Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 07:12 PM EST

PDB ID	:	2PM6
Title	:	Crystal Structure of yeast Sec13/31 edge element of the COPII vesicular coat, native version
Authors	:	Goldberg, J.; Fath, S.; Mancias, J.D.; Bi, X.
Deposited on	:	2007-04-20
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

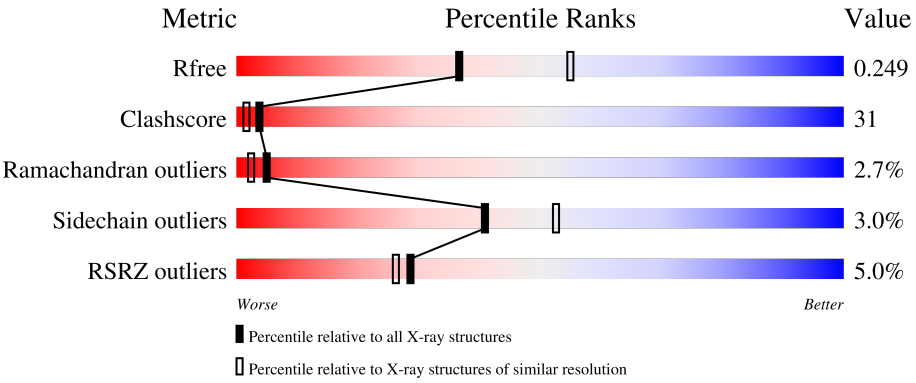
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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

Mol	Chain	Length	Quality of chain
1	A	399	4% 43% 40% · 14%
1	C	399	4% 50% 34% · 13%
2	B	297	4% 44% 49% · 6%
2	D	297	6% 52% 43% · ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10195 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 Protein transport protein SEC31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2729	1728	449	547	5			
1	C	347	Total	C	N	O	S	0	0	0
			2746	1739	452	550	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	GLY	-	cloning artifact	UNP P38968
A	366	ALA	-	cloning artifact	UNP P38968
A	367	MET	-	cloning artifact	UNP P38968
A	368	GLY	-	cloning artifact	UNP P38968
A	369	SER	-	cloning artifact	UNP P38968
C	365	GLY	-	cloning artifact	UNP P38968
C	366	ALA	-	cloning artifact	UNP P38968
C	367	MET	-	cloning artifact	UNP P38968
C	368	GLY	-	cloning artifact	UNP P38968
C	369	SER	-	cloning artifact	UNP P38968

- Molecule 2 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total	C	N	O	S	0	0	0
			2196	1403	375	415	3			
2	D	288	Total	C	N	O	S	0	0	0
			2263	1444	387	429	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		

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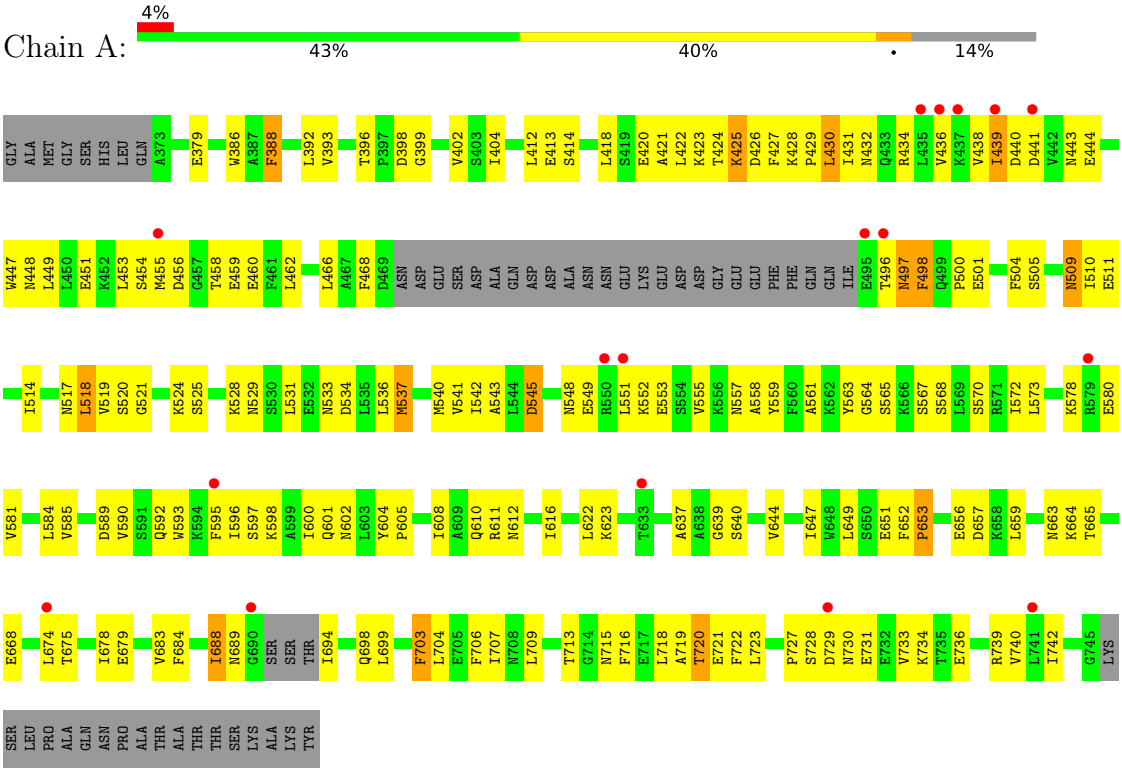
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	61	Total O 61 61	0	0
3	C	51	Total O 51 51	0	0
3	D	121	Total O 121 121	0	0

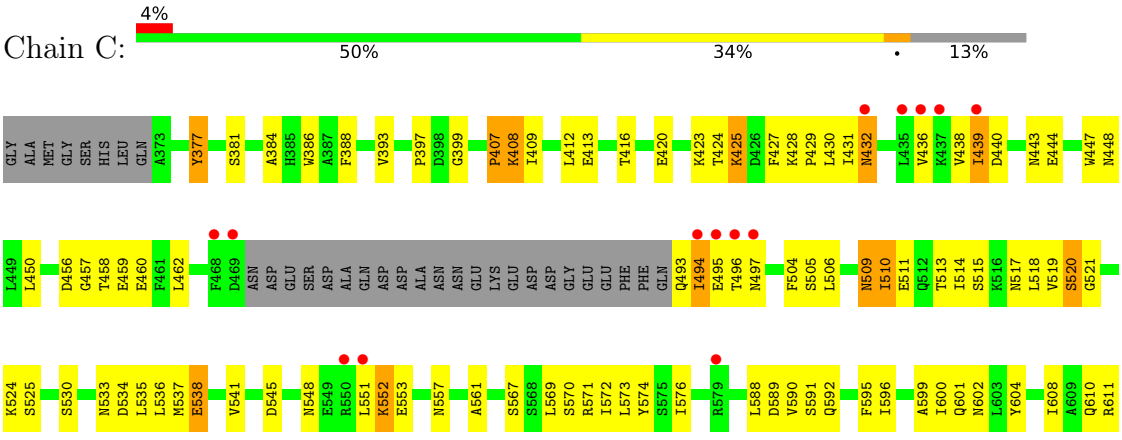
3 Residue-property plots (i)

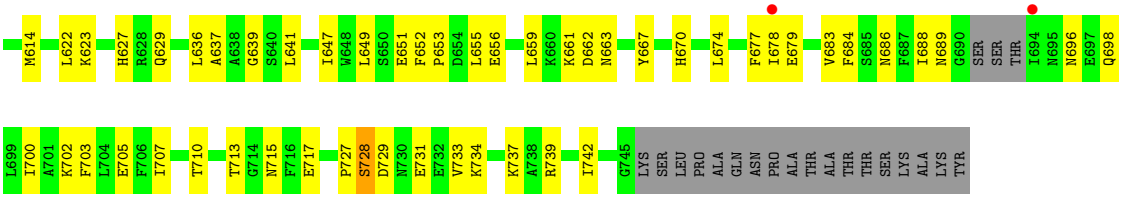
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein transport protein SEC31



