



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 07:27 AM EDT

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

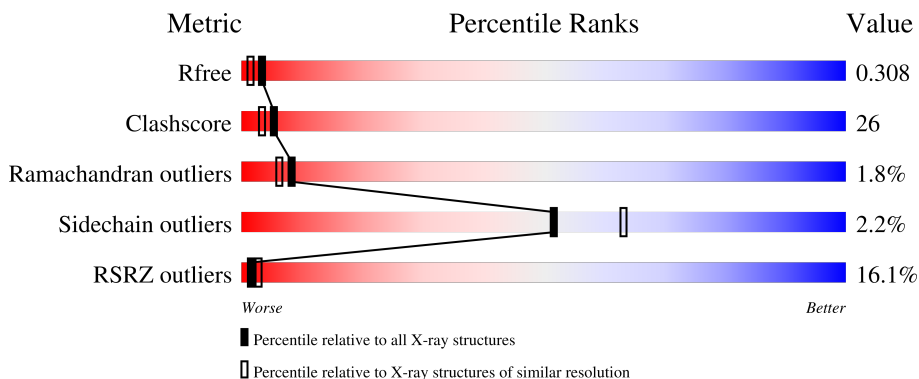
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	399	
1	C	399	
2	B	297	
2	D	297	

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
			Total	C	N	O	S	Se			
1	A	345	2729	1723	449	547	1	9	0	0	0
1	C	347	2746	1734	452	550	1	9	0	0	0

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 mutation	UNP P38968
A	455	MSE	MET	modified residue	UNP P38968
A	536	MSE	LEU	engineered mutation	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 mutation	UNP P38968
A	622	MSE	LEU	engineered mutation	UNP P38968
A	674	MSE	LEU	engineered mutation	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 mutation	UNP P38968
C	455	MSE	MET	modified residue	UNP P38968
C	536	MSE	LEU	engineered mutation	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 mutation	UNP P38968
C	622	MSE	LEU	engineered mutation	UNP P38968
C	674	MSE	LEU	engineered mutation	UNP P38968

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	279	2196	1397	375	415	3	6	0	0	0
2	D	288	2263	1438	387	429	3	6	0	0	0

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 mutation	UNP Q04491
B	17	MSE	LEU	engineered mutation	UNP Q04491
B	24	MSE	LEU	engineered mutation	UNP Q04491
B	80	MSE	LEU	engineered mutation	UNP Q04491
B	115	MSE	LEU	engineered mutation	UNP Q04491
B	222	MSE	LEU	engineered mutation	UNP Q04491
D	1	MSE	MET	modified residue	UNP Q04491
D	11	MSE	LEU	engineered mutation	UNP Q04491
D	17	MSE	LEU	engineered mutation	UNP Q04491
D	24	MSE	LEU	engineered mutation	UNP Q04491
D	80	MSE	LEU	engineered mutation	UNP Q04491
D	115	MSE	LEU	engineered mutation	UNP Q04491
D	222	MSE	LEU	engineered mutation	UNP Q04491

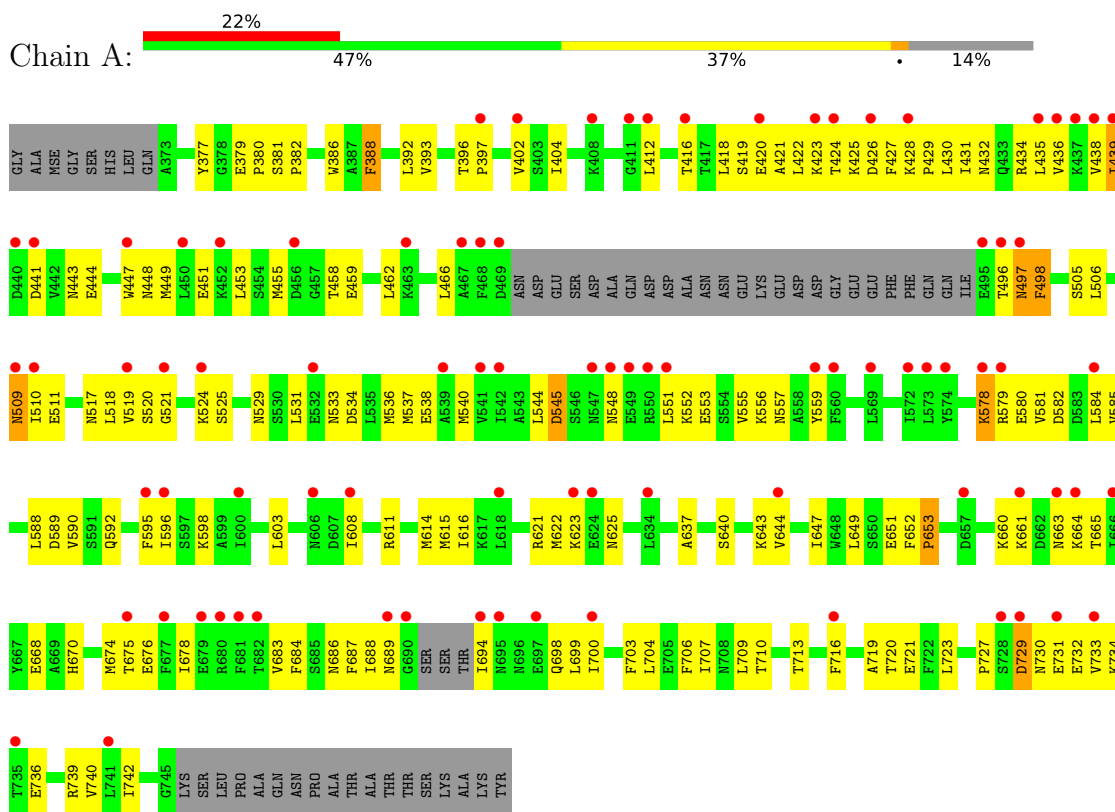
- Molecule 3 is water.

