1:B:567:ARG:HH22	2.05	0.58
1:C:190:ASP:OD1	1:C:284:PHE:HE1	1.87	0.58
1:A:576:VAL:HG22	1:A:577:ASP:N	2.19	0.57
1:C:213:LEU:HD12	1:C:214:PRO:HD2	1.86	0.57
1:A:146:ALA:HB2	1:A:156:THR:HB	1.86	0.57
1:C:563:ILE:HG23	1:C:564:PRO:HD2	1.85	0.57
1:A:442:ILE:O	1:A:446:LEU:O	2.22	0.57
1:A:133:PRO:HG2	1:A:440:TYR:CD2	2.38	0.57
1:A:516:ARG:HG3	1:A:520:HIS:CE1	2.40	0.56
1:B:432:HIS:O	1:B:433:ILE:HD12	2.05	0.56
1:B:134:TRP:CG	1:B:563:ILE:HG23	2.41	0.56
1:B:368:ILE:HA	1:B:409:ILE:HD12	1.88	0.56
1:A:352:VAL:HG11	1:A:359:SER:HA	1.87	0.56
1:B:161:VAL:HG11	1:B:194:LEU:HD21	1.86	0.56
1:A:350:ARG:HA	1:A:350:ARG:NE	2.20	0.56
1:C:442:ILE:O	1:C:443:VAL:HB	2.06	0.56
1:C:348:LEU:HD12	1:C:349:VAL:N	2.21	0.56
1:B:576:VAL:HG13	1:B:577:ASP:N	2.19	0.56
1:B:274:ASN:HB3	1:B:276:GLN:H	1.70	0.56
1:A:530:ASP:O	1:A:547:ARG:HD3	2.07	0.55
1:C:161:VAL:HG23	1:C:185:ARG:NH1	2.21	0.55
1:B:336:ARG:HG2	1:B:341:VAL:HB	1.87	0.55
1:C:117:ALA:CB	1:C:208:LEU:HD13	2.35	0.55
1:A:133:PRO:CB	1:A:438:PRO:HG2	2.37	0.55
1:C:362:LEU:O	1:C:363:LYS:HG3	2.07	0.55
1:A:262:ALA:HB2	1:A:294:ASN:HA	1.89	0.55
1:A:188:ASP:HB2	1:A:252:SER:OG	2.07	0.54
1:A:274:ASN:HB3	1:A:276:GLN:H	1.72	0.54
1:B:335:LEU:HD22	1:B:339:LEU:HD12	1.90	0.54
1:B:336:ARG:CG	1:B:341:VAL:HB	2.37	0.54
1:A:444:ALA:HB2	1:A:550:SER:HB3	1.88	0.54
1:A:379:GLU:HB2	4:A:769:HOH:O	2.08	0.54
1:B:157:ASN:OD1	1:B:268:SER:HB2	2.08	0.54
1:A:314:ASN:HB2	4:A:709:HOH:O	2.07	0.54
1:A:183:LEU:CD2	1:A:311:TYR:OH	2.56	0.54
1:A:145:SER:HB2	1:A:270:GLY:H	1.74	0.53
1:C:508:LEU:HD23	1:C:508:LEU:H	1.73	0.53
1:C:125:HIS:HE1	1:C:160:CYS:O	1.90	0.53
1:A:126:THR:HG22	1:A:136:LYS:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:VAL:HG21	1:C:499:TYR:O	2.08	0.53
1:A:443:VAL:HG21	1:A:525:ILE:CD1	2.36	0.53
1:C:534:VAL:HG22	1:C:544:VAL:HG22	1.91	0.53
1:C:341:VAL:O	1:C:341:VAL:HG23	2.09	0.53
1:A:132:LEU:HB3	1:A:134:TRP:CZ2	2.44	0.52
1:C:567:ARG:CG	1:C:571:LEU:HB2	2.39	0.52
1:A:432:HIS:O	1:A:433:ILE:CG1	2.54	0.52
1:A:341:VAL:HG12	1:A:343:THR:O	2.10	0.52
1:C:183:LEU:HD22	1:C:311:TYR:OH	2.10	0.52
1:B:198:SER:O	1:B:200:ASP:N	2.43	0.52