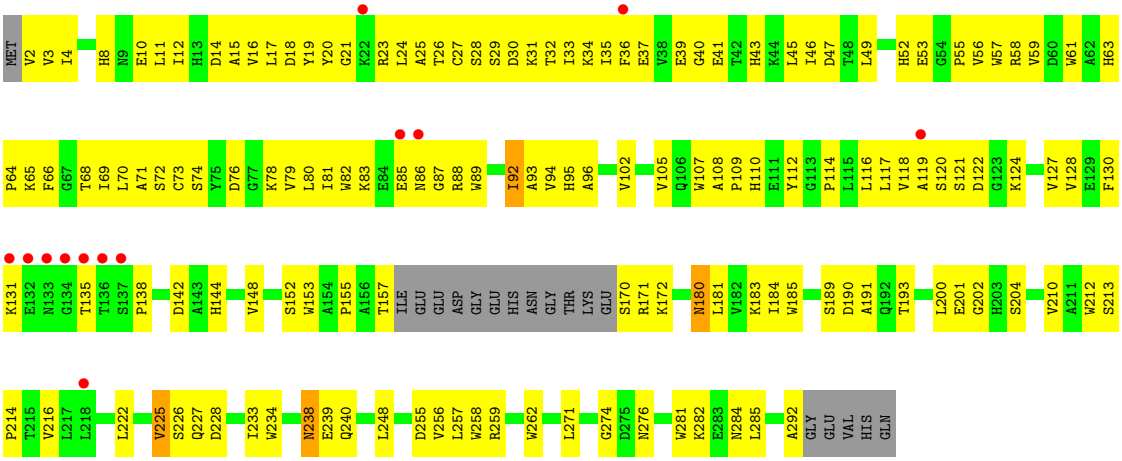
• Molecule 1: Protein transport protein SEC31





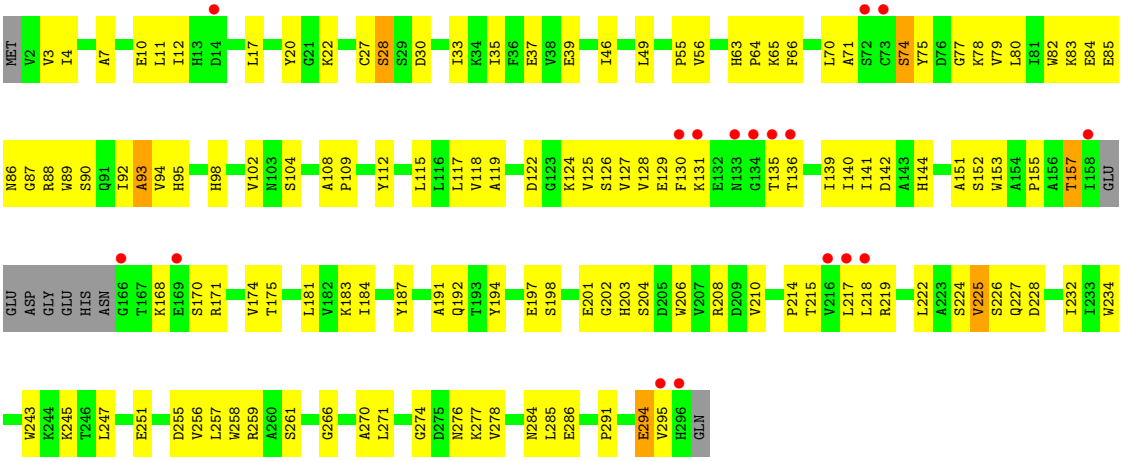
• Molecule 2: Protein transport protein SEC13

Chain B:



• Molecule 2: Protein transport protein SEC13

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	128.39Å 52.34Å 133.13Å 90.00° 108.62° 90.00°	Depositor
Resolution (Å)	30.00 – 2.45 26.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	88.0 (30.00-2.45) 88.0 (26.00-2.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.44Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.301 0.256 , 0.249	Depositor DCC
R_{free} test set	2997 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 71.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10195	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/2773	0.55	0/3744
1	C	0.38	0/2790	0.58	0/3767
2	B	0.39	0/2256	0.68	0/3079
2	D	0.44	0/2324	0.74	0/3170
All	All	0.39	0/10143	0.64	0/13760

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2729	0	2706	206	0
1	C	2746	0	2725	175	0
2	B	2196	0	2138	169	0
2	D	2263	0	2203	114	0
3	A	28	0	0	15	1
3	B	61	0	0	24	0
3	C	51	0	0	8	0
3	D	121	0	0	14	1
All	All	10195	0	9772	612	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 31.