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

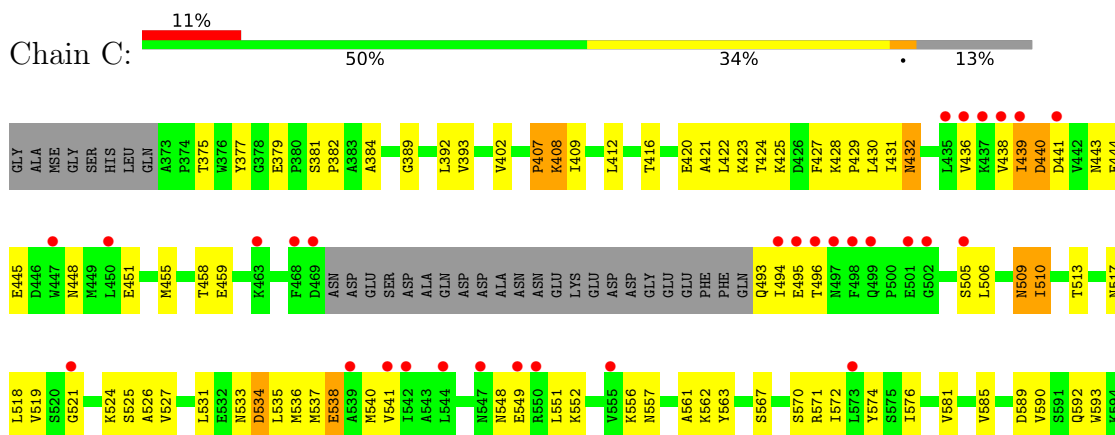
3 Residue-property plots [i](#)

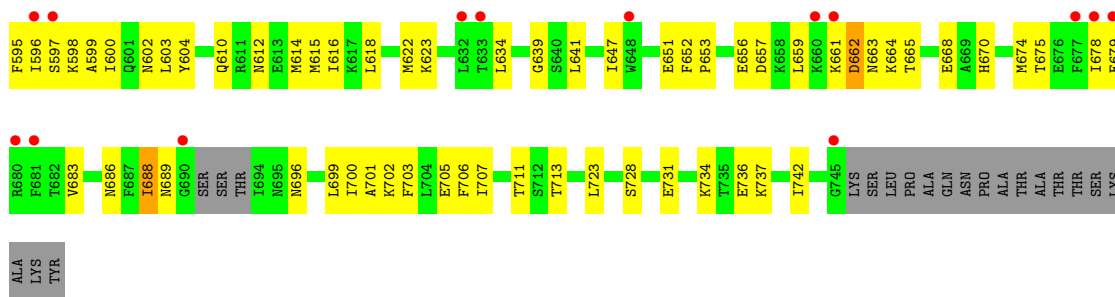
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

