Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:09 AM GMT

PDB ID	:	2PM7
Title	:	Crystal structure of yeast Sec13/31 edge element of the COPII vesicular coat, selenomethionine version
Authors	:	Goldberg, J.; Fath, S.; Mancias, J.D.; Bi, X.
Deposited on	:	2007-04-20
Resolution	:	2.35 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:

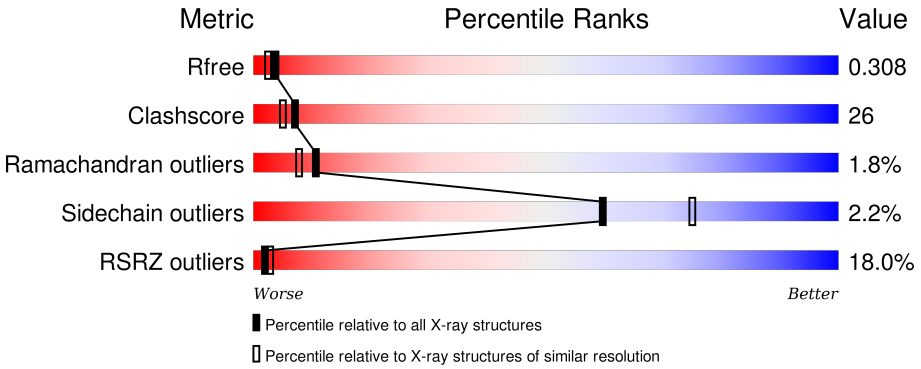
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	399	23% 47% 37% • 14%
1	C	399	12% 50% 34% • 13%
2	B	297	15% 54% 39% • 6%
2	D	297	12% 62% 33% • •

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	Se	0	0	0
			2729	1723	449	547	1	9			
1	C	347	Total	C	N	O	S	Se	0	0	0
			2746	1734	452	550	1	9			

There are 28 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	MSE	-	CLONING ARTIFACT	UNP P38968
A	368	GLY	-	CLONING ARTIFACT	UNP P38968
A	369	SER	-	CLONING ARTIFACT	UNP P38968
A	449	MSE	LEU	ENGINEERED	UNP P38968
A	455	MSE	MET	MODIFIED RESIDUE	UNP P38968
A	536	MSE	LEU	ENGINEERED	UNP P38968
A	537	MSE	MET	MODIFIED RESIDUE	UNP P38968
A	540	MSE	MET	MODIFIED RESIDUE	UNP P38968
A	614	MSE	MET	MODIFIED RESIDUE	UNP P38968
A	615	MSE	LEU	ENGINEERED	UNP P38968
A	622	MSE	LEU	ENGINEERED	UNP P38968
A	674	MSE	LEU	ENGINEERED	UNP P38968
C	365	GLY	-	CLONING ARTIFACT	UNP P38968
C	366	ALA	-	CLONING ARTIFACT	UNP P38968
C	367	MSE	-	CLONING ARTIFACT	UNP P38968
C	368	GLY	-	CLONING ARTIFACT	UNP P38968
C	369	SER	-	CLONING ARTIFACT	UNP P38968
C	449	MSE	LEU	ENGINEERED	UNP P38968
C	455	MSE	MET	MODIFIED RESIDUE	UNP P38968
C	536	MSE	LEU	ENGINEERED	UNP P38968
C	537	MSE	MET	MODIFIED RESIDUE	UNP P38968
C	540	MSE	MET	MODIFIED RESIDUE	UNP P38968
C	614	MSE	MET	MODIFIED RESIDUE	UNP P38968

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Chain	Residue	Modelled	Actual	Comment	Reference
C	615	MSE	LEU	ENGINEERED	UNP P38968
C	622	MSE	LEU	ENGINEERED	UNP P38968
C	674	MSE	LEU	ENGINEERED	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	Se	0	0	0
			2196	1397	375	415	3	6			
2	D	288	Total	C	N	O	S	Se	0	0	0
			2263	1438	387	429	3	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q04491
B	11	MSE	LEU	ENGINEERED	UNP Q04491
B	17	MSE	LEU	ENGINEERED	UNP Q04491
B	24	MSE	LEU	ENGINEERED	UNP Q04491
B	80	MSE	LEU	ENGINEERED	UNP Q04491
B	115	MSE	LEU	ENGINEERED	UNP Q04491
B	222	MSE	LEU	ENGINEERED	UNP Q04491
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q04491
D	11	MSE	LEU	ENGINEERED	UNP Q04491
D	17	MSE	LEU	ENGINEERED	UNP Q04491
D	24	MSE	LEU	ENGINEERED	UNP Q04491
D	80	MSE	LEU	ENGINEERED	UNP Q04491
D	115	MSE	LEU	ENGINEERED	UNP Q04491
D	222	MSE	LEU	ENGINEERED	UNP Q04491

- Molecule 3 is water.

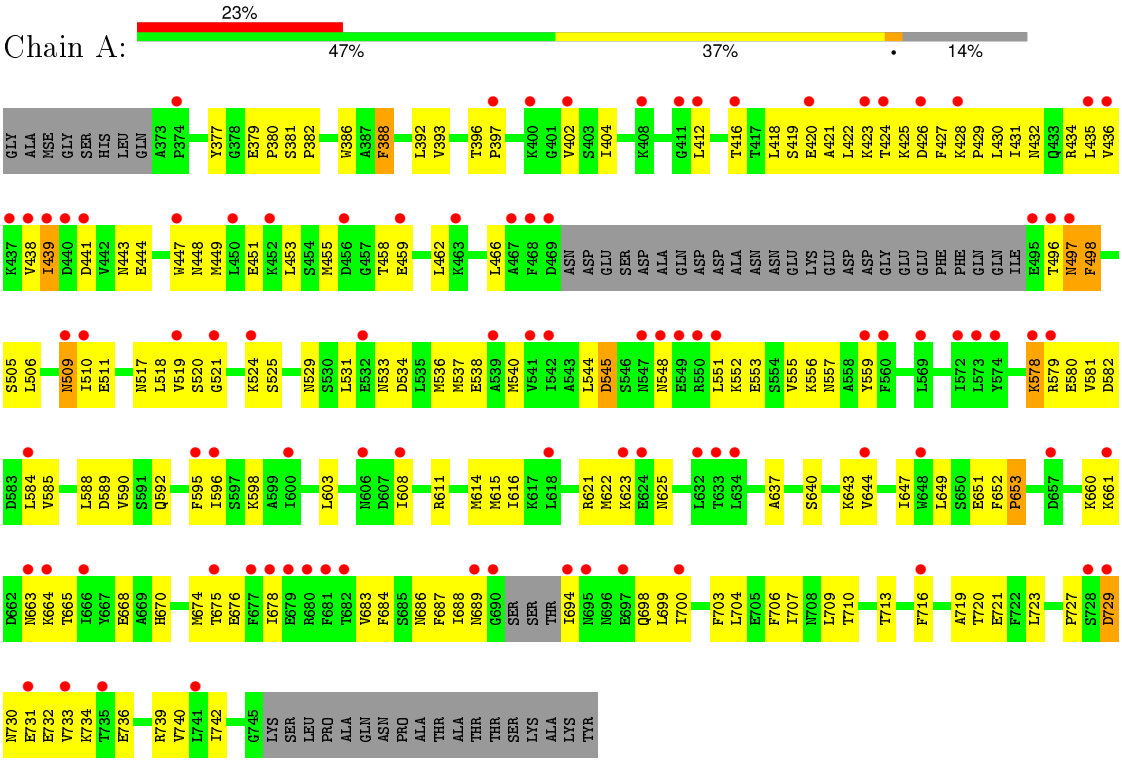
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	60	Total	O	0	0
			60	60		
3	C	50	Total	O	0	0
			50	50		
3	D	122	Total	O	0	0
			122	122		

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.