1:A:464:ILE:HD12	1:A:469:LEU:HD23	1.91	0.52
1:C:485:VAL:O	1:C:507:VAL:HG23	2.09	0.52
1:A:576:VAL:HG13	1:A:577:ASP:H	1.73	0.52
1:B:286:VAL:HG13	1:B:287:TYR:N	2.24	0.52
1:B:462:ASP:C	1:B:464:ILE:H	2.12	0.52
1:C:317:TYR:CZ	1:C:319:GLY:HA2	2.44	0.52
1:C:134:TRP:CD1	1:C:135:GLN:HG3	2.44	0.52
1:A:377:GLY:O	1:A:379:GLU:O	2.26	0.52
1:A:132:LEU:HB3	1:A:134:TRP:CE2	2.45	0.51
1:B:393:ARG:HG2	3:E:118:UNK:H	1.75	0.51
1:B:145:SER:HB2	1:B:270:GLY:H	1.75	0.51
1:C:440:TYR:CD2	1:C:568:SER:HB3	2.45	0.51
1:C:515:ILE:HD13	1:C:521:LEU:HD13	1.93	0.51
1:B:558:LEU:O	1:B:563:ILE:N	2.41	0.51
1:C:125:HIS:NE2	1:C:142:SER:OG	2.44	0.51
1:A:461:GLU:CA	1:A:464:ILE:HD11	2.36	0.50
1:A:134:TRP:CD1	1:A:135:GLN:HG3	2.47	0.50
1:A:311:TYR:O	1:A:313:ARG:O	2.29	0.50
1:B:305:SER:O	1:B:309:THR:HG23	2.11	0.50
1:A:313:ARG:O	1:A:315:GLY:N	2.44	0.50
1:C:193:LEU:HD13	1:C:307:PHE:HE2	1.77	0.50
1:A:469:LEU:HD11	1:A:473[A]:ARG:NH2	2.27	0.50
1:C:155:LEU:HD12	1:C:156:THR:H	1.77	0.50
1:A:168:LYS:HA	1:A:178:TYR:O	2.11	0.50
1:A:241:ARG:HH21	1:C:231:THR:H	1.58	0.50
1:C:368:ILE:HG13	1:C:368:ILE:O	2.11	0.50
1:C:284:PHE:CZ	1:C:286:VAL:HG13	2.46	0.50
1:C:508:LEU:HD21	1:C:538:GLU:HA	1.94	0.50
1:B:148:MET:SD	1:B:205:ALA:HB1	2.52	0.49
1:A:440:TYR:HA	1:A:448:PHE:O	2.10	0.49
1:C:450:PRO:HD3	1:C:518:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ALA:HB2	1:B:294:ASN:HA	1.95	0.49
1:C:329:LYS:HD2	1:C:379:GLU:HA	1.95	0.49
1:C:441:ILE:HG23	1:C:443:VAL:HG23	1.93	0.49
1:B:534:VAL:HG22	1:B:544:VAL:HG22	1.95	0.49
1:C:383:PRO:O	1:C:384:PHE:HB3	2.13	0.49
1:C:247:TYR:CE2	1:C:254:LEU:HB2	2.48	0.49
1:C:566:GLU:HG3	1:C:567:ARG:N	2.27	0.49
1:B:431:TYR:CE1	1:B:453:GLU:HG2	2.48	0.49
1:A:223:VAL:HG22	1:A:234:VAL:HG22	1.94	0.49
1:A:157:ASN:HB2	1:A:160:CYS:SG	2.53	0.49
1:A:443:VAL:CG2	1:A:525:ILE:HD13	2.37	0.49
1:C:382:VAL:HG11	1:C:395:LEU:CD1	2.43	0.49
1:B:182:VAL:HG11	1:B:185:ARG:NH2	2.28	0.49
1:C:404:ILE:N	1:C:404:ILE:HD12	2.27	0.49
1:B:226:PRO:HG3	1:B:233:SER:OG	2.12	0.49
1:A:268:SER:HB2	1:A:284:PHE:HA	1.94	0.48
1:A:314:ASN:O	1:A:316:LYS:HG2	2.13	0.48
1:C:563:ILE:HG22	1:C:565:SER:N	2.28	0.48
1:C:259:ILE:HG12	1:C:296:GLY:HA3	1.94	0.48