All (612) 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:D:129:GLU:HG2	2:D:130:PHE:H	1.14	1.08
1:C:425:LYS:HE2	1:C:686:ASN:HD21	1.21	1.06
1:C:408:LYS:HD3	1:C:408:LYS:H	1.22	1.04
1:C:688:ILE:HG13	1:C:689:ASN:H	1.21	1.04
2:D:55:PRO:HA	3:D:416:HOH:O	1.55	1.04
1:A:431:ILE:HD11	1:A:683:VAL:HG11	1.42	1.01
2:B:11:LEU:O	2:B:28:SER:HB2	1.61	1.00
2:B:128:VAL:HG22	2:B:138:PRO:HB3	1.43	0.98
1:A:720:THR:HA	1:A:723:LEU:HD12	1.46	0.98
1:A:438:VAL:HG23	1:A:443:ASN:HD22	1.28	0.96
1:C:623:LYS:HE3	1:C:647:ILE:HD12	1.44	0.95
1:C:535:LEU:HB3	1:C:538:GLU:HG3	1.48	0.95
2:D:83:LYS:HB2	2:D:92:ILE:HD13	1.49	0.94
1:C:407:PRO:HD2	3:C:214:HOH:O	1.67	0.94
2:D:124:LYS:HG3	3:D:408:HOH:O	1.69	0.91
1:A:639:GLY:HA2	1:A:688:ILE:HD11	1.51	0.90
1:C:420:GLU:O	1:C:423:LYS:HG2	1.71	0.90
1:A:496:THR:HG23	1:C:557:ASN:HB3	1.54	0.89
2:B:81:ILE:HB	3:B:320:HOH:O	1.73	0.88
1:A:428:LYS:HB2	1:A:429:PRO:HD3	1.54	0.88
2:B:81:ILE:HD13	2:B:93:ALA:HB3	1.54	0.87
1:A:412:LEU:HD21	1:A:713:THR:HG22	1.57	0.86
1:C:649:LEU:HD22	1:C:698:GLN:HG2	1.55	0.86
1:C:425:LYS:O	1:C:425:LYS:HD3	1.75	0.86
3:A:245:HOH:O	1:C:602:ASN:HB3	1.75	0.85
1:A:592:GLN:HE21	1:C:506:LEU:HD12	1.40	0.85
2:D:129:GLU:HG2	2:D:130:PHE:N	1.88	0.85
1:C:408:LYS:HE3	2:D:294:GLU:HG2	1.59	0.84
2:B:257:LEU:HD13	2:B:271:LEU:HD21	1.59	0.84
2:B:83:LYS:O	2:B:89:TRP:HA	1.76	0.84
1:C:524:LYS:HG3	1:C:525:SER:H	1.43	0.84
1:C:703:PHE:O	1:C:707:ILE:HG12	1.78	0.84
1:C:494:ILE:HG13	1:C:495:GLU:H	1.42	0.84
2:B:12:ILE:HA	2:B:28:SER:HB3	1.59	0.83
1:A:505:SER:HB3	1:C:589:ASP:HB2	1.62	0.81
1:C:439:ILE:HG21	1:C:659:LEU:HD21	1.63	0.80
1:A:420:GLU:HA	1:A:423:LYS:HE2	1.63	0.80
1:A:518:LEU:HB3	1:C:576:ILE:HD13	1.63	0.80
1:C:427:PHE:O	1:C:431:ILE:HG12	1.81	0.79
2:D:152:SER:HB2	3:D:407:HOH:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:LYS:HD3	1:C:408:LYS:N	1.97	0.78
1:A:590:VAL:HG13	1:A:622:LEU:HD23	1.65	0.78
1:C:652:PHE:HB3	1:C:653:PRO:HD3	1.64	0.78
1:C:688:ILE:HG13	1:C:689:ASN:N	1.98	0.78
1:C:393:VAL:HG21	2:D:17:LEU:HG	1.66	0.77
1:A:589:ASP:HB2	1:C:505:SER:HB3	1.67	0.77
2:D:95:HIS:CD2	2:D:128:VAL:HG21	2.20	0.76
1:A:393:VAL:HG22	1:A:404:ILE:HG13	1.67	0.76
2:D:144:HIS:CE1	2:D:183:LYS:HD2	2.19	0.76
1:C:513:THR:HB	3:C:202:HOH:O	1.84	0.75
1:C:524:LYS:HG3	1:C:525:SER:N	2.01	0.75
1:A:719:ALA:O	1:A:723:LEU:HG	1.87	0.75
1:A:723:LEU:HD11	1:A:740:VAL:HG21	1.69	0.75
2:B:10:GLU:HB2	3:B:336:HOH:O	1.86	0.75
1:C:408:LYS:HE3	2:D:294:GLU:CG	2.17	0.74
1:A:652:PHE:HB3	1:A:653:PRO:HD3	1.69	0.74
2:B:117:LEU:HA	3:B:340:HOH:O	1.86	0.73
1:A:578:LYS:O	1:A:580:GLU:HG3	1.88	0.73
1:A:393:VAL:HG21	2:B:17:LEU:HG	1.69	0.73
1:A:496:THR:O	1:A:497:ASN:HB2	1.89	0.73
1:C:592:GLN:HG3	1:C:595:PHE:HB3	1.69	0.72
1:C:428:LYS:HB2	1:C:429:PRO:HD3	1.69	0.72
1:C:510:ILE:HD12	1:C:510:ILE:H	1.55	0.72
2:D:259:ARG:HB2	3:D:413:HOH:O	1.90	0.72
2:B:255:ASP:OD2	2:B:274:GLY:HA3	1.89	0.72
1:C:548:ASN:O	1:C:552:LYS:HB2	1.89	0.72
1:A:431:ILE:HD13	1:A:447:TRP:HZ3	1.55	0.71
2:B:105:VAL:HG23	2:B:118:VAL:HG22	1.73	0.71
1:A:518:LEU:HD13	1:C:576:ILE:HD12	1.73	0.71
1:A:388:PHE:HB2	1:A:739:ARG:HH21	1.56	0.70
1:A:428:LYS:NZ	1:A:455:MET:HG2	2.06	0.70
1:C:567:SER:HB3	1:C:570:SER:HB2	1.73	0.70
1:A:665:THR:OG1	1:A:668:GLU:HG3	1.91	0.70
1:A:420:GLU:HG3	1:A:423:LYS:HE2	1.72	0.70
2:B:74:SER:HB3	2:B:76:ASP:OD1	1.91	0.70
1:A:595:PHE:CZ	1:C:515:SER:HB2	2.28	0.69
2:D:78:LYS:HD2	3:D:378:HOH:O	1.91	0.69
2:D:95:HIS:NE2	2:D:128:VAL:HG21	2.08	0.69
2:B:24:LEU:HB3	2:B:36:PHE:HB2	1.76	0.68
1:C:444:GLU:HG2	1:C:448:ASN:ND2	2.08	0.68
2:B:144:HIS:CE1	2:B:183:LYS:HD2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ILE:HD11	2:B:248:LEU:HD13	1.76	0.68
1:A:528:LYS:HG3	1:C:493:GLN:HE22	1.58	0.67
1:A:736:GLU:O	1:A:740:VAL:HG23	1.93	0.67
1:C:425:LYS:HE2	1:C:686:ASN:ND2	2.02	0.67
2:B:53:GLU:HG3	3:B:337:HOH:O	1.93	0.67
1:A:427:PHE:O	1:A:431:ILE:HG12	1.94	0.67
1:A:590:VAL:HG13	1:A:622:LEU:CD2	2.23	0.67
1:A:402:VAL:HG11	2:B:24:LEU:HD21	1.76	0.67
1:C:509:ASN:N	1:C:509:ASN:HD22	1.92	0.67
2:D:129:GLU:O	2:D:136:THR:HG22	1.94	0.66
1:A:536:LEU:O	1:A:540:MET:HG3	1.96	0.66
1:A:498:PHE:HB2	1:C:561:ALA:HA	1.77	0.66
1:A:639:GLY:CA	1:A:688:ILE:HD11	2.25	0.66
1:C:439:ILE:HG13	1:C:440:ASP:H	1.60	0.66
1:C:535:LEU:HB3	1:C:538:GLU:CG	2.23	0.66
1:A:557:ASN:HB3	1:C:496:THR:HG23	1.77	0.65
1:C:590:VAL:HG13	1:C:622:LEU:CD2	2.25	0.65
2:D:184:ILE:HD11	2:D:222:LEU:HD11	1.78	0.65
2:B:157:THR:OG1	2:B:170:SER:HB2	1.95	0.65
1:A:414:SER:OG	1:A:715:ASN:HB2	1.96	0.65
1:C:416:THR:HG22	1:C:420:GLU:OE2	1.96	0.65
1:C:647:ILE:O	1:C:651:GLU:HG3	1.96	0.65
2:D:33:ILE:CD1	2:D:56:VAL:HG11	2.27	0.65
2:D:225:VAL:HG22	2:D:257:LEU:HB3	1.77	0.65
1:A:519:VAL:HG13	1:C:599:ALA:HA	1.79	0.65
2:D:49:LEU:HB3	2:D:82:TRP:CZ3	2.32	0.65
1:A:427:PHE:CD2	1:A:683:VAL:HG22	2.31	0.65
1:A:608:ILE:HB	1:A:611:ARG:HH12	1.62	0.64
1:C:408:LYS:H	1:C:408:LYS:CD	2.05	0.64
1:A:557:ASN:HB3	1:C:496:THR:CG2	2.27	0.64
2:B:40:GLY:N	3:B:335:HOH:O	2.30	0.64
2:B:33:ILE:HD11	2:B:56:VAL:HG11	1.80	0.64
2:D:225:VAL:HG22	2:D:257:LEU:CB	2.27	0.64
1:A:727:PRO:C	1:A:729:ASP:H	2.01	0.64
2:B:18:ASP:HB2	3:B:317:HOH:O	1.97	0.63
2:B:102:VAL:CG2	3:B:353:HOH:O	2.45	0.63
2:B:274:GLY:C	2:B:276:ASN:H	2.00	0.63
1:A:608:ILE:HD13	1:A:611:ARG:HH11	1.62	0.63
2:B:238:ASN:HD22	2:B:240:GLN:H	1.44	0.63
1:A:458:THR:HG23	1:A:459:GLU:N	2.14	0.63
1:A:592:GLN:HG3	1:A:595:PHE:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:174:VAL:HG23	2:D:183:LYS:O	1.99	0.63
2:B:23:ARG:NH1	2:B:68:THR:HG21	2.14	0.63
1:C:519:VAL:C	1:C:521:GLY:H	2.02	0.63
1:A:438:VAL:HG23	1:A:443:ASN:ND2	2.07	0.62
1:C:641:LEU:HD13	1:C:688:ILE:HG21	1.82	0.62
1:C:510:ILE:HA	3:C:202:HOH:O	1.99	0.62
2:B:12:ILE:HA	2:B:28:SER:CB	2.30	0.62
1:A:596:ILE:O	1:A:600:ILE:HG12	2.00	0.62
1:A:703:PHE:HA	3:A:200:HOH:O	2.00	0.62
2:B:66:PHE:HE2	2:B:114:PRO:HD3	1.65	0.62
1:A:514:ILE:HA	1:A:517:ASN:HD22	1.65	0.62
1:C:639:GLY:HA2	1:C:688:ILE:HD11	1.81	0.62
1:A:517:ASN:ND2	1:A:529:ASN:HD22	1.98	0.61
1:A:592:GLN:HG3	1:A:592:GLN:O	1.99	0.61
2:B:102:VAL:HG23	3:B:353:HOH:O	2.00	0.61
2:B:157:THR:HG22	2:B:157:THR:O	2.00	0.61
1:A:392:LEU:HD13	3:A:219:HOH:O	2.00	0.61
1:A:458:THR:HG23	1:A:459:GLU:H	1.66	0.61
2:B:3:VAL:C	2:B:4:ILE:HD12	2.21	0.61
1:C:604:TYR:CE2	1:C:610:GLN:HG2	2.36	0.61
1:C:742:ILE:HD12	2:D:20:TYR:CE2	2.35	0.61
2:B:37:GLU:HG2	2:B:46:ILE:HG13	1.82	0.61
2:B:257:LEU:CD1	2:B:271:LEU:HD21	2.30	0.61
2:B:30:ASP:OD1	2:B:32:THR:N	2.34	0.61
1:A:742:ILE:HB	2:B:20:TYR:CD2	2.36	0.61
1:A:518:LEU:HB3	1:C:576:ILE:CD1	2.31	0.60
1:A:608:ILE:CD1	1:A:611:ARG:HH11	2.14	0.60
2:B:155:PRO:HG3	2:B:214:PRO:HA	1.83	0.60
1:A:675:THR:O	1:A:679:GLU:HG3	2.01	0.60