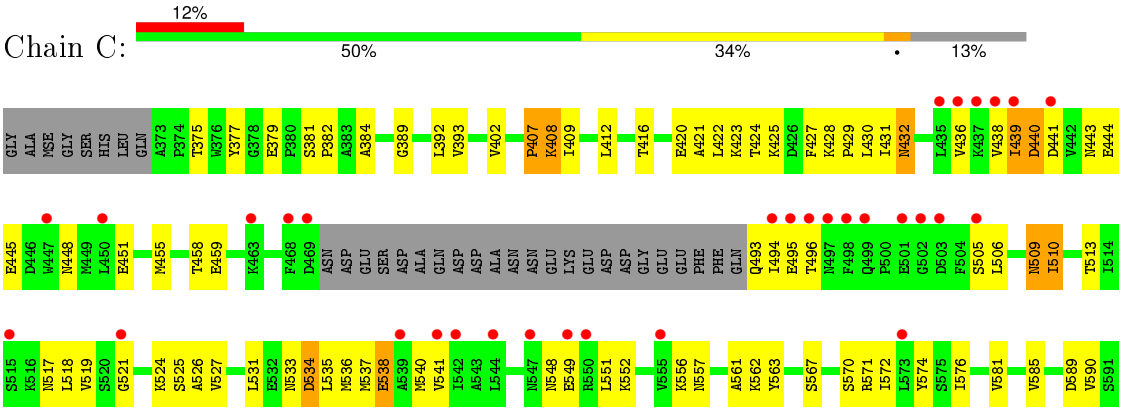
- Molecule 1: Protein transport protein SEC31

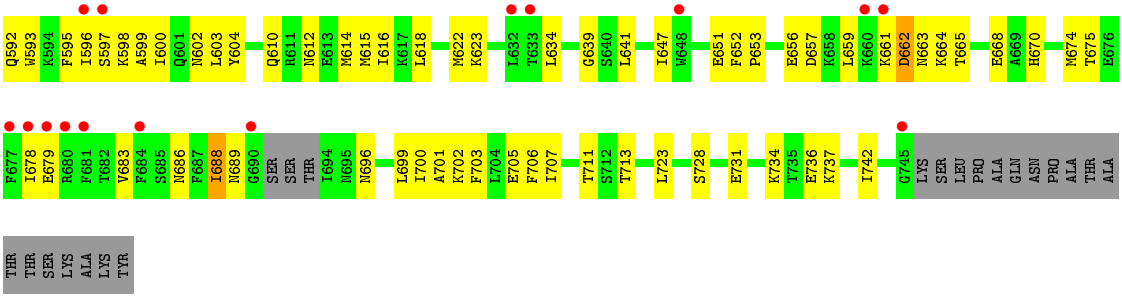
Chain A:



- Molecule 1: Protein transport protein SEC31

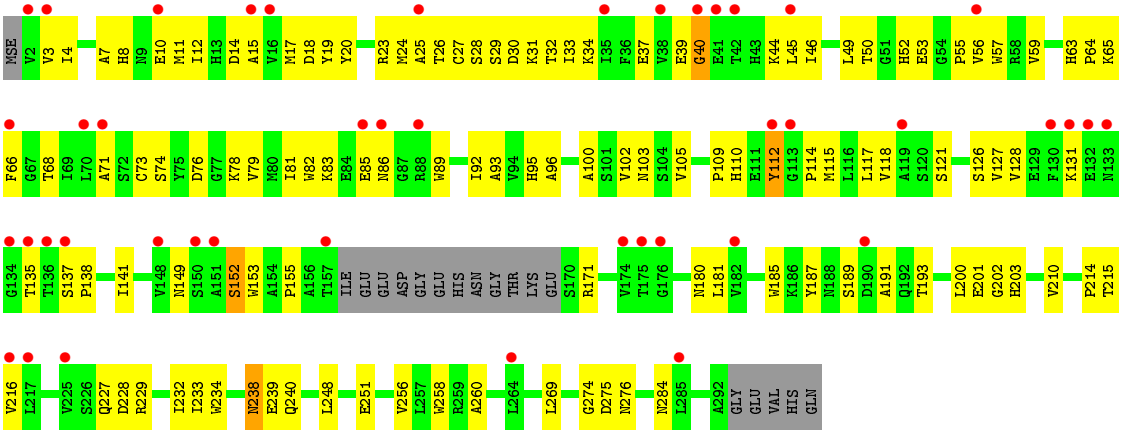
Chain C:





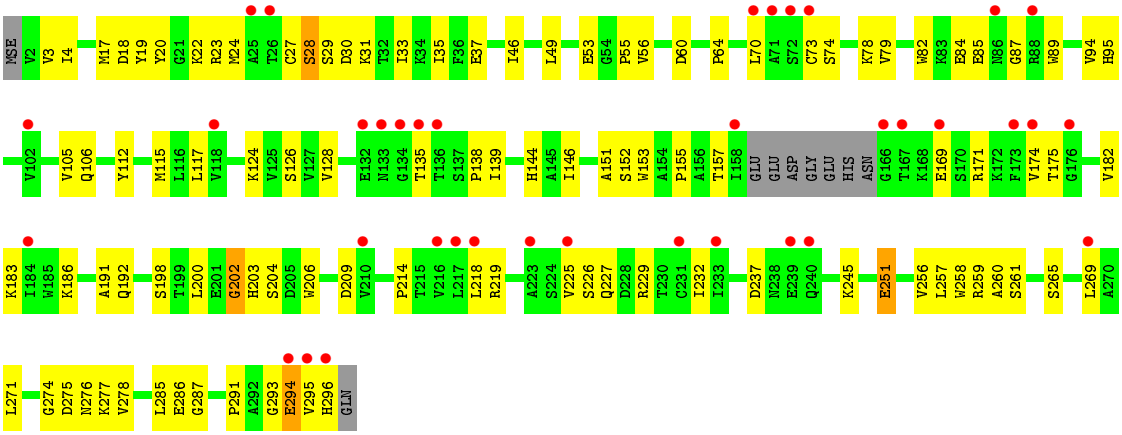
• Molecule 2: Protein transport protein SEC13

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	128.19Å 52.50Å 133.09Å 90.00° 108.34° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 24.83 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-2.35) 96.9 (24.83-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.47 (at 2.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.298 0.257 , 0.308	Depositor DCC
R_{free} test set	3487 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.883	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.5	EDS
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 68541 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10195	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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	0.31	0/2764	0.52	0/3712
1	C	0.35	0/2781	0.55	0/3735
2	B	0.36	0/2250	0.63	0/3055
2	D	0.43	0/2318	0.71	0/3146
All	All	0.36	0/10113	0.60	0/13648

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	2696	176	0
1	C	2746	0	2715	155	0
2	B	2196	0	2126	138	0
2	D	2263	0	2191	89	0
3	A	29	0	0	18	1
3	B	60	0	0	25	0
3	C	50	0	0	9	0
3	D	122	0	0	22	1
All	All	10195	0	9728	517	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 26.