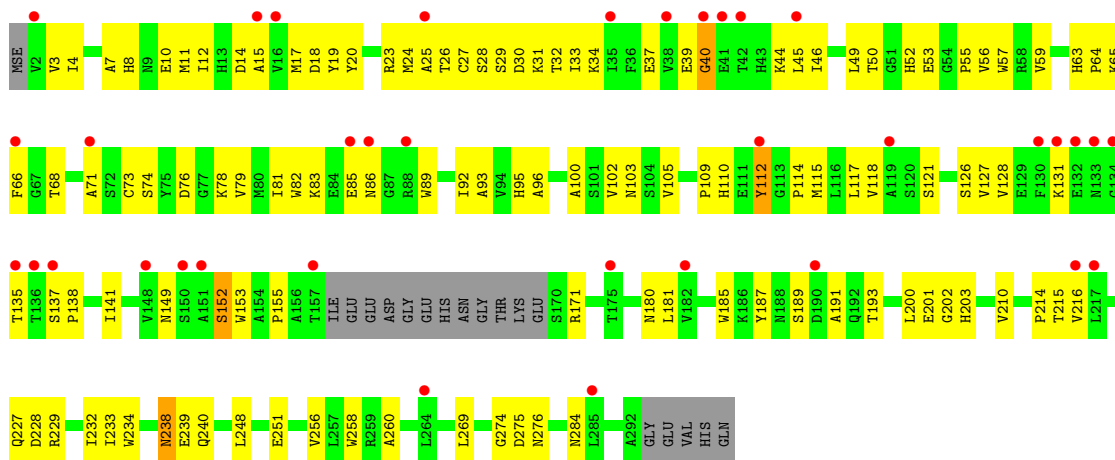


- Molecule 1: Protein transport protein SEC31

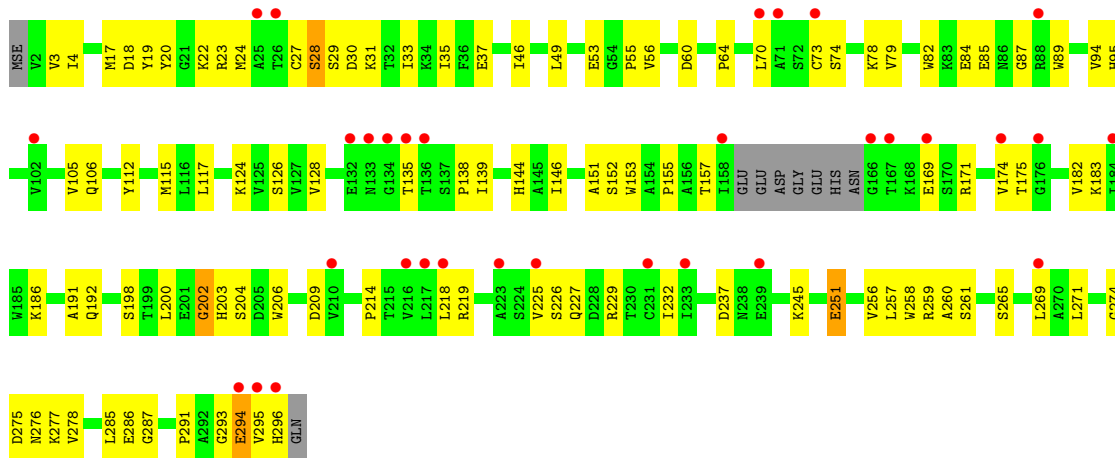




• Molecule 2: Protein transport protein SEC13



• Molecule 2: Protein transport protein SEC13



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	6.47 (at 2.36Å)	Xtrriage
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%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtrriage
Anisotropy	0.883	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.009 for l,-k,h	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	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 [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	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:HD3	1:C:408:LYS:H	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
1:A:412:LEU:HD21	1:A:713:THR:HG22	1.57	0.87
2:B:233:ILE:HD11	2:B:248:LEU:HD13	1.56	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
2:B:18:ASP:OD2	2:B:23:ARG:HB3	1.81	0.81
1:C:524:LYS:HG3	1:C:525:SER:H	1.46	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:HD3	1:C:408:LYS:N	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:A:590:VAL:HG13	1:A:622:MSE:SE	2.36	0.74
1:C:612:ASN:O	1:C:616:ILE:HG12	1.87	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:O	1:C:425:LYS:HD3	1.94	0.68
1:A:581:VAL:HG23	1:A:614:MSE:HE2	1.74	0.68
1:A:623:LYS:HE3	1:A:647:ILE:HD12	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
1:A:397:PRO:HG3	2:B:276:ASN:ND2	2.11	0.66
2:D:33:ILE:CD1	2:D:56:VAL:HG11	2.26	0.66
2:B:102:VAL:CG2	3:B:352:HOH:O	2.44	0.65
2:B:10:GLU:HB2	3:B:335:HOH:O	1.96	0.65
2:D:206:TRP:CE3	3:D:410:HOH:O	2.49	0.65
1:A:402:VAL:HG11	2:B:24:MSE:SE	2.47	0.65
1:C:675:THR:O	1:C:679:GLU:HG3	1.96	0.65
2:D:33:ILE:HB	2:D:49:LEU:HD12	1.79	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
1:A:404:ILE:N	1:A:404:ILE:HD12	2.12	0.64
1:A:531:LEU:C	1:A:533:ASN:H	2.01	0.64
2:B:112:TYR:HA	2:B:171:ARG:HH21	1.60	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:A:588:LEU:HB3	1:A:596:ILE:HD11	1.80	0.63
1:C:618:LEU:O	1:C:622:MSE:HG2	1.98	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
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:C:494:ILE:HG13	1:C:495:GLU:N	2.13	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:A:509:ASN:N	1:A:509:ASN:HD22	1.99	0.60
1:A:519:VAL:HG13	1:C:599:ALA:HA	1.83	0.60
1:C:493:GLN:HG3	1:C:494:ILE:H	1.66	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
2:B:66:PHE:CE2	2:B:114:PRO:HD3	2.36	0.60