2:B:4:ILE:HG13	2:B:43:HIS:ND1	2.16	0.60
1:C:553:GLU:HG2	1:C:557:ASN:HD21	1.66	0.60
1:A:559:TYR:CD2	1:C:541:VAL:HG21	2.35	0.60
1:A:519:VAL:C	1:A:521:GLY:H	2.05	0.60
1:C:458:THR:HG23	1:C:459:GLU:H	1.65	0.60
2:B:200:LEU:HB3	2:B:234:TRP:CZ3	2.36	0.60
1:A:537:MET:O	1:A:541:VAL:HG23	2.02	0.60
1:A:396:THR:HG23	3:A:251:HOH:O	2.01	0.60
2:D:274:GLY:C	2:D:276:ASN:H	2.05	0.60
2:B:29:SER:HA	2:B:55:PRO:HB3	1.84	0.59
1:C:377:TYR:HB3	3:C:113:HOH:O	2.02	0.59
2:D:291:PRO:CB	2:D:295:VAL:HG22	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ASN:N	2:B:180:ASN:HD22	2.00	0.59
1:C:670:HIS:HE1	1:C:705:GLU:OE1	1.86	0.59
1:A:709:LEU:O	1:A:713:THR:HG23	2.02	0.59
2:B:52:HIS:HA	3:B:337:HOH:O	2.01	0.59
2:B:216:VAL:HG12	2:B:216:VAL:O	2.03	0.59
1:A:386:TRP:HA	3:A:219:HOH:O	2.01	0.59
2:D:49:LEU:HD13	2:D:82:TRP:CD2	2.37	0.59
1:A:496:THR:O	1:A:497:ASN:CB	2.51	0.59
1:A:388:PHE:CD1	1:A:739:ARG:CZ	2.86	0.59
2:B:120:SER:HB3	2:B:122:ASP:OD1	2.03	0.59
1:A:674:LEU:O	1:A:678:ILE:HG12	2.03	0.59
1:A:730:ASN:O	1:A:733:VAL:HB	2.03	0.59
1:C:663:ASN:O	2:D:285:LEU:HD11	2.03	0.59
2:B:19:TYR:CD2	2:B:64:PRO:HG2	2.38	0.59
1:A:584:LEU:HD12	1:A:584:LEU:N	2.18	0.58
1:C:592:GLN:HG3	1:C:595:PHE:CB	2.33	0.58
1:A:496:THR:HG23	1:C:557:ASN:CB	2.31	0.58
1:A:511:GLU:HG3	3:A:107:HOH:O	2.03	0.58
2:B:68:THR:C	2:B:69:ILE:HD12	2.23	0.58
1:C:661:LYS:C	1:C:663:ASN:H	2.06	0.58
2:B:83:LYS:HB2	2:B:92:ILE:HD13	1.85	0.58
2:D:3:VAL:C	2:D:4:ILE:HD12	2.23	0.58
1:A:509:ASN:N	1:A:509:ASN:HD22	2.01	0.58
2:B:225:VAL:HG13	2:B:257:LEU:HB2	1.84	0.58
1:C:438:VAL:HG23	1:C:443:ASN:HD22	1.68	0.58
1:A:612:ASN:O	1:A:616:ILE:HG12	2.03	0.58
2:B:24:LEU:HG	2:B:25:ALA:N	2.19	0.58
2:B:108:ALA:HB1	2:B:109:PRO:CD	2.34	0.57
1:A:731:GLU:O	1:A:734:LYS:HB3	2.04	0.57
1:C:656:GLU:OE2	1:C:670:HIS:HA	2.04	0.57
2:D:255:ASP:OD1	2:D:256:VAL:N	2.35	0.57
1:A:438:VAL:HG22	1:A:439:ILE:N	2.20	0.57
2:B:222:LEU:HB2	2:B:234:TRP:HB2	1.85	0.57
1:A:423:LYS:HG3	1:A:424:THR:HG23	1.86	0.57
1:C:727:PRO:C	1:C:729:ASP:H	2.06	0.57
1:A:468:PHE:CE1	1:A:598:LYS:HE3	2.40	0.57
2:D:79:VAL:HB	2:D:95:HIS:HB3	1.86	0.57
1:A:418:LEU:HG	1:A:718:LEU:HD11	1.87	0.57
1:A:647:ILE:O	1:A:651:GLU:HG3	2.04	0.57
1:C:430:LEU:HD11	1:C:679:GLU:HG2	1.86	0.56
1:C:535:LEU:CB	1:C:538:GLU:HG3	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ILE:HG13	2:B:43:HIS:CG	2.40	0.56
2:B:189:SER:C	2:B:191:ALA:H	2.09	0.56
1:C:462:LEU:HD22	1:C:637:ALA:HB2	1.87	0.56
1:A:616:ILE:HD11	1:A:640:SER:HB2	1.88	0.56
1:A:584:LEU:HD12	1:A:584:LEU:H	1.71	0.56
1:C:509:ASN:N	1:C:509:ASN:ND2	2.51	0.56
2:B:4:ILE:HD12	2:B:4:ILE:N	2.20	0.56
1:C:431:ILE:HD11	1:C:683:VAL:HG11	1.88	0.56
2:D:155:PRO:HG3	2:D:214:PRO:HA	1.88	0.56
2:B:69:ILE:HD12	2:B:69:ILE:N	2.21	0.56
1:A:509:ASN:N	1:A:509:ASN:ND2	2.54	0.55
1:A:730:ASN:HB3	1:A:733:VAL:CG2	2.36	0.55
2:B:180:ASN:N	2:B:180:ASN:ND2	2.53	0.55
1:A:434:ARG:HG3	1:A:447:TRP:CZ2	2.41	0.55
1:C:519:VAL:HG23	1:C:520:SER:N	2.21	0.55
1:A:528:LYS:HG3	1:C:493:GLN:NE2	2.22	0.55
2:B:66:PHE:CE2	2:B:114:PRO:HD3	2.41	0.55
2:B:8:HIS:ND1	2:B:30:ASP:OD2	2.39	0.55
2:B:56:VAL:HA	2:B:74:SER:HB2	1.88	0.55
2:D:210:VAL:HG23	2:D:210:VAL:O	2.06	0.55
1:A:420:GLU:HG3	1:A:423:LYS:CE	2.37	0.55
1:C:444:GLU:HG2	1:C:448:ASN:HD21	1.71	0.55
1:C:663:ASN:C	2:D:285:LEU:HD11	2.26	0.55
2:B:73:CYS:HB2	2:B:102:VAL:CG1	2.37	0.55
2:D:4:ILE:HD12	2:D:4:ILE:N	2.22	0.55
2:D:33:ILE:HD11	2:D:56:VAL:HG11	1.87	0.54
1:C:535:LEU:HD22	1:C:538:GLU:HG3	1.88	0.54
1:C:733:VAL:O	1:C:737:LYS:HG3	2.07	0.54
2:D:226:SER:HB3	2:D:228:ASP:OD1	2.07	0.54
1:A:510:ILE:HB	3:A:107:HOH:O	2.06	0.54
1:A:623:LYS:HE3	1:A:647:ILE:HD12	1.89	0.54
1:A:517:ASN:HD21	1:A:529:ASN:ND2	2.04	0.54
1:C:590:VAL:HG13	1:C:622:LEU:HD23	1.90	0.54
2:D:271:LEU:O	2:D:278:VAL:HA	2.08	0.54
1:A:723:LEU:HA	3:A:255:HOH:O	2.08	0.54
2:B:45:LEU:O	2:B:46:ILE:HD13	2.08	0.54
1:C:423:LYS:CG	1:C:424:THR:N	2.71	0.54
2:D:86:ASN:O	2:D:88:ARG:N	2.40	0.54
1:A:418:LEU:HD23	1:A:718:LEU:HD21	1.89	0.53
2:D:28:SER:O	3:D:416:HOH:O	2.19	0.53
2:D:56:VAL:HA	2:D:74:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:TYR:CZ	1:C:610:GLN:HG2	2.43	0.53
1:C:510:ILE:HG21	1:C:533:ASN:ND2	2.23	0.53
1:C:696:ASN:O	1:C:700:ILE:HG13	2.08	0.53
1:A:742:ILE:H	1:A:742:ILE:HD12	1.73	0.53
2:D:104:SER:OG	2:D:119:ALA:HB3	2.08	0.53
2:B:49:LEU:HB3	2:B:82:TRP:CZ3	2.44	0.53
2:B:80:LEU:CD2	2:B:94:VAL:HG23	2.38	0.53
1:C:707:ILE:O	1:C:710:THR:HB	2.09	0.53
2:D:10:GLU:HG3	2:D:30:ASP:HB3	1.90	0.53
1:A:439:ILE:HG21	1:A:659:LEU:HD21	1.90	0.53
2:B:39:GLU:HB2	3:B:335:HOH:O	2.08	0.53
1:A:388:PHE:CD1	1:A:739:ARG:NH2	2.77	0.53
2:D:227:GLN:HA	2:D:256:VAL:HG13	1.90	0.53
1:A:649:LEU:HB3	1:A:698:GLN:OE1	2.09	0.53
2:D:225:VAL:CG2	2:D:271:LEU:HD11	2.38	0.53
2:D:232:ILE:HD13	2:D:247:LEU:HD23	1.91	0.53
1:A:531:LEU:C	1:A:533:ASN:H	2.13	0.52
2:B:25:ALA:HB2	2:B:61:TRP:CZ2	2.44	0.52
1:C:494:ILE:HG13	1:C:495:GLU:N	2.18	0.52
2:D:83:LYS:HB3	2:D:92:ILE:HG21	1.90	0.52
2:D:22:LYS:HE2	2:D:39:GLU:OE1	2.09	0.52
2:D:294:GLU:O	2:D:294:GLU:HG3	2.09	0.52
2:B:128:VAL:CG2	2:B:138:PRO:HB3	2.27	0.52
2:D:175:THR:C	3:D:369:HOH:O	2.47	0.52
1:A:608:ILE:HD13	1:A:611:ARG:NH1	2.24	0.52
1:A:505:SER:CB	1:C:589:ASP:HB2	2.37	0.52
1:A:584:LEU:H	1:A:584:LEU:CD1	2.22	0.52
2:B:80:LEU:HD23	2:B:94:VAL:HG23	1.90	0.52
1:A:593:TRP:C	1:A:595:PHE:H	2.13	0.52
1:A:451:GLU:O	1:A:454:SER:HB3	2.09	0.52
2:D:232:ILE:HG21	2:D:234:TRP:CE2	2.44	0.52
2:B:33:ILE:CD1	2:B:56:VAL:HG11	2.39	0.52
2:B:117:LEU:HD12	3:B:340:HOH:O	2.08	0.52
1:C:674:LEU:HD21	1:C:705:GLU:HB3	1.91	0.52
1:A:420:GLU:CA	1:A:423:LYS:HE2	2.38	0.52
2:B:69:ILE:HG22	2:B:70:LEU:N	2.25	0.52
1:A:688:ILE:HD13	1:A:689:ASN:N	2.25	0.51
1:A:551:LEU:C	1:A:553:GLU:H	2.11	0.51
1:C:377:TYR:HA	3:C:113:HOH:O	2.11	0.51
1:C:519:VAL:C	1:C:521:GLY:N	2.63	0.51
2:B:95:HIS:CE1	2:B:128:VAL:HG21	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:LEU:HD23	1:C:430:LEU:O	2.11	0.51
1:A:431:ILE:HD13	1:A:447:TRP:CZ3	2.40	0.51
1:A:519:VAL:CG1	1:C:599:ALA:HA	2.40	0.51
2:D:84:GLU:HB2	2:D:89:TRP:CE2	2.46	0.51
2:D:126:SER:HA	2:D:139:ILE:O	2.11	0.51
2:D:217:LEU:O	2:D:219:ARG:N	2.44	0.51
1:C:677:PHE:CD2	1:C:678:ILE:HD12	2.46	0.51
1:A:524:LYS:HG3	1:A:525:SER:N	2.26	0.50
2:B:238:ASN:HD22	2:B:240:GLN:N	2.07	0.50
2:D:115:LEU:HD11	2:D:127:VAL:HG12	1.93	0.50
1:C:494:ILE:HG23	1:C:495:GLU:N	2.26	0.50
1:C:636:LEU:HD12	1:C:688:ILE:HD12	1.93	0.50
2:D:11:LEU:O	2:D:28:SER:HB2	2.12	0.50
2:D:55:PRO:HD2	2:D:75:TYR:HB3	1.92	0.50
1:A:567:SER:HB3	1:A:570:SER:HB2	1.93	0.50
2:B:4:ILE:O	2:B:4:ILE:HG22	2.11	0.50
2:B:33:ILE:HB	2:B:49:LEU:HB2	1.92	0.50
1:A:664:LYS:HA	1:A:668:GLU:OE1	2.11	0.50
2:B:255:ASP:CG	2:B:256:VAL:H	2.14	0.50