All (517) 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:55:PRO:HA	3:D:417:HOH:O	1.51	1.10
1:A:496:THR:HG23	1:C:557:ASN:HB3	1.33	1.09
1:A:431:ILE:HD11	1:A:683:VAL:HG11	1.35	1.08
1:C:623:LYS:HE3	1:C:647:ILE:HD12	1.40	1.04
1:C:408:LYS:H	1:C:408:LYS:HD3	1.21	1.04
2:D:37:GLU:HG3	2:D:46:ILE:HD11	1.47	0.97
1:A:505:SER:HB3	1:C:589:ASP:HB2	1.48	0.95
1:A:536:MSE:HG2	1:A:540:MSE:HE2	1.46	0.94
1:A:506:LEU:HD21	1:C:572:ILE:HD12	1.47	0.93
2:B:12:ILE:HA	2:B:28:SER:HB3	1.50	0.91
1:C:535:LEU:HB3	1:C:538:GLU:HG3	1.49	0.91
1:A:592:GLN:HE21	1:C:506:LEU:HD12	1.34	0.90
2:B:117:LEU:HA	3:B:339:HOH:O	1.74	0.88
2:D:112:TYR:HB3	2:D:115:MSE:CE	2.03	0.88
2:B:233:ILE:HD11	2:B:248:LEU:HD13	1.56	0.87
1:A:412:LEU:HD21	1:A:713:THR:HG22	1.57	0.87
1:A:496:THR:HG22	1:A:497:ASN:H	1.39	0.86
2:B:81:ILE:HB	3:B:319:HOH:O	1.75	0.85
1:A:420:GLU:HA	1:A:423:LYS:HE2	1.56	0.85
1:C:602:ASN:HB3	3:C:245:HOH:O	1.77	0.83
2:B:238:ASN:HD22	2:B:240:GLN:H	1.27	0.82
1:A:703:PHE:HA	3:A:200:HOH:O	1.77	0.82
1:C:420:GLU:HA	1:C:423:LYS:HE2	1.60	0.82
2:B:37:GLU:HG2	2:B:46:ILE:HD11	1.62	0.81
2:B:112:TYR:HA	2:B:171:ARG:NH2	1.94	0.81
1:A:496:THR:HG22	1:A:497:ASN:N	1.94	0.81
1:C:524:LYS:HG3	1:C:525:SER:H	1.46	0.81
2:B:18:ASP:OD2	2:B:23:ARG:HB3	1.81	0.81
1:A:592:GLN:HG3	1:A:595:PHE:HB3	1.64	0.79
2:B:105:VAL:HG23	2:B:118:VAL:HG22	1.64	0.79
1:C:408:LYS:HE3	2:D:294:GLU:HG2	1.62	0.79
1:C:494:ILE:HG13	1:C:495:GLU:H	1.47	0.79
2:B:117:LEU:HD12	3:B:339:HOH:O	1.83	0.79
2:B:11:MSE:O	2:B:28:SER:HB2	1.82	0.78
1:C:407:PRO:HD2	3:C:214:HOH:O	1.82	0.78
1:C:535:LEU:HB3	1:C:538:GLU:CG	2.13	0.78
2:D:55:PRO:O	2:D:74:SER:HB2	1.83	0.78
1:C:513:THR:HB	3:C:202:HOH:O	1.83	0.78
2:B:53:GLU:HG3	3:B:336:HOH:O	1.84	0.78
1:A:733:VAL:HG13	3:A:255:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:VAL:HG22	2:B:138:PRO:HB3	1.67	0.77
1:A:428:LYS:HB2	1:A:429:PRO:HD3	1.66	0.77
1:C:674:MSE:HE1	1:C:702:LYS:HG2	1.67	0.76
2:B:37:GLU:HG2	2:B:46:ILE:CD1	2.16	0.76
1:A:496:THR:HG23	1:C:557:ASN:CB	2.14	0.76
1:C:408:LYS:N	1:C:408:LYS:HD3	1.97	0.76
1:A:720:THR:HA	1:A:723:LEU:HD12	1.66	0.76
1:A:589:ASP:HB2	1:C:505:SER:HB3	1.68	0.75
2:D:259:ARG:HB2	3:D:414:HOH:O	1.87	0.75
1:C:597:SER:OG	1:C:615:MSE:HE1	1.87	0.74
1:C:612:ASN:O	1:C:616:ILE:HG12	1.87	0.74
1:A:590:VAL:HG13	1:A:622:MSE:SE	2.36	0.74
1:C:428:LYS:HB2	1:C:429:PRO:HD3	1.68	0.74
2:B:44:LYS:O	2:B:46:ILE:HD12	1.87	0.74
1:C:427:PHE:O	1:C:431:ILE:HG12	1.88	0.73
1:C:585:VAL:HG21	1:C:614:MSE:HE3	1.70	0.73
2:B:102:VAL:HG23	3:B:352:HOH:O	1.87	0.73
1:A:706:PHE:HB3	3:A:200:HOH:O	1.89	0.72
1:C:592:GLN:HG3	1:C:595:PHE:HB3	1.71	0.72
1:A:496:THR:CG2	1:A:497:ASN:H	2.02	0.72
2:B:131:LYS:HE3	2:B:137:SER:HB2	1.71	0.72
1:C:590:VAL:HG13	1:C:622:MSE:SE	2.40	0.71
2:D:33:ILE:HD11	2:D:56:VAL:HG11	1.73	0.71
2:B:74:SER:HB3	2:B:76:ASP:OD1	1.91	0.71
1:C:431:ILE:HD11	1:C:683:VAL:HG11	1.73	0.70
1:C:393:VAL:HG21	2:D:17:MSE:HG3	1.73	0.70
1:A:652:PHE:HB3	1:A:653:PRO:HD3	1.74	0.70
2:B:274:GLY:C	2:B:276:ASN:H	1.94	0.70
1:A:518:LEU:HB3	1:C:576:ILE:HD13	1.74	0.69
1:C:408:LYS:HE3	2:D:294:GLU:CG	2.22	0.69
1:C:703:PHE:O	1:C:707:ILE:HG12	1.93	0.69
1:A:441:ASP:HA	3:A:212:HOH:O	1.92	0.69
1:A:386:TRP:HA	3:A:219:HOH:O	1.94	0.68
1:A:519:VAL:HG12	1:C:598:LYS:HG3	1.76	0.68
1:C:425:LYS:HD3	1:C:425:LYS:O	1.94	0.68
1:A:623:LYS:HE3	1:A:647:ILE:HD12	1.74	0.68
1:A:581:VAL:HG23	1:A:614:MSE:HE2	1.74	0.68
1:A:380:PRO:HG3	2:B:11:MSE:CE	2.24	0.67
2:D:27:CYS:HB2	2:D:56:VAL:HB	1.76	0.67
1:C:416:THR:HG22	1:C:420:GLU:OE2	1.95	0.66
1:C:674:MSE:O	1:C:678:ILE:HD12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:VAL:C	2:D:4:ILE:HD12	2.15	0.66
2:D:124:LYS:HG3	3:D:409:HOH:O	1.96	0.66
1:A:393:VAL:HG21	2:B:17:MSE:HG3	1.76	0.66
1:A:434:ARG:NH1	1:A:676:GLU:HB2	2.10	0.66
1:A:519:VAL:C	1:A:521:GLY:H	1.98	0.66
1:C:674:MSE:SE	1:C:678:ILE:HD11	2.46	0.66
2:D:33:ILE:CD1	2:D:56:VAL:HG11	2.26	0.66
1:A:397:PRO:HG3	2:B:276:ASN:ND2	2.11	0.66
2:B:102:VAL:CG2	3:B:352:HOH:O	2.44	0.65
2:D:206:TRP:CE3	3:D:410:HOH:O	2.49	0.65
2:B:10:GLU:HB2	3:B:335:HOH:O	1.96	0.65
1:A:402:VAL:HG11	2:B:24:MSE:SE	2.47	0.65
2:D:33:ILE:HB	2:D:49:LEU:HD12	1.79	0.65
1:C:675:THR:O	1:C:679:GLU:HG3	1.96	0.65
2:B:112:TYR:HB3	2:B:115:MSE:CE	2.26	0.65
1:C:510:ILE:HD12	1:C:510:ILE:H	1.63	0.64
1:C:510:ILE:HG21	1:C:533:ASN:ND2	2.12	0.64
2:B:112:TYR:HA	2:B:171:ARG:HH21	1.60	0.64
1:A:531:LEU:C	1:A:533:ASN:H	2.01	0.64
1:A:404:ILE:HD12	1:A:404:ILE:N	2.12	0.64
2:D:144:HIS:CE1	3:D:369:HOH:O	2.50	0.64
1:A:590:VAL:HG23	3:A:108:HOH:O	1.98	0.64
2:D:227:GLN:HA	2:D:256:VAL:HG13	1.79	0.64
2:B:39:GLU:HB2	3:B:334:HOH:O	1.97	0.63
2:B:49:LEU:HA	3:B:354:HOH:O	1.98	0.63
1:C:618:LEU:O	1:C:622:MSE:HG2	1.98	0.63
1:A:588:LEU:HB3	1:A:596:ILE:HD11	1.80	0.63
1:A:497:ASN:O	1:A:498:PHE:HB3	1.99	0.63
1:C:510:ILE:HA	3:C:202:HOH:O	1.98	0.63
2:B:200:LEU:HD13	2:B:234:TRP:CE3	2.33	0.63
2:D:112:TYR:HB3	2:D:115:MSE:HE1	1.80	0.63
1:C:444:GLU:HG2	1:C:448:ASN:HD21	1.63	0.62
2:B:10:GLU:HB3	2:B:29:SER:HB2	1.79	0.62
1:A:581:VAL:HG23	1:A:614:MSE:CE	2.29	0.62
2:B:26:THR:O	2:B:33:ILE:HG23	1.99	0.62
1:C:509:ASN:N	1:C:509:ASN:HD22	1.96	0.62
1:C:494:ILE:HG13	1:C:495:GLU:N	2.13	0.62
2:B:49:LEU:HD22	2:B:82:TRP:CE3	2.35	0.62
2:B:239:GLU:HG3	3:B:326:HOH:O	1.98	0.62
1:A:555:VAL:HB	3:A:199:HOH:O	1.99	0.62
2:D:183:LYS:N	3:D:369:HOH:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:THR:HG23	1:A:459:GLU:H	1.64	0.61
2:B:127:VAL:HA	3:B:339:HOH:O	2.00	0.61
1:C:536:MSE:HG2	1:C:540:MSE:HE3	1.81	0.61
1:A:496:THR:CG2	1:A:497:ASN:N	2.61	0.61
1:A:706:PHE:CB	3:A:200:HOH:O	2.47	0.61