1:C:723:LEU:HD21	1:C:736:GLU:HG2	1.83	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:A:665:THR:OG1	1:A:668:GLU:HG3	2.02	0.59
1:C:742:ILE:O	2:D:22:LYS:HD2	2.02	0.59
1:C:524:LYS:HG3	1:C:525:SER:N	2.16	0.59
2:D:18:ASP:OD2	2:D:23:ARG:HB3	2.02	0.59
2:D:245:LYS:NZ	3:D:335:HOH:O	2.34	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:379:GLU:HG2	2:B:258:TRP:CZ2	2.39	0.58
1:A:380:PRO:HG3	2:B:11:MSE:HE2	1.86	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
2:D:219:ARG:HG2	2:D:237:ASP:OD1	2.04	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
1:A:716:PHE:HD2	1:A:740:VAL:HG13	1.69	0.57
2:B:24:MSE:HE3	2:B:26:THR:HG23	1.84	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:402:VAL:HG11	2:B:24:MSE:HE1	1.86	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: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:402:VAL:HG11	2:D:24:MSE:SE	2.54	0.57
1:C:674:MSE:HE3	1:C:705:GLU:HB2	1.87	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
1:A:579:ARG:HB3	1:A:603:LEU:HD11	1.87	0.56
2:B:49:LEU:HB3	2:B:82:TRP:CZ3	2.40	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:A:688:ILE:HG12	1:A:689:ASN:N	2.22	0.55
2:B:33:ILE:N	2:B:33:ILE:HD12	2.21	0.55
1:C:533:ASN:OD1	1:C:534:ASP:N	2.39	0.55
2:D:285:LEU:C	2:D:287:GLY:H	2.10	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
1:A:418:LEU:O	1:A:422:LEU:HB2	2.05	0.55
2:B:33:ILE:HB	2:B:49:LEU:HD12	1.88	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:63:HIS:HB3	2:B:66:PHE:CE1	2.42	0.54
2:B:200:LEU:HB3	2:B:234:TRP:CH2	2.43	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:65:LYS:HE2	2:B:110:HIS:HB2	1.90	0.54
2:B:233:ILE:HD12	2:B:233:ILE:N	2.22	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:85:GLU:O	2:B:86:ASN:HB2	2.09	0.53
2:B:274:GLY:C	2:B:276:ASN:N	2.62	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:688:ILE:HG13	1:C:689:ASN:H	1.74	0.51
1:C:728:SER:HB3	1:C:737:LYS:NZ	2.25	0.51
2:B:30:ASP:OD1	2:B:32:THR:N	2.43	0.51
1:C:409:ILE:HB	1:C:412:LEU:HB3	1.93	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
1:A:551:LEU:C	1:A:551:LEU:HD23	2.30	0.51
2:B:19:TYR:CD2	2:B:64:PRO:HG2	2.45	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:432:ASN:O	1:C:436:VAL:HG23	2.10	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:A:742:ILE:HD12	2:B:20:TYR:CE2	2.46	0.50
2:B:46:ILE:HD12	2:B:46:ILE:N	2.26	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:A:438:VAL:HG23	1:A:443:ASN:HD22	1.76	0.50
1:C:663:ASN:C	2:D:285:LEU:HD11	2.32	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
2:B:14:ASP:HB3	2:B:27:CYS:SG	2.51	0.49