1:C:471:LYS:HD3	1:C:506:GLN:HE22	1.79	0.48
1:C:483:GLN:OE1	1:C:517:ASN:HB2	2.14	0.48
1:C:130:TYR:HE1	1:C:433:ILE:HG23	1.78	0.48
1:C:446:LEU:HD23	1:C:490:VAL:HG13	1.95	0.48
1:A:239:VAL:HG13	1:A:257:ILE:HG23	1.95	0.48
1:C:171:ARG:NH2	1:C:203:LYS:O	2.47	0.48
1:C:321:PRO:HA	1:C:424:PRO:HA	1.96	0.48
1:A:234:VAL:O	1:B:240:SER:HB3	2.13	0.48
1:B:238:VAL:H	1:B:260:ASP:HB3	1.79	0.48
1:A:368:ILE:HG13	1:A:369:VAL:N	2.28	0.48
1:B:149:ILE:HD11	1:B:193:LEU:HD11	1.96	0.48
1:B:507:VAL:HG13	1:B:537:PHE:CE1	2.48	0.48
1:C:253:ASP:O	1:C:254:LEU:HD23	2.13	0.47
1:C:558:LEU:HD13	1:C:565:SER:HA	1.96	0.47
1:C:433:ILE:HG12	1:C:454:PRO:CG	2.40	0.47
1:B:539:ASP:O	1:B:540:ASN:CB	2.62	0.47
1:B:385:ARG:HD3	1:B:388:GLU:CD	2.34	0.47
1:B:245:THR:O	1:B:253:ASP:HA	2.14	0.47
1:A:346:GLY:HA2	1:A:368:ILE:O	2.15	0.47
1:B:182:VAL:HG11	1:B:185:ARG:CZ	2.44	0.47
1:A:286:VAL:O	1:A:287:TYR:CB	2.62	0.47
1:C:440:TYR:CE2	1:C:568:SER:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:THR:O	1:B:504:ASN:ND2	2.33	0.47
1:C:344:ASN:ND2	1:C:344:ASN:O	2.48	0.47
1:C:148:MET:SD	1:C:205:ALA:HB1	2.54	0.46
1:A:235:THR:HG22	1:B:260:ASP:OD2	2.14	0.46
1:B:526:ASP:OD1	1:B:567:ARG:NH2	2.46	0.46
1:B:216:LEU:O	1:B:217:GLN:HB3	2.15	0.46
1:A:243:GLU:HG3	1:A:244:VAL:N	2.30	0.46
1:B:264:ASN:O	1:B:267:ASN:HB2	2.16	0.46
1:A:119:VAL:CG1	1:A:169:VAL:HB	2.43	0.46
1:B:330:LEU:HD22	1:B:335:LEU:HD13	1.97	0.46
1:B:407:ILE:HG22	1:B:409:ILE:CD1	2.45	0.46
1:A:370:SER:HA	1:A:374:LEU:O	2.16	0.46
1:C:531:LYS:O	1:C:531:LYS:HG3	2.16	0.46
1:A:562:GLY:C	1:A:563:ILE:HG13	2.35	0.46
1:A:442:ILE:O	1:A:443:VAL:HB	2.15	0.46
1:C:134:TRP:CZ3	1:C:442:ILE:HD11	2.51	0.46
1:A:462:ASP:C	1:A:464:ILE:N	2.70	0.46
1:A:182:VAL:HA	1:A:194:LEU:HD23	1.97	0.46
1:B:370:SER:OG	1:B:408:GLY:HA3	2.16	0.46
1:B:471:LYS:O	1:B:475:SER:HB3	2.16	0.46
1:C:265:PRO:HA	1:C:285:GLN:HB3	1.97	0.46
1:C:442:ILE:O	1:C:443:VAL:CB	2.64	0.45
1:A:183:LEU:HD21	1:A:311:TYR:OH	2.16	0.45
1:B:474:TYR:N	1:B:474:TYR:CD2	2.84	0.45
1:A:361:VAL:CG1	1:A:418:VAL:HB	2.46	0.45
1:C:390:ILE:HG13	1:C:391:ALA:N	2.29	0.45
1:C:491:LEU:O	1:C:496:ASN:ND2	2.47	0.45