1:A:458:THR:HG23	1:A:459:GLU:N	2.16	0.61
2:D:84:GLU:HB2	2:D:89:TRP:CE2	2.35	0.61
1:A:388:PHE:HB2	1:A:739:ARG:HH21	1.66	0.61
2:D:37:GLU:CG	2:D:46:ILE:HD11	2.27	0.61
2:B:83:LYS:O	2:B:89:TRP:HA	2.00	0.61
1:C:548:ASN:O	1:C:552:LYS:HB2	2.01	0.60
2:D:274:GLY:C	2:D:276:ASN:H	2.04	0.60
1:A:412:LEU:CD2	1:A:713:THR:HG22	2.29	0.60
1:C:493:GLN:HG3	1:C:494:ILE:H	1.66	0.60
1:A:519:VAL:HG13	1:C:599:ALA:HA	1.83	0.60
1:A:509:ASN:N	1:A:509:ASN:HD22	1.99	0.60
2:B:37:GLU:CG	2:B:46:ILE:HD11	2.31	0.60
1:A:719:ALA:O	1:A:723:LEU:HG	2.02	0.60
1:C:723:LEU:HD21	1:C:736:GLU:HG2	1.83	0.60
2:B:66:PHE:CE2	2:B:114:PRO:HD3	2.36	0.60
1:A:704:LEU:HD21	1:A:733:VAL:HG22	1.84	0.60
2:B:59:VAL:HA	2:B:71:ALA:O	2.02	0.60
2:B:103:ASN:ND2	3:B:337:HOH:O	2.36	0.59
1:C:742:ILE:O	2:D:22:LYS:HD2	2.02	0.59
1:A:665:THR:OG1	1:A:668:GLU:HG3	2.02	0.59
1:C:524:LYS:HG3	1:C:525:SER:N	2.16	0.59
2:D:245:LYS:NZ	3:D:335:HOH:O	2.34	0.59
2:D:18:ASP:OD2	2:D:23:ARG:HB3	2.02	0.59
1:C:493:GLN:HG3	1:C:494:ILE:N	2.17	0.59
1:A:510:ILE:HB	3:A:107:HOH:O	2.01	0.59
2:B:121:SER:HA	3:B:337:HOH:O	2.04	0.58
1:A:429:PRO:HD2	3:A:159:HOH:O	2.03	0.58
1:A:427:PHE:CD2	1:A:683:VAL:HG22	2.39	0.58
1:A:731:GLU:HA	1:A:734:LYS:HB3	1.84	0.58
1:A:585:VAL:HA	1:A:596:ILE:HG21	1.84	0.58
1:A:380:PRO:HG3	2:B:11:MSE:HE2	1.86	0.58
1:A:379:GLU:HG2	2:B:258:TRP:CZ2	2.39	0.58
2:D:219:ARG:HG2	2:D:237:ASP:OD1	2.04	0.58
1:C:567:SER:HB3	1:C:570:SER:HB3	1.84	0.58
1:C:665:THR:OG1	1:C:668:GLU:HG3	2.03	0.58
1:C:412:LEU:HD21	3:C:246:HOH:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:CYS:HB3	2:D:105:VAL:HG13	1.86	0.58
1:A:380:PRO:HG3	2:B:11:MSE:HE1	1.86	0.58
2:B:24:MSE:HE3	2:B:26:THR:HG23	1.84	0.57
1:A:716:PHE:HD2	1:A:740:VAL:HG13	1.69	0.57
1:C:439:ILE:HG12	1:C:443:ASN:HD22	1.67	0.57
1:A:427:PHE:O	1:A:431:ILE:HG12	2.04	0.57
1:A:519:VAL:CG1	1:C:598:LYS:HG3	2.34	0.57
1:A:402:VAL:HG11	2:B:24:MSE:HE1	1.86	0.57
1:A:402:VAL:HG11	2:B:24:MSE:CE	2.34	0.57
1:A:723:LEU:HA	3:A:255:HOH:O	2.05	0.57
1:C:581:VAL:HG23	1:C:614:MSE:HE2	1.86	0.57
1:C:661:LYS:C	1:C:663:ASN:H	2.07	0.57
2:B:155:PRO:HG3	2:B:214:PRO:HA	1.85	0.57
1:A:496:THR:O	1:A:497:ASN:CB	2.52	0.57
1:C:674:MSE:HE3	1:C:705:GLU:HB2	1.87	0.57
1:C:402:VAL:HG11	2:D:24:MSE:SE	2.54	0.57
1:A:421:ALA:O	1:A:425:LYS:HA	2.05	0.57
2:B:78:LYS:HG2	2:B:96:ALA:HB2	1.87	0.56
1:A:432:ASN:O	1:A:436:VAL:HG23	2.05	0.56
2:B:49:LEU:HB3	2:B:82:TRP:CZ3	2.40	0.56
1:A:579:ARG:HB3	1:A:603:LEU:HD11	1.87	0.56
1:A:498:PHE:HB2	1:C:561:ALA:HA	1.88	0.56
1:C:424:THR:O	1:C:425:LYS:HB3	2.05	0.56
1:C:593:TRP:HA	1:C:596:ILE:HD12	1.85	0.56
1:A:643:LYS:O	1:A:647:ILE:HG12	2.06	0.56
1:C:652:PHE:HB3	1:C:653:PRO:HD3	1.86	0.56
1:A:644:VAL:HG21	1:A:684:PHE:CZ	2.41	0.56
2:D:4:ILE:HD12	2:D:4:ILE:N	2.21	0.56
2:D:31:LYS:N	3:D:417:HOH:O	2.39	0.55
1:A:431:ILE:HD13	1:A:447:TRP:HZ3	1.71	0.55
1:C:533:ASN:OD1	1:C:534:ASP:N	2.39	0.55
2:B:33:ILE:N	2:B:33:ILE:HD12	2.21	0.55
2:D:285:LEU:C	2:D:287:GLY:H	2.10	0.55
1:A:688:ILE:HG12	1:A:689:ASN:N	2.22	0.55
2:B:73:CYS:HB2	2:B:102:VAL:CG1	2.36	0.55
1:C:439:ILE:HG12	1:C:443:ASN:ND2	2.21	0.55
2:B:33:ILE:HB	2:B:49:LEU:HD12	1.88	0.55
1:A:418:LEU:O	1:A:422:LEU:HB2	2.05	0.55
1:A:431:ILE:HG21	1:A:451:GLU:HA	1.88	0.55
1:A:435:LEU:HD11	1:A:448:ASN:OD1	2.07	0.54
1:C:615:MSE:HE3	1:C:634:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:ILE:HA	2:B:28:SER:CB	2.33	0.54
2:B:200:LEU:HB3	2:B:234:TRP:CH2	2.43	0.54
2:B:63:HIS:HB3	2:B:66:PHE:CE1	2.42	0.54
1:A:496:THR:O	1:A:497:ASN:HB2	2.06	0.54
2:B:44:LYS:O	2:B:46:ILE:CD1	2.55	0.54
1:C:659:LEU:HD22	1:C:664:LYS:HZ2	1.73	0.54
1:A:703:PHE:O	1:A:707:ILE:HG12	2.08	0.54
1:C:377:TYR:HA	3:C:113:HOH:O	2.07	0.54
2:B:112:TYR:HB3	2:B:115:MSE:HE2	1.89	0.54
1:C:412:LEU:HD21	1:C:713:THR:HG22	1.89	0.54
2:D:126:SER:HA	2:D:139:ILE:O	2.08	0.54
2:B:233:ILE:HD12	2:B:233:ILE:N	2.22	0.54
2:B:65:LYS:HE2	2:B:110:HIS:HB2	1.90	0.54
1:C:742:ILE:HD12	2:D:20:TYR:CE2	2.42	0.54
1:A:449:MSE:O	1:A:453:LEU:HB2	2.08	0.53
1:C:517:ASN:HB3	1:C:526:ALA:HB2	1.90	0.53
1:A:730:ASN:HB3	1:A:733:VAL:CG2	2.39	0.53
2:B:274:GLY:C	2:B:276:ASN:N	2.62	0.53
2:B:85:GLU:O	2:B:86:ASN:HB2	2.09	0.53
2:D:128:VAL:HG22	2:D:138:PRO:HB3	1.91	0.53
2:D:291:PRO:CB	2:D:295:VAL:HG22	2.38	0.53
2:B:189:SER:C	2:B:191:ALA:H	2.12	0.53
2:D:35:ILE:HG22	2:D:46:ILE:HD12	1.91	0.53
1:C:581:VAL:HG13	1:C:603:LEU:HD22	1.91	0.53
1:C:659:LEU:HD22	1:C:664:LYS:NZ	2.23	0.52
2:D:79:VAL:HB	2:D:95:HIS:HB3	1.92	0.52
1:A:434:ARG:HG3	1:A:447:TRP:CZ2	2.45	0.52
1:A:540:MSE:HE1	1:C:537:MSE:HG2	1.91	0.52
1:C:412:LEU:CD2	1:C:713:THR:HG22	2.40	0.52
1:A:506:LEU:HD21	1:C:572:ILE:CD1	2.29	0.52
1:A:509:ASN:N	1:A:509:ASN:ND2	2.56	0.52
1:C:509:ASN:N	1:C:509:ASN:ND2	2.58	0.52
1:A:397:PRO:HG3	2:B:276:ASN:HD22	1.75	0.52
1:C:696:ASN:HB3	1:C:699:LEU:HB3	1.92	0.52
1:C:678:ILE:HD13	1:C:706:PHE:CD1	2.45	0.52
1:A:736:GLU:O	1:A:740:VAL:HG23	2.10	0.52
2:B:49:LEU:HD13	2:B:82:TRP:CD2	2.45	0.51
1:C:728:SER:HB3	1:C:737:LYS:NZ	2.25	0.51
1:C:688:ILE:HG13	1:C:689:ASN:H	1.74	0.51
1:C:409:ILE:HB	1:C:412:LEU:HB3	1.93	0.51
2:B:30:ASP:OD1	2:B:32:THR:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:HD11	1:C:552:LYS:HG3	1.93	0.51
2:B:19:TYR:CD2	2:B:64:PRO:HG2	2.45	0.51
1:A:551:LEU:HD23	1:A:551:LEU:C	2.30	0.51
2:B:100:ALA:O	3:B:352:HOH:O	2.19	0.51
2:D:78:LYS:HD2	3:D:378:HOH:O	2.10	0.51
2:D:169:GLU:O	2:D:186:LYS:HE2	2.11	0.51
1:A:518:LEU:HB3	1:C:576:ILE:CD1	2.40	0.51
2:D:227:GLN:CG	3:D:410:HOH:O	2.59	0.51
2:B:93:ALA:N	3:B:319:HOH:O	2.24	0.50
1:C:688:ILE:CG1	1:C:689:ASN:H	2.23	0.50
2:D:257:LEU:HD22	2:D:271:LEU:HD21	1.92	0.50
1:C:432:ASN:O	1:C:436:VAL:HG23	2.10	0.50