1:C:423:LYS:HG3	1:C:424:THR:N	2.27	0.49
1:A:462:LEU:HD13	1:A:637:ALA:HB2	1.94	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:420:GLU:HG3	1:A:423:LYS:HE2	1.93	0.49
1:A:438:VAL:HG21	1:A:444:GLU:HA	1.93	0.49
2:B:121:SER:CA	3:B:337:HOH:O	2.60	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:C:604:TYR:CE2	1:C:610:GLN:HG2	2.47	0.49
1:A:423:LYS:HG3	1:A:424:THR:N	2.27	0.49
1:A:524:LYS:HG3	1:A:525:SER:N	2.27	0.49
2:D:19:TYR:CD2	2:D:64:PRO:HG2	2.48	0.49
2:D:182:VAL:HB	2:D:200:LEU:HB2	1.95	0.49
1:A:538:GLU:OE1	1:A:538:GLU:N	2.41	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
2:B:4:ILE:O	2:B:4:ILE:HG22	2.12	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:A:616:ILE:HD11	1:A:640:SER:CB	2.43	0.48
1:C:548:ASN:O	1:C:552:LYS:CB	2.62	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:109:PRO:HD2	2:B:112:TYR:CD1	2.48	0.48
2:B:238:ASN:HD22	2:B:240:GLN:N	2.05	0.48
2:D:226:SER:OG	2:D:227:GLN:N	2.47	0.48
1:A:428:LYS:NZ	1:A:455:MSE:HG2	2.29	0.48
2:D:294:GLU:O	2:D:294:GLU:HG3	2.13	0.48
1:A:517:ASN:ND2	1:A:529:ASN:HD22	2.11	0.48
2:B:238:ASN:ND2	2:B:240:GLN:HB2	2.28	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:615:MSE:HE3	1:C:634:LEU:HD23	1.96	0.47
1:C:701:ALA:O	1:C:705:GLU:HG3	2.14	0.47
2:D:251:GLU:H	2:D:251:GLU:CD	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:430:LEU:C	1:C:430:LEU:HD23	2.35	0.47
1:C:548:ASN:OD1	1:C:549:GLU:N	2.47	0.47
1:A:444:GLU:HG2	1:A:448:ASN:HD21	1.80	0.47
1:A:518:LEU:HD13	1:C:576:ILE:HD12	1.96	0.47
1:A:730:ASN:O	1:A:733:VAL:HB	2.15	0.47
1:C:439:ILE:HG13	1:C:440:ASP:H	1.80	0.47
2:D:191:ALA:O	2:D:192:GLN:HB2	2.15	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:B:117:LEU:HB2	2:B:153:TRP:NE1	2.30	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: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: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:517:ASN:HD21	1:A:529:ASN:ND2	2.12	0.46
1:A:427:PHE:CD1	1:A:427:PHE:N	2.83	0.46
1:A:434:ARG:HH21	1:A:675:THR:HG22	1.80	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:B:112:TYR:N	2:B:112:TYR:HD2	2.13	0.46
2:D:31:LYS:HA	3:D:417:HOH:O	2.14	0.46
2:B:15:ALA:HA	2:B:25:ALA:O	2.16	0.46
2:B:152:SER:OG	2:B:210:VAL:O	2.34	0.46
1:C:451:GLU:O	1:C:455:MSE:HG3	2.15	0.46
1:C:524:LYS:CG	1:C:525:SER:H	2.24	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
1:A:388:PHE:HB2	1:A:739:ARG:NH2	2.28	0.45
1:A:709:LEU:O	1:A:713:THR:HG23	2.16	0.45
2:D:112:TYR:HB3	2:D:115:MSE:HE3	1.96	0.45
2:D:293:GLY:O	2:D:294:GLU:C	2.55	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:HG3	1:A:592:GLN:O	2.16	0.45