1:A:462:ASP:O	1:A:464:ILE:N	2.49	0.45
1:A:221:THR:HA	1:A:235:THR:O	2.16	0.45
1:B:350:ARG:HA	1:B:350:ARG:NE	2.31	0.45
1:B:221:THR:HA	1:B:235:THR:O	2.16	0.45
1:C:323:LEU:HB2	1:C:396:ILE:HD13	1.98	0.45
1:C:133:PRO:CG	1:C:440:TYR:HB3	2.45	0.45
1:A:529:LYS:HA	1:A:547:ARG:CZ	2.47	0.45
1:A:411:ARG:O	1:A:412:ALA:HB3	2.16	0.45
1:B:197:GLU:CA	1:B:198:SER:CB	2.95	0.45
1:B:231:THR:HB	1:C:243:GLU:OE1	2.17	0.45
1:A:330:LEU:O	1:A:378:CYS:HB2	2.16	0.45
1:B:161:VAL:O	1:B:164:ASP:HB3	2.17	0.45
1:C:567:ARG:HG2	1:C:571:LEU:HB2	1.97	0.45
1:C:432:HIS:C	1:C:433:ILE:HG13	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ILE:HD13	1:C:407:ILE:HG23	1.99	0.44
1:B:474:TYR:N	1:B:474:TYR:HD2	2.14	0.44
1:A:275:ASP:OD1	1:A:275:ASP:N	2.39	0.44
1:A:431:TYR:CE1	1:A:453:GLU:HG2	2.52	0.44
1:C:126:THR:HG22	1:C:136:LYS:HD3	2.00	0.44
1:C:369:VAL:N	1:C:408:GLY:O	2.32	0.44
1:B:122:TYR:HB2	1:B:168:LYS:HD2	1.99	0.44
1:C:348:LEU:HD11	1:C:365:GLY:HA2	2.00	0.44
1:A:576:VAL:HG13	1:A:577:ASP:N	2.32	0.44
1:C:238:VAL:H	1:C:260:ASP:CB	2.23	0.44
1:A:132:LEU:HD13	1:A:134:TRP:CZ2	2.53	0.44
1:B:432:HIS:C	1:B:433:ILE:HD12	2.38	0.44
1:C:272:ALA:O	1:C:280:ILE:HG13	2.17	0.44
1:C:384:PHE:HB2	1:C:390:ILE:CG2	2.48	0.44
1:C:515:ILE:CD1	1:C:521:LEU:HD13	2.48	0.44
1:A:563:ILE:HA	1:A:564:PRO:HD3	1.88	0.44
1:A:133:PRO:HB2	1:A:438:PRO:HG2	2.00	0.44
1:C:125:HIS:CE1	1:C:160:CYS:O	2.71	0.44
1:B:355:THR:HG23	4:B:726:HOH:O	2.18	0.44
1:C:188:ASP:N	1:C:188:ASP:OD1	2.39	0.44
1:A:561:TYR:N	1:A:562:GLY:HA2	2.33	0.44
1:A:464:ILE:HG13	1:A:465:GLY:H	1.83	0.43
1:A:133:PRO:HB3	1:A:438:PRO:HG2	1.99	0.43
1:C:264:ASN:O	1:C:267:ASN:HB2	2.18	0.43
1:A:185:ARG:NH1	4:A:757:HOH:O	2.30	0.43
1:C:462:ASP:O	1:C:463:THR:CB	2.66	0.43
1:A:468:LEU:HD23	1:A:468:LEU:HA	1.57	0.43
1:C:317:TYR:CE2	1:C:319:GLY:HA2	2.53	0.43
1:B:210:LEU:N	1:B:210:LEU:HD23	2.34	0.43
1:A:341:VAL:HA	1:A:342:PRO:HD3	1.82	0.43
1:C:464:ILE:HD13	1:C:464:ILE:HA	1.91	0.43
1:C:206:GLU:HA	1:C:207:PRO:HD2	1.86	0.43
1:A:186:GLY:HA2	1:A:317:TYR:CD2	2.53	0.43
1:A:268:SER:CB	1:A:285:GLN:H	2.32	0.43
1:B:356:SER:O	1:B:358:ALA:O	2.36	0.43