2:B:46:ILE:N	2:B:46:ILE:HD12	2.26	0.50
1:A:742:ILE:HD12	2:B:20:TYR:CE2	2.46	0.50
2:B:92:ILE:O	3:B:317:HOH:O	2.19	0.50
2:B:112:TYR:HB3	2:B:115:MSE:HE3	1.93	0.50
1:C:641:LEU:HD13	1:C:688:ILE:HG21	1.93	0.50
1:C:519:VAL:C	1:C:521:GLY:H	2.15	0.50
1:C:562:LYS:HE3	1:C:563:TYR:CE1	2.47	0.50
2:D:152:SER:HB2	3:D:408:HOH:O	2.11	0.50
2:B:200:LEU:HB3	2:B:234:TRP:CZ3	2.47	0.50
1:C:663:ASN:C	2:D:285:LEU:HD11	2.32	0.50
1:A:438:VAL:HG23	1:A:443:ASN:HD22	1.76	0.50
2:D:73:CYS:HB3	2:D:105:VAL:CG1	2.42	0.49
1:C:384:ALA:N	3:D:414:HOH:O	2.44	0.49
1:C:423:LYS:HG3	1:C:424:THR:N	2.27	0.49
2:B:14:ASP:HB3	2:B:27:CYS:SG	2.51	0.49
1:A:731:GLU:O	1:A:734:LYS:HB3	2.13	0.49
2:B:78:LYS:HG2	2:B:96:ALA:CB	2.43	0.49
1:A:462:LEU:HD13	1:A:637:ALA:HB2	1.94	0.49
1:A:420:GLU:HG3	1:A:423:LYS:HE2	1.93	0.49
2:B:121:SER:CA	3:B:337:HOH:O	2.60	0.49
1:A:438:VAL:HG21	1:A:444:GLU:HA	1.93	0.49
1:C:604:TYR:CE2	1:C:610:GLN:HG2	2.47	0.49
2:B:3:VAL:HG12	2:B:4:ILE:N	2.28	0.49
2:B:228:ASP:O	2:B:229:ARG:HB2	2.13	0.49
1:A:423:LYS:HG3	1:A:424:THR:N	2.27	0.49
2:D:19:TYR:CD2	2:D:64:PRO:HG2	2.48	0.49
1:A:524:LYS:HG3	1:A:525:SER:N	2.27	0.49
2:D:182:VAL:HB	2:D:200:LEU:HB2	1.95	0.49
2:B:4:ILE:O	2:B:4:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ASP:OD2	1:C:556:LYS:NZ	2.41	0.49
1:A:538:GLU:OE1	1:A:538:GLU:N	2.41	0.49
1:C:731:GLU:HA	1:C:734:LYS:HB3	1.94	0.48
1:C:420:GLU:O	1:C:423:LYS:HG2	2.13	0.48
2:D:53:GLU:HG3	3:D:378:HOH:O	2.13	0.48
1:A:537:MSE:HA	1:A:540:MSE:HE3	1.96	0.48
1:C:548:ASN:O	1:C:552:LYS:CB	2.62	0.48
1:A:616:ILE:HD11	1:A:640:SER:CB	2.43	0.48
1:A:540:MSE:HE1	1:C:537:MSE:CG	2.44	0.48
1:A:694:ILE:HB	1:A:700:ILE:HD11	1.94	0.48
2:B:238:ASN:HD22	2:B:240:GLN:N	2.05	0.48
2:B:109:PRO:HD2	2:B:112:TYR:CD1	2.48	0.48
2:D:226:SER:OG	2:D:227:GLN:N	2.47	0.48
2:D:294:GLU:O	2:D:294:GLU:HG3	2.13	0.48
1:A:428:LYS:NZ	1:A:455:MSE:HG2	2.29	0.48
2:B:238:ASN:ND2	2:B:240:GLN:HB2	2.28	0.48
1:A:517:ASN:ND2	1:A:529:ASN:HD22	2.11	0.48
1:A:426:ASP:OD1	1:A:429:PRO:HD3	2.13	0.48
1:C:412:LEU:HD11	3:C:246:HOH:O	2.14	0.48
2:B:33:ILE:HB	2:B:49:LEU:HB2	1.96	0.47
1:C:701:ALA:O	1:C:705:GLU:HG3	2.14	0.47
1:C:615:MSE:HE3	1:C:634:LEU:HD23	1.96	0.47
2:D:251:GLU:CD	2:D:251:GLU:H	2.17	0.47
1:A:732:GLU:O	1:A:736:GLU:HG2	2.15	0.47
1:A:420:GLU:CA	1:A:423:LYS:HE2	2.36	0.47
2:B:112:TYR:N	2:B:112:TYR:CD2	2.82	0.47
2:D:151:ALA:HA	2:D:174:VAL:O	2.15	0.47
1:A:557:ASN:HB3	1:C:496:THR:HG23	1.95	0.47
2:D:271:LEU:O	2:D:278:VAL:HA	2.15	0.47
1:C:548:ASN:OD1	1:C:549:GLU:N	2.47	0.47
1:C:430:LEU:C	1:C:430:LEU:HD23	2.35	0.47
1:A:730:ASN:O	1:A:733:VAL:HB	2.15	0.47
1:A:518:LEU:HD13	1:C:576:ILE:HD12	1.96	0.47
1:C:439:ILE:HG13	1:C:440:ASP:H	1.80	0.47
1:A:444:GLU:HG2	1:A:448:ASN:HD21	1.80	0.47
2:D:191:ALA:O	2:D:192:GLN:HB2	2.15	0.47
2:B:117:LEU:HB2	2:B:153:TRP:NE1	2.30	0.47
1:A:412:LEU:C	1:A:412:LEU:HD23	2.36	0.47
1:A:423:LYS:HG3	1:A:424:THR:HG23	1.97	0.47
2:B:49:LEU:HB3	2:B:82:TRP:CH2	2.50	0.47
2:D:30:ASP:OD1	2:D:30:ASP:C	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:LEU:O	1:C:533:ASN:O	2.33	0.46
2:D:175:THR:O	3:D:369:HOH:O	2.21	0.46
1:A:422:LEU:HD23	1:A:721:GLU:HG2	1.97	0.46
1:A:466:LEU:O	1:A:598:LYS:HE2	2.15	0.46
1:A:517:ASN:HD21	1:A:529:ASN:ND2	2.12	0.46
1:A:427:PHE:N	1:A:427:PHE:CD1	2.83	0.46
1:A:434:ARG:HH21	1:A:675:THR:HG22	1.80	0.46
2:B:112:TYR:N	2:B:112:TYR:HD2	2.13	0.46
1:A:388:PHE:CD1	1:A:739:ARG:CZ	2.99	0.46
2:B:63:HIS:HB3	2:B:66:PHE:CD1	2.51	0.46
2:D:31:LYS:HA	3:D:417:HOH:O	2.14	0.46
1:C:524:LYS:CG	1:C:525:SER:H	2.24	0.46
2:B:15:ALA:HA	2:B:25:ALA:O	2.16	0.46
1:C:451:GLU:O	1:C:455:MSE:HG3	2.15	0.46
2:B:152:SER:OG	2:B:210:VAL:O	2.34	0.46
2:B:63:HIS:CE1	2:B:65:LYS:HB3	2.50	0.46
1:C:562:LYS:HE3	1:C:563:TYR:CZ	2.51	0.46
2:D:293:GLY:O	2:D:294:GLU:C	2.55	0.45
2:D:112:TYR:HB3	2:D:115:MSE:HE3	1.96	0.45
1:A:709:LEU:O	1:A:713:THR:HG23	2.16	0.45
1:A:388:PHE:HB2	1:A:739:ARG:NH2	2.28	0.45
2:D:28:SER:OG	2:D:29:SER:N	2.49	0.45
2:D:260:ALA:HB1	2:D:269:LEU:HD11	1.97	0.45
1:A:431:ILE:HD13	1:A:447:TRP:CZ3	2.50	0.45
2:B:29:SER:C	2:B:31:LYS:H	2.20	0.45
1:A:592:GLN:O	1:A:592:GLN:HG3	2.16	0.45
2:B:30:ASP:C	2:B:30:ASP:OD1	2.55	0.45
1:C:551:LEU:C	1:C:551:LEU:HD23	2.36	0.45
2:B:227:GLN:HA	2:B:256:VAL:HG13	1.99	0.45
2:B:95:HIS:HE1	2:B:138:PRO:HG3	1.80	0.45
1:C:458:THR:HG23	1:C:459:GLU:N	2.31	0.45
1:A:727:PRO:C	1:A:729:ASP:H	2.20	0.45
2:B:26:THR:O	2:B:33:ILE:HA	2.16	0.45
2:B:40:GLY:N	3:B:334:HOH:O	2.49	0.45
1:A:555:VAL:N	3:A:199:HOH:O	2.47	0.45
2:D:274:GLY:C	2:D:276:ASN:N	2.70	0.45
1:C:375:THR:OG1	1:C:379:GLU:OE1	2.35	0.45
2:D:60:ASP:O	2:D:70:LEU:HD12	2.17	0.45
1:C:647:ILE:O	1:C:651:GLU:HG3	2.17	0.45
2:B:117:LEU:HB2	2:B:153:TRP:CE2	2.52	0.45
1:A:590:VAL:CG1	1:A:622:MSE:SE	3.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:TYR:CA	3:C:113:HOH:O	2.63	0.45
1:A:545:ASP:CG	1:C:556:LYS:HZ3	2.20	0.45
1:A:683:VAL:O	1:A:686:ASN:HB3	2.17	0.45
2:B:27:CYS:HB2	2:B:56:VAL:HB	1.98	0.45
1:C:444:GLU:O	1:C:448:ASN:ND2	2.50	0.45
1:A:416:THR:O	1:A:419:SER:N	2.50	0.45
1:C:493:GLN:CG	1:C:494:ILE:N	2.79	0.44
2:D:285:LEU:C	2:D:287:GLY:N	2.71	0.44
1:A:519:VAL:C	1:A:521:GLY:N	2.64	0.44
2:B:24:MSE:HG2	2:B:25:ALA:N	2.32	0.44
2:B:260:ALA:HB1	2:B:269:LEU:HD11	2.00	0.44
1:C:510:ILE:HG21	1:C:533:ASN:HD22	1.80	0.44
2:B:63:HIS:CE1	2:B:65:LYS:H	2.32	0.44
1:A:578:LYS:O	1:A:580:GLU:HG3	2.16	0.44
2:D:265:SER:HA	3:D:353:HOH:O	2.17	0.44
2:B:203:HIS:CE1	2:B:232:ILE:HD12	2.52	0.44
2:B:18:ASP:HB2	3:B:316:HOH:O	2.17	0.44
1:C:639:GLY:HA2	1:C:688:ILE:HG13	1.99	0.44
2:B:180:ASN:N	2:B:180:ASN:HD22	2.15	0.44