2:B:30:ASP:OD1	2:B:30:ASP:C	2.55	0.45
1:C:551:LEU:HD23	1:C:551:LEU:C	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:555:VAL:N	3:A:199:HOH:O	2.47	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: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
2:D:274:GLY:C	2:D:276:ASN:N	2.70	0.45
1:A:545:ASP:CG	1:C:556:LYS:HZ3	2.20	0.45
1:A:590:VAL:CG1	1:A:622:MSE:SE	3.13	0.45
2:B:117:LEU:HB2	2:B:153:TRP:CE2	2.52	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:C:647:ILE:O	1:C:651:GLU:HG3	2.17	0.45
1:A:416:THR:O	1:A:419:SER:N	2.50	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: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:A:578:LYS:O	1:A:580:GLU:HG3	2.16	0.44
2:B:63:HIS:CE1	2:B:65:LYS:H	2.32	0.44
2:B:203:HIS:CE1	2:B:232:ILE:HD12	2.52	0.44
1:C:510:ILE:HG21	1:C:533:ASN:HD22	1.80	0.44
2:D:265:SER:HA	3:D:353:HOH:O	2.17	0.44
2:B:18:ASP:HB2	3:B:316:HOH:O	2.17	0.44
2:B:180:ASN:N	2:B:180:ASN:HD22	2.15	0.44
1:C:639:GLY:HA2	1:C:688:ILE:HG13	1.99	0.44
1:A:621:ARG:O	1:A:625:ASN:ND2	2.49	0.44
1:C:571:ARG:O	1:C:574:TYR:HB3	2.18	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:O	1:A:578:LYS:HG2	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: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
1:C:592:GLN:HG3	1:C:595:PHE:CB	2.44	0.43
2:D:117:LEU:HB2	2:D:153:TRP:CE2	2.54	0.43
1:A:582:ASP:HA	1:A:614:MSE:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:421:ALA:HB1	1:C:427:PHE:CD2	2.53	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:H	1:C:408:LYS:CD	2.10	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
2:D:227:GLN:HG2	3:D:410:HOH:O	2.16	0.43
1:A:434:ARG:NH2	1:A:675:THR:HG22	2.34	0.43
1:A:674:MSE:O	1:A:678:ILE:HG12	2.18	0.43
1:A:699:LEU:O	1:A:703:PHE:HD1	2.02	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:C:422:LEU:HD12	1:C:422:LEU:HA	1.83	0.43
1:C:674:MSE:SE	1:C:678:ILE:CD1	3.16	0.43
2:D:275:ASP:OD1	2:D:277:LYS:CB	2.67	0.43
1:A:396:THR:HG23	3:A:251:HOH:O	2.18	0.43
2:D:209:ASP:HB2	2:D:258:TRP:O	2.19	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
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
2:D:33:ILE:HB	2:D:49:LEU:HB2	2.01	0.42
1:A:649:LEU:HB3	1:A:698:GLN:OE1	2.20	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
2:B:131:LYS:HD2	2:B:135:THR:OG1	2.19	0.42
1:C:494:ILE:CG1	1:C:495:GLU:H	2.23	0.42
1:C:590:VAL:HG13	1:C:622:MSE:CE	2.49	0.42
1:A:421:ALA:O	1:A:425:LYS:N	2.52	0.42
1:C:408:LYS:O	1:C:408:LYS:HG2	2.19	0.42
2:D:155:PRO:HG3	2:D:214:PRO:HA	2.00	0.42
2:D:227:GLN:C	2:D:229:ARG:H	2.22	0.42