1:B:206:GLU:HA	1:B:207:PRO:HD2	1.90	0.43
1:B:196:VAL:HG11	1:B:201:PHE:CD2	2.53	0.43
1:C:519:HIS:CD2	1:C:575:TYR:HB2	2.50	0.43
1:C:469:LEU:HD21	1:C:473[A]:ARG:CZ	2.48	0.43
1:C:133:PRO:HB3	1:C:438:PRO:HG2	2.00	0.43
1:B:329:LYS:HG2	1:B:379:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:TYR:N	1:A:431:TYR:CD2	2.86	0.43
1:A:182:VAL:HA	1:A:194:LEU:CD2	2.49	0.43
1:C:353:GLU:HA	1:C:354:PRO:HD3	1.80	0.42
1:C:513:ILE:CG2	1:C:524:LEU:HD11	2.47	0.42
1:C:451:LEU:HA	1:C:451:LEU:HD23	1.78	0.42
1:C:155:LEU:HD12	1:C:156:THR:N	2.34	0.42
1:C:508:LEU:CD2	1:C:508:LEU:H	2.31	0.42
1:A:223:VAL:O	1:A:271:PRO:HD2	2.20	0.42
1:B:383:PRO:HD3	1:B:389:ARG:NH2	2.34	0.42
1:A:303:VAL:HG13	1:A:320:TYR:OH	2.19	0.42
1:B:488:SER:O	1:B:503:ASN:HA	2.19	0.42
1:B:528:CYS:SG	1:B:547:ARG:HD2	2.59	0.42
1:B:253:ASP:OD2	1:B:393:ARG:NH1	2.52	0.42
1:A:565:SER:OG	1:A:566:GLU:N	2.52	0.42
1:A:563:ILE:HG23	1:A:564:PRO:HD2	2.01	0.42
1:C:132:LEU:HB3	1:C:134:TRP:CH2	2.54	0.42
1:A:253:ASP:O	1:A:254:LEU:HD23	2.20	0.42
1:A:158:ALA:HB3	1:A:190:ASP:OD1	2.18	0.42
1:B:188:ASP:N	1:B:188:ASP:OD1	2.43	0.42
1:A:183:LEU:HD22	1:A:311:TYR:OH	2.20	0.42
1:A:210:LEU:HD13	1:A:301:THR:HG23	2.02	0.42
1:C:382:VAL:HG13	1:C:383:PRO:HD2	2.02	0.42
1:A:466:LEU:HD12	1:A:466:LEU:HA	1.74	0.42
1:B:357:ASP:C	1:B:358:ALA:O	2.57	0.42
1:C:445:GLY:O	1:C:490:VAL:HA	2.20	0.42
1:C:350:ARG:CA	1:C:350:ARG:NE	2.81	0.42
1:A:501:ASP:O	1:A:502:MET:C	2.58	0.41
1:B:464:ILE:HA	1:B:464:ILE:HD13	1.89	0.41
1:C:470:THR:O	1:C:474:TYR:HB2	2.20	0.41
1:B:358:ALA:O	1:B:359:SER:OG	2.27	0.41
1:A:453:GLU:N	1:A:454:PRO:CD	2.82	0.41
1:C:182:VAL:HG11	1:C:185:ARG:CZ	2.51	0.41
1:B:358:ALA:C	1:B:360:LYS:H	2.23	0.41
1:A:163:HIS:NE2	1:A:433:ILE:HD11	2.35	0.41
1:C:441:ILE:CG2	1:C:443:VAL:HG23	2.50	0.41
1:B:335:LEU:HA	1:B:335:LEU:HD23	1.82	0.41
1:B:134:TRP:CD1	1:B:135:GLN:HG3	2.55	0.41
1:A:309:THR:O	1:A:313:ARG:HG3	2.20	0.41
1:B:353:GLU:HA	1:B:354:PRO:HD3	1.90	0.41
1:C:350:ARG:CA	1:C:350:ARG:HE	2.29	0.41
1:A:575:TYR:O	1:A:575:TYR:CD2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:VAL:O	1:A:143:THR:HA	2.20	0.41
1:A:325:VAL:HG23	1:A:352:VAL:HG22	2.02	0.41