1:C:571:ARG:O	1:C:574:TYR:HB3	2.18	0.44
1:A:621:ARG:O	1:A:625:ASN:ND2	2.49	0.44
1:A:531:LEU:C	1:A:533:ASN:N	2.70	0.44
1:A:551:LEU:C	1:A:553:GLU:H	2.20	0.44
2:B:180:ASN:N	2:B:180:ASN:ND2	2.65	0.44
1:A:420:GLU:O	1:A:423:LYS:HG2	2.18	0.44
1:C:590:VAL:O	1:C:590:VAL:CG1	2.66	0.44
1:C:696:ASN:O	1:C:700:ILE:HG13	2.18	0.44
1:A:392:LEU:HD13	3:A:219:HOH:O	2.17	0.44
1:A:578:LYS:HG2	1:A:578:LYS:O	2.16	0.44
2:B:52:HIS:HA	3:B:336:HOH:O	2.18	0.44
2:B:149:ASN:ND2	3:B:357:HOH:O	2.46	0.44
1:A:700:ILE:HD12	1:A:727:PRO:HD2	2.00	0.43
2:B:73:CYS:HB2	2:B:102:VAL:HG12	2.00	0.43
2:B:74:SER:CB	2:B:76:ASP:OD1	2.64	0.43
1:C:596:ILE:O	1:C:600:ILE:HG13	2.18	0.43
1:C:604:TYR:CZ	1:C:610:GLN:HG2	2.53	0.43
1:C:592:GLN:HG3	1:C:595:PHE:CB	2.44	0.43
1:A:647:ILE:O	1:A:651:GLU:HG3	2.18	0.43
1:C:438:VAL:HG22	1:C:439:ILE:N	2.33	0.43
2:D:117:LEU:HB2	2:D:153:TRP:CE2	2.54	0.43
1:C:421:ALA:HB1	1:C:427:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ASP:HA	1:A:614:MSE:HE1	2.00	0.43
2:B:29:SER:HA	2:B:55:PRO:HB3	1.99	0.43
1:C:381:SER:HA	1:C:382:PRO:HD3	1.86	0.43
1:C:389:GLY:HA2	1:C:711:THR:O	2.18	0.43
1:A:519:VAL:O	1:A:521:GLY:N	2.51	0.43
2:B:24:MSE:HE3	2:B:26:THR:CG2	2.48	0.43
2:B:141:ILE:HD13	2:B:185:TRP:CZ3	2.54	0.43
1:A:438:VAL:HG21	1:A:444:GLU:CA	2.48	0.43
1:A:557:ASN:HB3	1:C:496:THR:CG2	2.48	0.43
1:C:408:LYS:CD	1:C:408:LYS:H	2.10	0.43
2:D:227:GLN:HG2	3:D:410:HOH:O	2.16	0.43
1:C:567:SER:HB3	1:C:570:SER:CB	2.47	0.43
1:C:656:GLU:OE2	1:C:670:HIS:HA	2.18	0.43
2:D:203:HIS:CE1	2:D:232:ILE:HD12	2.53	0.43
1:A:434:ARG:NH2	1:A:675:THR:HG22	2.34	0.43
1:A:699:LEU:O	1:A:703:PHE:HD1	2.02	0.43
1:C:674:MSE:SE	1:C:678:ILE:CD1	3.16	0.43
2:B:34:LYS:HB3	2:B:45:LEU:HD11	2.00	0.43
2:B:181:LEU:CD2	2:B:201:GLU:HG2	2.49	0.43
1:A:674:MSE:O	1:A:678:ILE:HG12	2.18	0.43
1:C:422:LEU:HA	1:C:422:LEU:HD12	1.83	0.43
2:D:275:ASP:OD1	2:D:277:LYS:CB	2.67	0.43
2:D:209:ASP:HB2	2:D:258:TRP:O	2.19	0.43
1:A:396:THR:HG23	3:A:251:HOH:O	2.18	0.43
1:A:444:GLU:O	1:A:448:ASN:ND2	2.52	0.43
2:B:284:ASN:HB2	3:B:351:HOH:O	2.18	0.43
2:D:33:ILE:HB	2:D:49:LEU:HB2	2.01	0.42
1:A:420:GLU:HG3	1:A:423:LYS:CE	2.49	0.42
2:B:8:HIS:CE1	2:B:34:LYS:HG3	2.54	0.42
1:C:494:ILE:CG1	1:C:495:GLU:H	2.23	0.42
2:B:131:LYS:HD2	2:B:135:THR:OG1	2.19	0.42
1:C:590:VAL:HG13	1:C:622:MSE:CE	2.49	0.42
2:B:29:SER:C	2:B:31:LYS:N	2.73	0.42
2:B:121:SER:N	3:B:337:HOH:O	2.52	0.42
1:A:649:LEU:HB3	1:A:698:GLN:OE1	2.20	0.42
1:C:408:LYS:O	1:C:408:LYS:HG2	2.19	0.42
2:D:227:GLN:C	2:D:229:ARG:H	2.22	0.42
1:A:421:ALA:O	1:A:425:LYS:N	2.52	0.42
2:D:155:PRO:HG3	2:D:214:PRO:HA	2.00	0.42
2:D:261:SER:HA	3:D:351:HOH:O	2.19	0.42
2:D:49:LEU:HD22	2:D:82:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:CD1	3:A:219:HOH:O	2.67	0.42
1:A:688:ILE:HG12	1:A:689:ASN:H	1.84	0.42
1:C:430:LEU:HD23	1:C:430:LEU:O	2.18	0.42
2:D:202:GLY:O	2:D:232:ILE:HD11	2.19	0.42
1:A:559:TYR:CD2	1:C:541:VAL:HG21	2.54	0.42
1:A:670:HIS:HD2	3:A:241:HOH:O	2.01	0.42
2:D:94:VAL:O	2:D:94:VAL:HG13	2.19	0.42
1:A:683:VAL:O	1:A:687:PHE:HD1	2.03	0.42
1:A:707:ILE:O	1:A:710:THR:HB	2.18	0.42
2:B:27:CYS:HB2	2:B:56:VAL:CG1	2.49	0.42
1:C:592:GLN:NE2	3:C:229:HOH:O	2.51	0.42
2:D:174:VAL:HG23	2:D:183:LYS:O	2.19	0.42
1:A:381:SER:HA	1:A:382:PRO:HD3	1.90	0.42
2:D:295:VAL:HG12	2:D:296:HIS:H	1.85	0.42
3:A:251:HOH:O	2:B:3:VAL:HG13	2.19	0.42
1:A:438:VAL:HG22	1:A:439:ILE:N	2.35	0.42
2:D:106:GLN:NE2	3:D:408:HOH:O	2.53	0.42
1:A:540:MSE:HE1	1:C:537:MSE:SE	2.70	0.42
2:B:50:THR:O	2:B:82:TRP:HH2	2.03	0.42
1:A:660:LYS:HD2	1:A:664:LYS:O	2.20	0.42
1:A:616:ILE:HD11	1:A:640:SER:HB2	2.01	0.42
2:B:189:SER:C	2:B:191:ALA:N	2.73	0.41
1:A:661:LYS:C	1:A:663:ASN:H	2.23	0.41
2:B:216:VAL:HG12	2:B:216:VAL:O	2.19	0.41
1:A:552:LYS:HG2	1:A:552:LYS:O	2.20	0.41
1:A:582:ASP:OD1	1:A:614:MSE:HE1	2.20	0.41
1:C:723:LEU:HD21	1:C:736:GLU:CG	2.50	0.41
2:B:214:PRO:O	2:B:215:THR:C	2.59	0.41
1:A:556:LYS:O	1:A:559:TYR:HB3	2.21	0.41
1:A:430:LEU:HD23	1:A:430:LEU:O	2.19	0.41
2:B:57:TRP:HA	2:B:57:TRP:CE3	2.55	0.41
1:C:384:ALA:HA	1:C:393:VAL:O	2.21	0.41
1:C:683:VAL:O	1:C:686:ASN:HB3	2.21	0.41
1:A:388:PHE:CE2	1:A:716:PHE:HE2	2.37	0.41
2:B:64:PRO:HD2	3:B:333:HOH:O	2.20	0.41
2:D:251:GLU:OE1	2:D:251:GLU:N	2.41	0.41
2:B:187:TYR:HE1	2:B:193:THR:N	2.18	0.41
2:B:52:HIS:CD2	2:B:56:VAL:HG22	2.55	0.41
2:B:8:HIS:ND1	2:B:30:ASP:OD2	2.53	0.41
2:D:49:LEU:HB3	2:D:82:TRP:CZ3	2.56	0.41
1:A:694:ILE:HG23	1:A:699:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:PHE:CD1	1:A:739:ARG:NH2	2.89	0.41
1:A:511:GLU:HG3	3:A:107:HOH:O	2.21	0.41
1:C:661:LYS:C	1:C:663:ASN:N	2.73	0.41
1:C:661:LYS:O	1:C:663:ASN:N	2.53	0.41
2:D:112:TYR:CZ	2:D:171:ARG:HG2	2.56	0.41
2:B:23:ARG:NH1	2:B:68:THR:HG21	2.36	0.41
2:D:209:ASP:OD1	2:D:259:ARG:HA	2.20	0.41
2:D:78:LYS:NZ	3:D:378:HOH:O	2.52	0.41
2:B:251:GLU:OE1	2:B:251:GLU:N	2.54	0.41
2:D:105:VAL:HG23	2:D:105:VAL:O	2.21	0.41
1:C:440:ASP:OD1	1:C:443:ASN:HB2	2.20	0.41
1:C:392:LEU:HB2	1:C:407:PRO:HG2	2.03	0.40
2:B:66:PHE:HE2	2:B:114:PRO:HD3	1.81	0.40
2:B:7:ALA:O	2:B:34:LYS:HD2	2.21	0.40
2:D:56:VAL:HA	2:D:74:SER:HB2	2.02	0.40
1:C:662:ASP:OD1	1:C:662:ASP:O	2.39	0.40
2:D:29:SER:C	3:D:417:HOH:O	2.59	0.40
2:B:79:VAL:HB	2:B:95:HIS:HB3	2.04	0.40
2:D:225:VAL:HG13	2:D:257:LEU:HB2	2.03	0.40
1:C:527:VAL:HG21	1:C:551:LEU:HD21	2.03	0.40
1:A:584:LEU:CD1	1:A:584:LEU:N	2.83	0.40
1:A:700:ILE:O	1:A:703:PHE:HB2	2.21	0.40
2:D:124:LYS:CG	3:D:409:HOH:O	2.61	0.40
1:C:441:ASP:O	1:C:445:GLU:HG3	2.21	0.40
1:A:608:ILE:HB	1:A:611:ARG:HH12	1.86	0.40
2:B:126:SER:O	3:B:339:HOH:O	2.22	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]	2.14	0.06