2:B:259:ARG:HG3	2:B:259:ARG:HH11	1.77	0.50
1:C:397:PRO:HA	2:D:276:ASN:HD21	1.77	0.50
1:A:608:ILE:HB	1:A:611:ARG:NH1	2.27	0.50
2:B:26:THR:O	2:B:33:ILE:HG23	2.12	0.50
2:D:215:THR:HG23	2:D:215:THR:O	2.11	0.50
2:B:112:TYR:CZ	2:B:171:ARG:HG2	2.47	0.50
1:C:601:GLN:HE22	1:C:611:ARG:HD3	1.77	0.50
1:A:402:VAL:HG11	2:B:24:LEU:CD2	2.42	0.49
2:B:105:VAL:CG2	2:B:116:LEU:HD21	2.41	0.49
2:B:200:LEU:HD13	2:B:234:TRP:CE3	2.47	0.49
2:D:33:ILE:HB	2:D:49:LEU:HB2	1.94	0.49
1:A:432:ASN:O	1:A:436:VAL:HG23	2.11	0.49
1:A:663:ASN:HA	2:B:285:LEU:HD11	1.94	0.49
2:B:95:HIS:HE1	2:B:138:PRO:HG3	1.77	0.49
1:C:551:LEU:HD23	1:C:551:LEU:C	2.33	0.49
2:D:10:GLU:CG	2:D:30:ASP:HB3	2.42	0.49
2:D:203:HIS:CE1	2:D:232:ILE:HG12	2.48	0.49
2:B:63:HIS:CD2	3:B:334:HOH:O	2.65	0.49
2:B:148:VAL:O	3:B:338:HOH:O	2.20	0.49
2:D:261:SER:HA	3:D:351:HOH:O	2.13	0.49
1:C:530:SER:O	1:C:533:ASN:O	2.31	0.49
1:A:585:VAL:HA	1:A:596:ILE:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:222:LEU:HG	2:D:243:TRP:CZ3	2.48	0.49
1:A:430:LEU:O	1:A:430:LEU:HD23	2.13	0.49
1:A:731:GLU:HA	1:A:734:LYS:HB3	1.93	0.49
1:A:555:VAL:O	1:A:558:ALA:HB3	2.12	0.49
1:A:568:SER:HB2	1:C:511:GLU:OE1	2.13	0.49
1:A:496:THR:HG22	1:A:497:ASN:N	2.27	0.49
2:B:184:ILE:N	2:B:184:ILE:HD12	2.28	0.49
2:D:70:LEU:HG	2:D:71:ALA:N	2.28	0.49
1:A:593:TRP:C	1:A:595:PHE:N	2.66	0.48
2:B:57:TRP:O	2:B:58:ARG:HG2	2.14	0.48
1:A:466:LEU:O	1:A:598:LYS:HE2	2.13	0.48
1:A:536:LEU:HD23	1:C:537:MET:HE3	1.94	0.48
1:A:644:VAL:HG11	1:A:684:PHE:CE2	2.48	0.48
2:D:94:VAL:O	2:D:94:VAL:HG13	2.11	0.48
2:B:108:ALA:HA	2:B:153:TRP:CD1	2.49	0.48
2:B:225:VAL:HG13	2:B:257:LEU:CB	2.43	0.48
2:D:27:CYS:HB2	2:D:56:VAL:HB	1.94	0.48
1:C:388:PHE:CE1	1:C:739:ARG:HD3	2.49	0.48
1:C:728:SER:HB3	1:C:737:LYS:NZ	2.29	0.48
1:C:733:VAL:HG12	1:C:737:LYS:HE3	1.95	0.48
2:D:10:GLU:HB2	2:D:28:SER:OG	2.14	0.48
2:B:29:SER:C	2:B:31:LYS:H	2.16	0.48
2:B:59:VAL:HA	2:B:71:ALA:O	2.14	0.48
2:B:212:TRP:CD2	2:B:222:LEU:HD21	2.49	0.48
1:C:514:ILE:HA	1:C:517:ASN:HD22	1.79	0.48
2:D:227:GLN:HG2	3:D:409:HOH:O	2.13	0.48
2:D:90:SER:O	2:D:92:ILE:HG23	2.14	0.48
2:B:69:ILE:CG2	2:B:70:LEU:N	2.77	0.48
1:C:439:ILE:HG13	1:C:440:ASP:N	2.27	0.48
1:A:514:ILE:HA	1:A:517:ASN:ND2	2.28	0.48
2:B:8:HIS:CE1	2:B:34:LYS:HE2	2.48	0.47
2:B:15:ALA:HA	2:B:25:ALA:O	2.14	0.47
1:C:456:ASP:O	1:C:460:GLU:HB2	2.14	0.47
1:C:727:PRO:C	1:C:729:ASP:N	2.67	0.47
1:A:664:LYS:HB3	1:A:668:GLU:HB2	1.95	0.47
2:B:74:SER:CB	2:B:76:ASP:OD1	2.61	0.47
2:B:93:ALA:HB1	3:B:344:HOH:O	2.14	0.47
1:A:412:LEU:C	1:A:412:LEU:HD23	2.35	0.47
2:B:72:SER:O	2:B:79:VAL:HG13	2.14	0.47
2:B:172:LYS:HA	2:B:185:TRP:O	2.14	0.47
2:B:119:ALA:HB1	2:B:148:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:LYS:CE	2:D:294:GLU:HG2	2.36	0.47
1:A:426:ASP:OD1	1:A:429:PRO:HD3	2.14	0.47
2:B:27:CYS:HB2	2:B:56:VAL:CG1	2.45	0.47
1:C:424:THR:O	1:C:425:LYS:CB	2.62	0.47
2:B:34:LYS:HB3	2:B:36:PHE:HE1	1.80	0.47
1:C:438:VAL:HG21	1:C:444:GLU:HA	1.97	0.47
2:D:276:ASN:ND2	3:D:310:HOH:O	2.47	0.47
2:B:109:PRO:HD2	2:B:112:TYR:CD1	2.50	0.47
2:B:119:ALA:HB1	2:B:148:VAL:CG1	2.45	0.47
1:C:386:TRP:NE1	2:D:270:ALA:HB2	2.30	0.47
1:A:593:TRP:O	1:A:595:PHE:N	2.48	0.47
2:B:29:SER:O	2:B:31:LYS:HG3	2.14	0.47
2:D:92:ILE:O	2:D:93:ALA:HB2	2.15	0.47
1:A:392:LEU:CD1	3:A:219:HOH:O	2.61	0.47
1:A:652:PHE:HB3	1:A:653:PRO:CD	2.44	0.47
1:A:572:ILE:CD1	1:C:504:PHE:HE1	2.28	0.47
1:A:608:ILE:CD1	1:A:611:ARG:NH1	2.78	0.47
2:B:18:ASP:OD2	2:B:23:ARG:HB3	2.14	0.47
2:B:233:ILE:CD1	2:B:248:LEU:HD13	2.43	0.47
1:C:412:LEU:CD2	1:C:713:THR:HG22	2.45	0.47
1:C:641:LEU:HD12	1:C:684:PHE:HE2	1.80	0.47
1:C:731:GLU:HA	1:C:734:LYS:HB3	1.97	0.47
2:D:35:ILE:HG13	2:D:89:TRP:CE2	2.50	0.47
2:D:108:ALA:HB2	2:D:153:TRP:CE2	2.50	0.47
1:A:536:LEU:HD23	1:C:537:MET:CE	2.46	0.46
1:C:553:GLU:HG2	1:C:557:ASN:ND2	2.28	0.46
2:D:225:VAL:HG21	2:D:271:LEU:HD11	1.97	0.46
2:D:277:LYS:HG3	2:D:278:VAL:N	2.30	0.46
2:B:259:ARG:HG3	2:B:259:ARG:NH1	2.30	0.46
2:D:222:LEU:HB2	2:D:234:TRP:HB2	1.97	0.46
1:A:462:LEU:HD13	1:A:637:ALA:HB2	1.97	0.46
1:A:542:ILE:HD11	1:C:573:LEU:CD2	2.44	0.46
1:A:542:ILE:HD11	1:C:573:LEU:HD21	1.96	0.46
1:C:438:VAL:HG23	1:C:443:ASN:ND2	2.30	0.46
2:D:141:ILE:HG22	3:D:322:HOH:O	2.14	0.46
2:D:274:GLY:C	2:D:276:ASN:N	2.69	0.46
2:B:37:GLU:HG2	2:B:46:ILE:CG1	2.44	0.46
2:D:245:LYS:NZ	3:D:335:HOH:O	2.44	0.46
1:A:441:ASP:HA	3:A:212:HOH:O	2.15	0.46
2:B:124:LYS:HE2	2:B:142:ASP:OD1	2.15	0.46
2:B:200:LEU:HB3	2:B:234:TRP:CH2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:TRP:HZ3	3:C:214:HOH:O	1.98	0.46
2:D:98:HIS:ND1	2:D:122:ASP:OD2	2.49	0.46
1:A:727:PRO:C	1:A:729:ASP:N	2.69	0.46
1:A:739:ARG:HD2	2:B:19:TYR:CZ	2.50	0.46
2:D:65:LYS:HE2	2:D:66:PHE:CZ	2.50	0.46
1:A:718:LEU:O	1:A:722:PHE:HD1	1.98	0.46
2:B:31:LYS:O	3:B:321:HOH:O	2.20	0.46
1:C:641:LEU:HD12	1:C:684:PHE:CE2	2.51	0.46
1:A:436:VAL:HG12	1:A:436:VAL:O	2.16	0.46
1:A:663:ASN:CA	2:B:285:LEU:HD11	2.46	0.46
2:B:25:ALA:HB2	2:B:61:TRP:HZ2	1.81	0.46
2:B:117:LEU:HB2	2:B:153:TRP:NE1	2.31	0.46
2:D:284:ASN:OD1	2:D:286:GLU:N	2.49	0.46
2:B:127:VAL:HA	3:B:340:HOH:O	2.15	0.46
2:B:29:SER:C	2:B:31:LYS:N	2.70	0.45
1:A:392:LEU:HA	3:A:219:HOH:O	2.16	0.45
1:A:412:LEU:CD2	1:A:713:THR:HG22	2.38	0.45
2:B:121:SER:HA	3:B:338:HOH:O	2.15	0.45
1:C:458:THR:HG23	1:C:459:GLU:N	2.30	0.45
2:D:77:GLY:HA2	2:D:102:VAL:HG23	1.98	0.45
1:A:581:VAL:HG11	1:A:600:ILE:HD13	1.98	0.45
2:D:80:LEU:HD23	2:D:94:VAL:HG23	1.98	0.45
2:B:30:ASP:OD1	2:B:30:ASP:C	2.55	0.45
1:C:596:ILE:O	1:C:600:ILE:HG13	2.16	0.45
1:A:543:ALA:C	1:A:545:ASP:H	2.19	0.45
1:A:601:GLN:HE22	1:A:611:ARG:HD3	1.82	0.45
2:B:284:ASN:HB2	3:B:352:HOH:O	2.16	0.45
1:C:431:ILE:HD13	1:C:447:TRP:HZ3	1.82	0.45
1:C:639:GLY:HA2	1:C:688:ILE:CD1	2.47	0.45
2:D:37:GLU:HB2	2:D:46:ILE:HD11	1.98	0.45
1:A:559:TYR:CE2	1:C:541:VAL:HG21	2.52	0.45
2:B:274:GLY:C	2:B:276:ASN:N	2.69	0.45
1:C:524:LYS:CG	1:C:525:SER:H	2.24	0.45
2:B:66:PHE:CD2	2:B:114:PRO:HB3	2.51	0.45
2:B:191:ALA:HB1	2:B:193:THR:HG22	1.99	0.45
1:C:590:VAL:O	1:C:590:VAL:CG1	2.64	0.45
1:C:674:LEU:O	1:C:678:ILE:HD13	2.15	0.45
2:D:30:ASP:OD1	2:D:30:ASP:C	2.54	0.45
1:A:564:GLY:HA2	1:A:570:SER:OG	2.16	0.45
2:B:239:GLU:HG3	3:B:327:HOH:O	2.16	0.45
1:C:727:PRO:O	1:C:729:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:LYS:CB	2:D:92:ILE:HG21	2.47	0.45
2:D:139:ILE:O	2:D:140:ILE:HD13	2.16	0.45
2:B:30:ASP:OD1	2:B:32:THR:HG23	2.17	0.45
2:B:35:ILE:HG13	2:B:89:TRP:CE2	2.51	0.45
1:C:399:GLY:O	2:D:11:LEU:HD12	2.17	0.45
1:C:432:ASN:O	1:C:436:VAL:HG23	2.16	0.45
2:B:4:ILE:HG21	2:B:36:PHE:CE2	2.52	0.45
2:B:181:LEU:CD2	2:B:201:GLU:HG2	2.47	0.45
1:A:399:GLY:O	2:B:11:LEU:HD12	2.17	0.44