2:D:261:SER:HA	3:D:351:HOH:O	2.19	0.42
1:A:392:LEU:CD1	3:A:219:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:49:LEU:HD22	2:D:82:TRP:CE3	2.54	0.42
2:D:94:VAL:O	2:D:94:VAL:HG13	2.19	0.42
2:D:202:GLY:O	2:D:232:ILE:HD11	2.19	0.42
1:A:381:SER:HA	1:A:382:PRO:HD3	1.90	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
3:A:251:HOH:O	2:B:3:VAL:HG13	2.19	0.42
2:D:295:VAL:HG12	2:D:296:HIS:H	1.85	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
1:A:660:LYS:HD2	1:A:664:LYS:O	2.20	0.42
2:B:50:THR:O	2:B:82:TRP:HH2	2.03	0.42
1:A:616:ILE:HD11	1:A:640:SER:HB2	2.01	0.42
1:A:552:LYS:O	1:A:552:LYS:HG2	2.20	0.41
1:A:661:LYS:C	1:A:663:ASN:H	2.23	0.41
2:B:189:SER:C	2:B:191:ALA:N	2.73	0.41
2:B:216:VAL:HG12	2:B:216:VAL:O	2.19	0.41
1:A:430:LEU:O	1:A:430:LEU:HD23	2.19	0.41
1:A:556:LYS:O	1:A:559:TYR:HB3	2.21	0.41
1:A:582:ASP:OD1	1:A:614:MSE:HE1	2.20	0.41
2:B:57:TRP:HA	2:B:57:TRP:CE3	2.55	0.41
2:B:214:PRO:O	2:B:215:THR:C	2.59	0.41
1:C:723:LEU:HD21	1:C:736:GLU:CG	2.50	0.41
1:A:388:PHE:CE2	1:A:716:PHE:HE2	2.37	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
2:B:64:PRO:HD2	3:B:333:HOH:O	2.20	0.41
2:B:187:TYR:HE1	2:B:193:THR:N	2.18	0.41
2:D:251:GLU:OE1	2:D:251:GLU:N	2.41	0.41
2:B:8:HIS:ND1	2:B:30:ASP:OD2	2.53	0.41
2:B:52:HIS:CD2	2:B:56:VAL:HG22	2.55	0.41
1:A:694:ILE:HG23	1:A:699:LEU:HD23	2.03	0.41
2:D:49:LEU:HB3	2:D:82:TRP:CZ3	2.56	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:B:23:ARG:NH1	2:B:68:THR:HG21	2.36	0.41
2:B:251:GLU:OE1	2:B:251:GLU:N	2.54	0.41
2:D:78:LYS:NZ	3:D:378:HOH:O	2.52	0.41
2:D:112:TYR:CZ	2:D:171:ARG:HG2	2.56	0.41
2:D:209:ASP:OD1	2:D:259:ARG:HA	2.20	0.41
1:C:440:ASP:OD1	1:C:443:ASN:HB2	2.20	0.41
2:D:105:VAL:O	2:D:105:VAL:HG23	2.21	0.41
2:B:7:ALA:O	2:B:34:LYS:HD2	2.21	0.40
2:B:66:PHE:HE2	2:B:114:PRO:HD3	1.81	0.40
1:C:392:LEU:HB2	1:C:407:PRO:HG2	2.03	0.40
1:C:662:ASP:OD1	1:C:662:ASP:O	2.39	0.40
2:D:56:VAL:HA	2:D:74:SER:HB2	2.02	0.40
1:A:584:LEU:N	1:A:584:LEU:CD1	2.83	0.40
2:B:79:VAL:HB	2:B:95:HIS:HB3	2.04	0.40
1:C:527:VAL:HG21	1:C:551:LEU:HD21	2.03	0.40
2:D:29:SER:C	3:D:417:HOH:O	2.59	0.40
2:D:225:VAL:HG13	2:D:257:LEU:HB2	2.03	0.40
1:A:608:ILE:HB	1:A:611:ARG:HH12	1.86	0.40
1:A:700:ILE:O	1:A:703:PHE:HB2	2.21	0.40
1:C:441:ASP:O	1:C:445:GLU:HG3	2.21	0.40
2:D:124:LYS:CG	3:D:409:HOH:O	2.61	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%)	6	4
1	C	341/399 (86%)	315 (92%)	22 (6%)	4 (1%)	13	11
2	B	275/297 (93%)	246 (90%)	26 (10%)	3 (1%)	14	13
2	D	284/297 (96%)	258 (91%)	19 (7%)	7 (2%)	5	3
All	All	1239/1392 (89%)	1111 (90%)	106 (9%)	22 (2%)	8	6