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%)	292 (86%)	39 (12%)	8 (2%)	7 5
1	C	341/399 (86%)	315 (92%)	22 (6%)	4 (1%)	16 15
2	B	275/297 (93%)	246 (90%)	26 (10%)	3 (1%)	17 17
2	D	284/297 (96%)	258 (91%)	19 (7%)	7 (2%)	7 4
All	All	1239/1392 (89%)	1111 (90%)	106 (9%)	22 (2%)	11 8

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	ILE
1	A	497	ASN
2	D	135	THR
2	D	294	GLU
1	C	439	ILE
2	D	218	LEU
1	A	520	SER
2	B	202	GLY
1	A	548	ASN
1	A	578	LYS
2	B	275	ASP
1	C	662	ASP
2	D	202	GLY
1	A	388	PHE
1	A	498	PHE
1	C	518	LEU
2	D	87	GLY
2	D	286	GLU
1	A	653	PRO
2	B	40	GLY
2	D	146	ILE
1	C	407	PRO

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	306/340 (90%)	300 (98%)	6 (2%)	63 77
1	C	308/340 (91%)	299 (97%)	9 (3%)	50 64
2	B	237/245 (97%)	234 (99%)	3 (1%)	76 87
2	D	244/245 (100%)	238 (98%)	6 (2%)	55 70
All	All	1095/1170 (94%)	1071 (98%)	24 (2%)	60 75