1:A:449:LEU:O	1:A:453:LEU:HB2	2.17	0.44
1:C:377:TYR:CA	3:C:113:HOH:O	2.64	0.44
1:C:622:LEU:O	1:C:627:HIS:HB2	2.16	0.44
2:D:108:ALA:HB1	2:D:109:PRO:HD2	2.00	0.44
1:A:537:MET:CE	1:C:536:LEU:HD23	2.48	0.44
1:A:604:TYR:N	1:A:605:PRO:CD	2.81	0.44
1:A:573:LEU:HD23	1:C:518:LEU:CD1	2.47	0.44
2:B:14:ASP:HB3	2:B:27:CYS:SG	2.58	0.44
1:C:652:PHE:HB3	1:C:653:PRO:CD	2.42	0.44
1:A:379:GLU:HG2	2:B:258:TRP:CZ2	2.53	0.44
1:A:504:PHE:CZ	1:C:588:LEU:HD13	2.52	0.44
1:A:688:ILE:HG12	1:A:689:ASN:H	1.82	0.44
2:B:105:VAL:HG22	2:B:116:LEU:HD11	1.99	0.44
2:D:142:ASP:HB3	3:D:366:HOH:O	2.17	0.44
2:D:187:TYR:HB2	2:D:194:TYR:CE2	2.53	0.44
1:A:688:ILE:CG1	1:A:689:ASN:H	2.31	0.44
1:C:608:ILE:HD13	1:C:611:ARG:NH1	2.33	0.44
2:D:112:TYR:CZ	2:D:171:ARG:HG2	2.53	0.44
1:A:706:PHE:CB	3:A:200:HOH:O	2.66	0.44
2:B:85:GLU:O	2:B:86:ASN:HB2	2.18	0.44
2:D:184:ILE:O	2:D:197:GLU:HB2	2.17	0.44
1:A:551:LEU:C	1:A:553:GLU:N	2.71	0.44
2:B:102:VAL:HG22	3:B:353:HOH:O	2.13	0.44
2:B:213:SER:HB2	2:B:262:TRP:CE2	2.53	0.44
2:D:63:HIS:ND1	2:D:64:PRO:HD2	2.32	0.43
2:D:108:ALA:HB1	2:D:109:PRO:CD	2.48	0.43
1:A:639:GLY:HA2	1:A:688:ILE:CD1	2.35	0.43
2:B:63:HIS:CE1	2:B:65:LYS:HB3	2.53	0.43
2:B:112:TYR:N	2:B:112:TYR:CD2	2.86	0.43
1:C:571:ARG:O	1:C:574:TYR:HB3	2.18	0.43
1:C:614:MET:HA	1:C:614:MET:HE2	1.99	0.43
2:D:10:GLU:HB2	2:D:28:SER:HG	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LYS:HG3	1:A:424:THR:N	2.33	0.43
1:C:384:ALA:N	3:D:413:HOH:O	2.50	0.43
1:C:420:GLU:HA	1:C:423:LYS:HD3	2.01	0.43
1:C:636:LEU:HD12	1:C:688:ILE:CD1	2.48	0.43
1:A:422:LEU:CD2	1:A:721:GLU:HG2	2.49	0.43
1:A:519:VAL:C	1:A:521:GLY:N	2.71	0.43
1:A:595:PHE:C	1:A:597:SER:N	2.72	0.43
2:B:227:GLN:HA	2:B:256:VAL:HG13	2.01	0.43
2:B:255:ASP:CG	2:B:256:VAL:N	2.72	0.43
1:C:661:LYS:C	1:C:663:ASN:N	2.72	0.43
2:D:208:ARG:CZ	2:D:258:TRP:HZ3	2.32	0.43
2:B:238:ASN:ND2	2:B:240:GLN:H	2.14	0.43
2:B:74:SER:C	2:B:76:ASP:N	2.71	0.43
2:B:87:GLY:C	2:B:88:ARG:HG3	2.39	0.43
1:C:439:ILE:CG2	1:C:659:LEU:HD21	2.39	0.43
1:C:519:VAL:O	1:C:521:GLY:N	2.51	0.43
1:A:388:PHE:CE2	1:A:716:PHE:HE2	2.37	0.43
1:A:496:THR:CG2	1:A:497:ASN:N	2.81	0.43
1:A:504:PHE:CE1	1:C:588:LEU:HD13	2.53	0.43
2:B:18:ASP:CG	2:B:23:ARG:HB3	2.39	0.43
2:B:107:TRP:CH2	2:B:130:PHE:HE1	2.37	0.43
1:C:412:LEU:HD21	1:C:713:THR:HG22	2.01	0.43
2:B:46:ILE:HG22	2:B:46:ILE:O	2.19	0.43
2:B:64:PRO:HD2	3:B:334:HOH:O	2.18	0.43
1:A:608:ILE:HA	1:A:611:ARG:NH1	2.34	0.42
1:C:590:VAL:HG13	1:C:622:LEU:HD22	1.99	0.42
1:A:438:VAL:CG2	1:A:439:ILE:N	2.81	0.42
1:A:511:GLU:HG2	1:C:569:LEU:HB2	1.99	0.42
2:B:225:VAL:CG2	2:B:271:LEU:HD11	2.50	0.42
2:B:226:SER:HB3	2:B:228:ASP:OD1	2.19	0.42
1:A:399:GLY:HA3	2:B:11:LEU:CD1	2.49	0.42
1:A:414:SER:HG	1:A:715:ASN:HB2	1.82	0.42
1:A:610:GLN:HA	1:A:610:GLN:OE1	2.20	0.42
1:A:706:PHE:HB2	3:A:200:HOH:O	2.19	0.42
2:D:124:LYS:HE3	2:D:142:ASP:OD1	2.19	0.42
2:D:224:SER:OG	2:D:232:ILE:HB	2.19	0.42
1:A:404:ILE:N	1:A:404:ILE:HD12	2.35	0.42
2:B:16:VAL:HG12	2:B:61:TRP:HD1	1.84	0.42
1:A:584:LEU:N	1:A:584:LEU:CD1	2.81	0.42
1:A:733:VAL:HG13	3:A:255:HOH:O	2.20	0.42
2:B:49:LEU:HA	3:B:355:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:PRO:CG	2:B:214:PRO:HA	2.49	0.42
1:C:420:GLU:HA	1:C:423:LYS:CD	2.50	0.42
1:C:536:LEU:O	1:C:537:MET:C	2.57	0.42
2:D:157:THR:HG21	2:D:170:SER:HB2	2.00	0.42
2:D:225:VAL:HG22	2:D:257:LEU:HB2	2.00	0.42
1:A:428:LYS:HB2	1:A:429:PRO:CD	2.38	0.42
1:A:497:ASN:OD1	1:A:498:PHE:N	2.53	0.42
2:B:52:HIS:CD2	2:B:56:VAL:HG22	2.55	0.42
1:A:500:PRO:O	1:A:501:GLU:HG2	2.20	0.42
2:B:63:HIS:CD2	2:B:110:HIS:HB3	2.54	0.42
2:B:281:TRP:CD1	2:B:281:TRP:N	2.87	0.42
1:C:655:LEU:HD12	1:C:655:LEU:HA	1.78	0.42
1:A:431:ILE:HG21	1:A:451:GLU:HA	2.02	0.42
1:A:429:PRO:HD2	3:A:159:HOH:O	2.18	0.42
1:A:447:TRP:O	1:A:451:GLU:N	2.53	0.42
1:A:458:THR:CG2	1:A:459:GLU:N	2.81	0.42
1:C:408:LYS:HG3	2:D:294:GLU:OE1	2.19	0.42
1:C:493:GLN:HG3	1:C:494:ILE:N	2.35	0.42
1:A:549:GLU:HA	1:A:552:LYS:HB3	2.01	0.42
2:B:233:ILE:HD12	2:B:233:ILE:N	2.35	0.42
1:C:589:ASP:C	1:C:591:SER:H	2.23	0.42
2:D:118:VAL:O	2:D:125:VAL:HA	2.20	0.42
2:D:118:VAL:HB	2:D:126:SER:OG	2.20	0.42
1:A:644:VAL:HG21	1:A:684:PHE:CZ	2.55	0.41
1:A:517:ASN:HD21	1:A:529:ASN:HD22	1.60	0.41
2:B:121:SER:CA	3:B:338:HOH:O	2.68	0.41
2:B:225:VAL:CG1	2:B:257:LEU:O	2.68	0.41
2:B:282:LYS:HB3	2:B:292:ALA:HB2	2.02	0.41
1:C:667:TYR:CD1	2:D:266:GLY:HA2	2.55	0.41
1:A:412:LEU:HD23	1:A:413:GLU:N	2.36	0.41
2:B:213:SER:HB2	2:B:262:TRP:CD2	2.55	0.41
1:C:424:THR:O	1:C:425:LYS:HB3	2.19	0.41
2:D:7:ALA:HB3	2:D:12:ILE:HD11	2.01	0.41
2:D:277:LYS:HG3	2:D:278:VAL:H	1.86	0.41
1:A:517:ASN:ND2	1:A:529:ASN:ND2	2.63	0.41
1:A:653:PRO:O	1:A:656:GLU:N	2.54	0.41
2:B:2:VAL:HG13	2:B:41:GLU:HA	2.03	0.41
2:B:17:LEU:HB3	2:B:21:GLY:HA2	2.03	0.41
2:B:152:SER:OG	2:B:210:VAL:O	2.33	0.41
2:B:238:ASN:HB2	3:B:327:HOH:O	2.20	0.41
1:C:447:TRP:CE3	1:C:450:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:ALA:O	2:D:192:GLN:HB2	2.20	0.41
1:A:420:GLU:O	1:A:423:LYS:HG2	2.20	0.41
1:A:434:ARG:HG3	1:A:447:TRP:CH2	2.55	0.41
2:B:212:TRP:HA	2:B:222:LEU:HD23	2.03	0.41
1:A:551:LEU:C	1:A:551:LEU:HD23	2.41	0.41
1:A:578:LYS:HD3	1:A:580:GLU:OE2	2.21	0.41
2:D:181:LEU:CD2	2:D:201:GLU:HG2	2.50	0.41
2:D:203:HIS:NE2	2:D:232:ILE:HG12	2.35	0.41
1:A:694:ILE:HG23	1:A:699:LEU:HD23	2.02	0.41
1:C:438:VAL:HG21	1:C:444:GLU:CA	2.50	0.41
1:A:396:THR:HB	1:A:398:ASP:OD1	2.21	0.41
1:A:421:ALA:O	1:A:425:LYS:HA	2.21	0.41
1:A:444:GLU:HG2	1:A:448:ASN:ND2	2.36	0.41
1:A:704:LEU:O	1:A:707:ILE:HB	2.21	0.41
1:C:497:ASN:O	1:C:497:ASN:CG	2.59	0.41
1:A:388:PHE:HB2	1:A:739:ARG:NH2	2.30	0.41
2:B:46:ILE:O	2:B:47:ASP:HB2	2.21	0.41
1:C:457:GLY:O	1:C:458:THR:C	2.59	0.41
1:A:497:ASN:O	1:A:498:PHE:HB3	2.20	0.40
1:A:519:VAL:O	1:A:521:GLY:N	2.52	0.40
2:B:23:ARG:NH1	2:B:68:THR:CG2	2.83	0.40
2:B:78:LYS:HG2	2:B:96:ALA:CB	2.52	0.40
1:C:438:VAL:HG22	1:C:439:ILE:N	2.36	0.40
1:C:649:LEU:CD2	1:C:698:GLN:HG2	2.38	0.40
2:D:33:ILE:HB	2:D:49:LEU:HD12	2.03	0.40
1:A:439:ILE:HG13	1:A:440:ASP:H	1.85	0.40
1:A:563:TYR:C	1:A:565:SER:H	2.24	0.40
1:A:598:LYS:O	1:A:602:ASN:HB2	2.20	0.40
1:C:551:LEU:O	1:C:553:GLU:N	2.54	0.40
1:C:677:PHE:HD2	1:C:678:ILE:HD12	1.83	0.40
2:D:117:LEU:HD21	2:D:151:ALA:HB1	2.03	0.40
1:A:456:ASP:O	1:A:460:GLU:HB2	2.22	0.40
1:C:572:ILE:HG22	1:C:573:LEU:N	2.35	0.40
1:C:652:PHE:CE2	1:C:702:LYS:HE2	2.56	0.40
2:B:24:LEU:HG	2:B:25:ALA:H	1.85	0.40
1:C:409:ILE:HB	1:C:412:LEU:HB3	2.04	0.40
1:C:412:LEU:C	1:C:412:LEU:HD23	2.42	0.40
1:C:535:LEU:CD2	1:C:538:GLU:HG3	2.52	0.40
1:C:717:GLU:N	3:C:127:HOH:O	2.55	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)
3:A:118:HOH:O	3:D:311:HOH:O[1_644]	2.02	0.18