1:C:473[A]:ARG:HH11	1:C:473[A]:ARG:HG3	1.86	0.41
1:C:168:LYS:HB2	1:C:168:LYS:HE3	1.88	0.41
1:A:153:LYS:HD2	1:A:193:LEU:HD23	2.02	0.41
1:B:432:HIS:O	1:B:432:HIS:CG	2.74	0.41
1:A:528:CYS:O	1:A:529:LYS:HB2	2.21	0.41
1:B:119:VAL:HG11	1:B:169:VAL:HB	2.02	0.41
1:C:563:ILE:CG2	1:C:565:SER:O	2.69	0.41
1:C:133:PRO:HD3	1:C:449:THR:HG21	2.03	0.40
1:C:158:ALA:HA	1:C:192:ALA:HB2	2.03	0.40
1:A:558:LEU:HB2	1:A:563:ILE:HB	2.03	0.40
1:B:441:ILE:HG22	1:B:518:ILE:HD11	2.03	0.40
1:B:272:ALA:O	1:B:280:ILE:HG13	2.22	0.40
1:A:542:VAL:O	1:A:542:VAL:HG13	2.21	0.40
1:B:497:ILE:HA	1:B:500:GLU:OE2	2.21	0.40
1:A:429:VAL:HA	1:A:430:PRO:HD2	1.89	0.40
1:C:190:ASP:OD1	1:C:284:PHE:CE1	2.71	0.40
1:C:188:ASP:OD1	1:C:317:TYR:HE2	2.05	0.40
1:A:119:VAL:HG13	1:A:170:LYS:O	2.21	0.40
1:A:154:LEU:HD11	1:A:201:PHE:CZ	2.57	0.40
1:B:286:VAL:O	1:B:287:TYR:CB	2.70	0.40
1:C:170:LYS:NZ	4:C:728:HOH:O	2.49	0.40

All (1) 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:A:139:GLN:NE2	1:A:490:VAL:O[3_555]	2.15	0.05

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	463/539 (86%)	423 (91%)	36 (8%)	4 (1%)	21 55
1	B	460/539 (85%)	430 (94%)	29 (6%)	1 (0%)	52 84
1	C	461/539 (86%)	427 (93%)	31 (7%)	3 (1%)	26 62
2	D	1/4 (25%)	1 (100%)	0	0	100 100
2	F	1/4 (25%)	1 (100%)	0	0	100 100
3	E	2/20 (10%)	2 (100%)	0	0	100 100
All	All	1388/1645 (84%)	1284 (92%)	96 (7%)	8 (1%)	30 65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	ILE
1	B	433	ILE
1	C	433	ILE
1	A	442	ILE
1	A	576	VAL
1	C	442	ILE
1	A	443	VAL
1	C	443	VAL

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	381/463 (82%)	340 (89%)	41 (11%)	8 23
1	B	373/463 (81%)	334 (90%)	39 (10%)	8 24
1	C	367/463 (79%)	336 (92%)	31 (8%)	14 37
2	D	1/1 (100%)	1 (100%)	0	100 100
2	F	1/1 (100%)	1 (100%)	0	100 100
3	E	2/2 (100%)	2 (100%)	0	100 100
All	All	1125/1393 (81%)	1014 (90%)	111 (10%)	10 28

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LYS
1	A	155	LEU
1	A	179	VAL
1	A	183	LEU
1	A	185	ARG
1	A	197	GLU
1	A	198	SER
1	A	208	LEU
1	A	231	THR
1	A	246	SER
1	A	275	ASP
1	A	309	THR
1	A	312	GLU
1	A	325	VAL
1	A	326	LEU
1	A	335	LEU