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	TYR
1	A	509	ASN
1	A	534	ASP
1	A	545	ASP
1	A	615	MSE
1	A	729	ASP
2	B	112	TYR
2	B	152	SER
2	B	238	ASN
1	C	408	LYS
1	C	432	ASN
1	C	440	ASP
1	C	509	ASN
1	C	510	ILE
1	C	534	ASP
1	C	538	GLU
1	C	657	ASP
1	C	688	ILE
2	D	28	SER
2	D	85	GLU
2	D	157	THR
2	D	198	SER
2	D	204	SER
2	D	251	GLU

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

Mol	Chain	Res	Type
1	A	433	GLN
1	A	443	ASN

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Mol	Chain	Res	Type
1	A	448	ASN
1	A	509	ASN
1	A	517	ASN
1	A	592	GLN
1	A	601	GLN
1	A	670	HIS
2	B	149	ASN
2	B	180	ASN
2	B	238	ASN
2	B	240	GLN
2	B	276	ASN
1	C	433	GLN
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	606	ASN
1	C	686	ASN
2	D	110	HIS
2	D	149	ASN
2	D	180	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

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	336/399 (84%)	1.39	93 (27%)	1	1	52, 87, 110, 119	0
1	C	338/399 (84%)	0.88	47 (13%)	4	7	35, 67, 99, 117	0
2	B	273/297 (91%)	0.98	44 (16%)	3	4	28, 64, 105, 120	0
2	D	282/297 (94%)	0.81	37 (13%)	5	8	27, 49, 90, 113	0
All	All	1229/1392 (88%)	1.03	221 (17%)	2	3	27, 70, 106, 120	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	216	VAL	8.7
2	B	216	VAL	6.9
1	C	494	ILE	6.8
1	A	439	ILE	6.5
1	A	550	ARG	6.4
1	A	690	GLY	5.9
2	D	158	ILE	5.9
1	A	496	THR	5.7
1	A	495	GLU	5.7
2	B	25	ALA	5.4
2	D	296	HIS	5.3
1	A	741	LEU	5.2
2	B	133	ASN	5.2
1	A	694	ILE	5.2
2	D	133	ASN	5.1
2	D	295	VAL	5.0
1	A	663	ASN	4.9
1	A	468	PHE	4.7
1	C	438	VAL	4.6
1	C	678	ILE	4.5
2	D	217	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	135	THR	4.4
1	A	689	ASN	4.4
2	D	88	ARG	4.3
1	A	573	LEU	4.3
1	A	452	LYS	4.3
1	A	408	LYS	4.3
1	C	495	GLU	4.2
2	B	135	THR	4.1
1	C	499	GLN	4.1
1	C	496	THR	4.1
1	A	436	VAL	4.0
1	A	437	LYS	4.0
1	A	551	LEU	4.0
2	B	131	LYS	4.0
1	C	541	VAL	3.9
1	A	467	ALA	3.9
1	C	690	GLY	3.9
2	B	86	ASN	3.9
1	C	437	LYS	3.8
1	A	435	LEU	3.8
2	B	42	THR	3.8
2	B	88	ARG	3.7
1	C	469	ASP	3.7
2	D	25	ALA	3.7
1	A	677	PHE	3.6
1	C	502	GLY	3.6
1	C	547	ASN	3.6
1	A	664	LYS	3.5
2	B	190	ASP	3.5
1	A	596	ILE	3.5
2	B	132	GLU	3.5
2	D	167	THR	3.5
1	A	695	ASN	3.5
1	A	733	VAL	3.4
1	C	542	ILE	3.4
1	C	680	ARG	3.4
1	A	572	ILE	3.4
1	C	436	VAL	3.4
1	C	681	PHE	3.4
2	B	148	VAL	3.3
1	A	634	LEU	3.3
1	C	497	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	447	TRP	3.3
2	B	137	SER	3.3
2	B	38	VAL	3.3
1	C	745	GLY	3.3
2	B	157	THR	3.3
1	A	579	ARG	3.3
1	A	680	ARG	3.3
1	A	441	ASP	3.3
1	C	549	GLU	3.2
2	B	175	THR	3.2
2	D	218	LEU	3.2
2	D	233	ILE	3.2
1	A	519	VAL	3.2
2	B	45	LEU	3.2
1	A	731	GLU	3.1
2	B	134	GLY	3.1
2	D	176	GLY	3.1
2	D	70	LEU	3.1
2	D	136	THR	3.1
1	A	450	LEU	3.1
1	C	498	PHE	3.1
1	A	463	LYS	3.1
2	B	66	PHE	3.1
2	B	85	GLU	3.0
1	A	666	ILE	3.0
1	A	584	LEU	3.0
2	B	35	ILE	3.0
2	B	285	LEU	3.0
2	B	41	GLU	3.0
1	A	416	THR	2.9
1	A	541	VAL	2.9
2	B	16	VAL	2.9
1	A	547	ASN	2.9
1	A	608	ILE	2.9
1	A	560	PHE	2.9
2	B	136	THR	2.8
2	D	166	GLY	2.8
1	A	447	TRP	2.8
1	A	497	ASN	2.8
1	C	439	ILE	2.8
1	C	555	VAL	2.7
1	A	574	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	411	GLY	2.7
1	A	428	LYS	2.7
1	A	509	ASN	2.7
1	A	624	GLU	2.7
1	A	548	ASN	2.7
1	C	435	LEU	2.7
1	A	424	THR	2.7
1	C	550	ARG	2.7
2	B	2	VAL	2.7
1	A	606	ASN	2.7
2	B	130	PHE	2.6
1	A	402	VAL	2.6
1	A	644	VAL	2.6
1	A	682	THR	2.6
1	A	716	PHE	2.6
2	D	169	GLU	2.6
1	A	420	GLU	2.6
1	A	697	GLU	2.6
2	B	182	VAL	2.6
2	D	210	VAL	2.6
1	A	440	ASP	2.6
1	C	539	ALA	2.6
2	B	40	GLY	2.5
1	A	524	LYS	2.5
2	D	102	VAL	2.5
2	D	132	GLU	2.5
2	D	294	GLU	2.5
1	A	521	GLY	2.5
1	C	597	SER	2.5
1	C	463	LYS	2.5
1	C	648	TRP	2.5
2	D	269	LEU	2.5
1	A	623	LYS	2.5
1	A	397	PRO	2.5
1	A	542	ILE	2.5
1	C	596	ILE	2.5
2	B	151	ALA	2.5
1	A	559	TYR	2.5
1	C	633	THR	2.5
1	A	438	VAL	2.5
1	C	677	PHE	2.5
2	D	223	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	544	LEU	2.5
1	C	632	LEU	2.5
1	A	578	LYS	2.4
1	A	735	THR	2.4
2	B	112	TYR	2.4
1	A	423	LYS	2.4
1	C	505	SER	2.4
2	B	150	SER	2.4
2	B	264	LEU	2.4
1	A	729	ASP	2.4
2	B	119	ALA	2.4
1	C	450	LEU	2.4
1	A	657	ASP	2.4
2	D	184	ILE	2.4
1	C	468	PHE	2.4
1	A	539	ALA	2.4
1	A	569	LEU	2.3
1	A	600	ILE	2.3
2	B	15	ALA	2.3
1	C	441	ASP	2.3
2	D	73	CYS	2.3
2	D	239	GLU	2.3
2	D	134	GLY	2.3
1	A	510	ILE	2.3
1	A	675	THR	2.3
2	D	71	ALA	2.3
1	A	681	PHE	2.3
2	B	217	LEU	2.3
2	D	231	CYS	2.3
1	A	456	ASP	2.3
1	A	412	LEU	2.3
1	C	573	LEU	2.3
2	B	71	ALA	2.3
1	C	501	GLU	2.3
2	D	174	VAL	2.2
1	A	618	LEU	2.2
1	A	469	ASP	2.2
2	D	26	THR	2.2
1	C	661	LYS	2.2
1	A	595	PHE	2.2
1	A	426	ASP	2.2
1	A	679	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	700	ILE	2.2
2	D	225	VAL	2.2
1	A	728	SER	2.2
1	A	661	LYS	2.1
1	C	521	GLY	2.1
1	A	532	GLU	2.1
1	A	374	PRO	2.1
2	B	225	VAL	2.1
1	C	679	GLU	2.1
1	A	633	THR	2.1
1	A	678	ILE	2.1
1	A	549	GLU	2.1
2	B	113	GLY	2.1
1	A	459	GLU	2.1
2	B	3	VAL	2.1
2	B	174	VAL	2.1
1	A	632	LEU	2.1
2	B	70	LEU	2.1
1	A	648	TRP	2.1
2	D	240	GLN	2.1
1	C	515	SER	2.1
1	A	400	LYS	2.1
1	C	660	LYS	2.1
2	D	86	ASN	2.0
1	C	503	ASP	2.0
2	D	72	SER	2.0
2	B	56	VAL	2.0
1	C	684	PHE	2.0
2	B	176	GLY	2.0
2	D	118	VAL	2.0
2	B	10	GLU	2.0
2	D	173	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.