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	339/399 (85%)	285 (84%)	43 (13%)	11 (3%)	4 1
1	C	341/399 (86%)	298 (87%)	34 (10%)	9 (3%)	5 3
2	B	275/297 (93%)	241 (88%)	30 (11%)	4 (2%)	10 9
2	D	284/297 (96%)	255 (90%)	20 (7%)	9 (3%)	4 1
All	All	1239/1392 (89%)	1079 (87%)	127 (10%)	33 (3%)	5 2

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	ASN
2	B	131	LYS
1	C	715	ASN
2	D	131	LYS
2	D	218	LEU
2	D	294	GLU
1	A	388	PHE
1	A	425	LYS
1	A	518	LEU
2	B	135	THR
1	C	425	LYS
2	D	87	GLY
2	D	135	THR
1	A	520	SER
1	A	728	SER
2	B	190	ASP
1	C	439	ILE

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Mol	Chain	Res	Type
1	C	552	LYS
1	C	728	SER
1	A	439	ILE
1	A	498	PHE
1	A	561	ALA
2	B	202	GLY
1	C	407	PRO
2	D	168	LYS
2	D	206	TRP
1	A	548	ASN
1	A	653	PRO
1	C	520	SER
1	C	662	ASP
2	D	202	GLY
2	D	93	ALA
1	C	494	ILE