1	A	368	ILE
1	A	369	VAL
1	A	382	VAL
1	A	385	ARG
1	A	423[A]	ARG
1	A	423[B]	ARG
1	A	434	ASP
1	A	441	ILE
1	A	446	LEU
1	A	449	THR
1	A	451	LEU
1	A	457	GLU
1	A	459	GLU
1	A	463	THR
1	A	466	LEU
1	A	469	LEU
1	A	473[A]	ARG
1	A	473[B]	ARG
1	A	494	GLU
1	A	500	GLU
1	A	539	ASP
1	A	546	GLU
1	A	550	SER
1	A	567	ARG
1	A	570	ASP
1	B	171	ARG

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Mol	Chain	Res	Type
1	B	177	LYS
1	B	196	VAL
1	B	198	SER
1	B	200	ASP
1	B	208	LEU
1	B	230	ASP
1	B	231	THR
1	B	253	ASP
1	B	279	CYS
1	B	295	ILE
1	B	309	THR
1	B	326	LEU
1	B	335	LEU
1	B	351	ARG
1	B	368	ILE
1	B	369	VAL
1	B	381	THR
1	B	382	VAL
1	B	385	ARG
1	B	386	SER
1	B	387	SER
1	B	409	ILE
1	B	423	ARG
1	B	433	ILE
1	B	451	LEU
1	B	453	GLU
1	B	457	GLU
1	B	459	GLU
1	B	461	GLU
1	B	466	LEU
1	B	468	LEU
1	B	469	LEU
1	B	495	VAL
1	B	507	VAL
1	B	529	LYS
1	B	542	VAL
1	B	545	LEU
1	B	566	GLU
1	C	139	GLN
1	C	164	ASP
1	C	165	THR
1	C	166	GLN

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Mol	Chain	Res	Type
1	C	193	LEU
1	C	208	LEU
1	C	209	ARG
1	C	231	THR
1	C	302	THR
1	C	312	GLU
1	C	313	ARG
1	C	326	LEU
1	C	330	LEU
1	C	368	ILE
1	C	370	SER
1	C	411	ARG
1	C	414	GLU
1	C	417	LYS
1	C	434	ASP
1	C	441	ILE
1	C	451	LEU
1	C	457	GLU
1	C	469	LEU
1	C	478	ARG
1	C	495	VAL
1	C	502	MET
1	C	508	LEU
1	C	529	LYS
1	C	530	ASP
1	C	542	VAL
1	C	577	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	HIS
1	C	267	ASN
1	C	519	HIS

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	463/539 (85%)	-0.47	3 (0%) 90 86	30, 53, 93, 140	0
1	B	464/539 (86%)	-0.39	1 (0%) 95 94	34, 60, 104, 137	0
1	C	463/539 (85%)	-0.13	6 (1%) 79 71	38, 78, 121, 144	0
2	D	1/4 (25%)	-0.65	0 100 100	72, 72, 72, 72	0
2	F	1/4 (25%)	-1.04	0 100 100	73, 73, 73, 73	0
3	E	2/20 (10%)	-0.67	0 100 100	56, 56, 56, 75	0
All	All	1394/1645 (84%)	-0.33	10 (0%) 89 84	30, 64, 111, 144	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	HIS	4.0
1	A	460	CYS	3.6
1	C	114	PHE	3.3
1	A	463	THR	2.8
1	C	113	SER	2.6
1	C	205	ALA	2.4
1	C	527	MET	2.3
1	B	110	HIS	2.3
1	A	110	HIS	2.2
1	C	111	ASP	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.