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	306/350 (87%)	297 (97%)	9 (3%)	42	53
1	C	308/350 (88%)	297 (96%)	11 (4%)	35	46
2	B	237/252 (94%)	232 (98%)	5 (2%)	53	66
2	D	244/252 (97%)	236 (97%)	8 (3%)	38	49
All	All	1095/1204 (91%)	1062 (97%)	33 (3%)	41	52

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	430	LEU
1	A	509	ASN
1	A	534	ASP
1	A	537	MET
1	A	545	ASP

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Mol	Chain	Res	Type
1	A	657	ASP
1	A	688	ILE
1	A	703	PHE
1	A	720	THR
2	B	92	ILE
2	B	180	ASN
2	B	204	SER
2	B	225	VAL
2	B	238	ASN
1	C	377	TYR
1	C	381	SER
1	C	408	LYS
1	C	413	GLU
1	C	432	ASN
1	C	509	ASN
1	C	510	ILE
1	C	534	ASP
1	C	538	GLU
1	C	545	ASP
1	C	629	GLN
2	D	28	SER
2	D	74	SER
2	D	85	GLU
2	D	157	THR
2	D	198	SER
2	D	204	SER
2	D	225	VAL
2	D	251	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	433	GLN
1	A	443	ASN
1	A	448	ASN
1	A	509	ASN
1	A	517	ASN
1	A	592	GLN
1	A	601	GLN
2	B	95	HIS
2	B	149	ASN
2	B	180	ASN

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Mol	Chain	Res	Type
2	B	238	ASN
2	B	240	GLN
2	B	276	ASN
1	C	443	ASN
1	C	448	ASN
1	C	493	GLN
1	C	509	ASN
1	C	517	ASN
1	C	557	ASN
1	C	592	GLN
1	C	601	GLN
1	C	606	ASN
1	C	670	HIS
1	C	686	ASN
2	D	149	ASN
2	D	180	ASN
2	D	276	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 monosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	345/399 (86%)	0.39	17 (4%)	29	27	49, 83, 114, 130	0
1	C	347/399 (86%)	0.15	16 (4%)	32	30	30, 66, 103, 130	0
2	B	279/297 (93%)	0.35	13 (4%)	31	29	15, 62, 110, 142	0
2	D	288/297 (96%)	0.16	17 (5%)	22	19	16, 47, 96, 135	0
All	All	1259/1392 (90%)	0.26	63 (5%)	28	26	15, 68, 109, 142	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	THR	8.0
2	B	133	ASN	7.5
2	B	136	THR	7.1
2	D	296	HIS	7.0
2	D	295	VAL	6.8
2	B	134	GLY	6.5
2	B	135	THR	6.2
2	D	135	THR	6.1
2	D	133	ASN	5.8
2	D	216	VAL	5.6
1	C	496	THR	5.4
2	D	134	GLY	4.9
2	D	158	ILE	4.6
1	C	494	ILE	4.1
2	B	137	SER	4.1
1	A	595	PHE	4.1
1	C	469	ASP	4.1
2	D	136	THR	4.1
1	C	436	VAL	4.0
1	A	550	ARG	3.7
2	D	166	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	131	LYS	3.7
2	B	218	LEU	3.7
1	A	436	VAL	3.7
1	A	435	LEU	3.6
1	A	741	LEU	3.3
2	B	132	GLU	3.2
1	C	694	ILE	3.0
2	D	72	SER	2.9
2	D	169	GLU	2.8
2	D	130	PHE	2.7
1	A	551	LEU	2.7
1	A	633	THR	2.7
1	C	468	PHE	2.7
2	D	73	CYS	2.6
1	C	550	ARG	2.6
1	A	495	GLU	2.6
2	B	22	LYS	2.5
1	A	579	ARG	2.4
2	B	85	GLU	2.4
1	C	435	LEU	2.4
1	A	439	ILE	2.3
1	A	455	MET	2.3
1	A	441	ASP	2.3
2	D	217	LEU	2.3
2	D	131	LYS	2.3
1	C	497	ASN	2.2
1	C	495	GLU	2.2
1	C	437	LYS	2.2
1	C	678	ILE	2.2
1	A	690	GLY	2.2
1	C	551	LEU	2.2
2	D	218	LEU	2.2
2	B	36	PHE	2.2
1	A	729	ASP	2.1
1	C	432	ASN	2.1
1	A	674	LEU	2.1
1	C	579	ARG	2.1
1	A	437	LYS	2.1
2	D	14	ASP	2.0
2	B	86	ASN	2.0
1	C	439	ILE	2.0
2	B	119	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.