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%)	55	66
1	C	308/340 (91%)	299 (97%)	9 (3%)	42	52
2	B	237/245 (97%)	234 (99%)	3 (1%)	69	80
2	D	244/245 (100%)	238 (98%)	6 (2%)	47	58
All	All	1095/1170 (94%)	1071 (98%)	24 (2%)	52	63

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

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	336/399 (84%)	1.30	86 (25%) 0 1	52, 87, 110, 119	0
1	C	338/399 (84%)	0.81	44 (13%) 3 5	35, 67, 99, 117	0
2	B	273/297 (91%)	0.90	36 (13%) 3 5	28, 64, 105, 120	0
2	D	282/297 (94%)	0.74	32 (11%) 5 8	27, 49, 90, 113	0
All	All	1229/1392 (88%)	0.95	198 (16%) 1 3	27, 70, 106, 120	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	216	VAL	8.3
2	B	216	VAL	6.6
1	C	494	ILE	6.5
1	A	439	ILE	6.3
1	A	550	ARG	6.3
1	A	690	GLY	5.7
2	D	158	ILE	5.6
1	A	495	GLU	5.5
1	A	496	THR	5.5
2	B	25	ALA	5.2
2	D	296	HIS	5.1
1	A	741	LEU	5.0
2	B	133	ASN	5.0
1	A	694	ILE	5.0
2	D	133	ASN	4.9
2	D	295	VAL	4.8
1	A	663	ASN	4.7
1	A	468	PHE	4.5
1	C	438	VAL	4.4
1	C	678	ILE	4.3
2	D	217	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
2	D	88	ARG	4.2
2	D	135	THR	4.2
1	A	689	ASN	4.2
1	A	408	LYS	4.2
1	A	452	LYS	4.2
1	A	573	LEU	4.1
1	C	495	GLU	4.1
1	C	499	GLN	4.0
2	B	135	THR	4.0
1	C	496	THR	4.0
1	A	437	LYS	3.9
1	A	436	VAL	3.9
2	B	131	LYS	3.9
1	A	551	LEU	3.8
1	C	437	LYS	3.7
1	C	541	VAL	3.7
1	A	435	LEU	3.7
1	C	690	GLY	3.7
1	A	467	ALA	3.7
2	B	86	ASN	3.7
2	B	88	ARG	3.6
2	B	42	THR	3.6
1	C	469	ASP	3.5
2	D	25	ALA	3.5
1	C	502	GLY	3.5
1	A	677	PHE	3.4
1	C	547	ASN	3.4
1	A	664	LYS	3.4
2	B	190	ASP	3.4
2	B	132	GLU	3.4
1	C	680	ARG	3.3
1	A	695	ASN	3.3
1	A	596	ILE	3.3
2	D	167	THR	3.3
1	C	542	ILE	3.3
1	A	733	VAL	3.3
1	A	572	ILE	3.3
1	C	497	ASN	3.2
1	C	681	PHE	3.2
1	C	436	VAL	3.2
2	B	137	SER	3.2
1	C	447	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	148	VAL	3.2
1	A	634	LEU	3.2
1	A	579	ARG	3.2
1	A	680	ARG	3.2
1	C	549	GLU	3.1
2	B	38	VAL	3.1
1	A	441	ASP	3.1
1	C	745	GLY	3.1
2	B	157	THR	3.1
2	D	218	LEU	3.1
2	B	175	THR	3.1
2	B	45	LEU	3.0
2	D	233	ILE	3.0
1	A	519	VAL	3.0
1	A	731	GLU	3.0
1	A	463	LYS	3.0
2	D	176	GLY	3.0
2	D	136	THR	3.0
2	D	70	LEU	3.0
2	B	85	GLU	3.0
2	B	134	GLY	3.0
2	B	66	PHE	2.9
1	A	450	LEU	2.9
1	C	498	PHE	2.9
1	A	666	ILE	2.9
2	B	41	GLU	2.9
1	A	584	LEU	2.9
2	B	285	LEU	2.9
2	B	35	ILE	2.8
1	A	547	ASN	2.8
1	A	416	THR	2.8
1	A	541	VAL	2.7
2	B	16	VAL	2.7
1	A	560	PHE	2.7
2	B	136	THR	2.7
1	A	608	ILE	2.7
2	D	166	GLY	2.7
1	A	497	ASN	2.7
1	A	447	TRP	2.7
1	A	574	TYR	2.7
1	A	428	LYS	2.6
1	C	439	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	624	GLU	2.6
1	C	555	VAL	2.6
1	C	550	ARG	2.6
1	A	411	GLY	2.6
1	A	509	ASN	2.6
1	A	548	ASN	2.6
1	C	435	LEU	2.6
1	A	606	ASN	2.6
1	A	424	THR	2.5
2	B	2	VAL	2.5
1	A	420	GLU	2.5
1	A	697	GLU	2.5
2	D	169	GLU	2.5
1	A	524	LYS	2.5
1	A	644	VAL	2.5
1	A	716	PHE	2.5
2	B	130	PHE	2.5
1	A	682	THR	2.5
2	D	294	GLU	2.5
1	A	623	LYS	2.5
1	C	463	LYS	2.5
1	A	440	ASP	2.5
1	C	539	ALA	2.4
2	D	132	GLU	2.4
1	A	402	VAL	2.4
2	B	182	VAL	2.4
2	D	210	VAL	2.4
1	A	521	GLY	2.4
2	B	40	GLY	2.4
1	C	597	SER	2.4
1	C	648	TRP	2.4
2	D	269	LEU	2.4
2	D	102	VAL	2.4
1	A	559	TYR	2.4
1	A	542	ILE	2.4
1	A	578	LYS	2.4
1	C	596	ILE	2.4
1	A	397	PRO	2.4
2	B	151	ALA	2.4
1	C	633	THR	2.4
1	C	677	PHE	2.4
1	C	544	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	632	LEU	2.3
2	D	223	ALA	2.3
1	A	423	LYS	2.3
1	A	438	VAL	2.3
2	B	112	TYR	2.3
1	A	735	THR	2.3
1	C	505	SER	2.3
2	B	150	SER	2.3
1	A	729	ASP	2.3
2	B	119	ALA	2.3
1	C	450	LEU	2.3
2	B	264	LEU	2.3
1	A	657	ASP	2.3
2	D	239	GLU	2.2
1	A	539	ALA	2.2
2	D	184	ILE	2.2
1	A	569	LEU	2.2
1	C	441	ASP	2.2
1	C	468	PHE	2.2
1	A	600	ILE	2.2
1	A	675	THR	2.2
2	B	15	ALA	2.2
2	D	134	GLY	2.2
2	D	71	ALA	2.2
1	A	456	ASP	2.2
1	A	681	PHE	2.2
1	A	510	ILE	2.2
1	C	573	LEU	2.2
2	D	73	CYS	2.2
2	B	217	LEU	2.2
2	B	71	ALA	2.1
1	C	501	GLU	2.1
1	A	412	LEU	2.1
1	C	661	LYS	2.1
2	D	231	CYS	2.1
1	A	469	ASP	2.1
1	A	426	ASP	2.1
2	D	26	THR	2.1
2	D	174	VAL	2.1
1	A	679	GLU	2.1
1	A	618	LEU	2.1
1	A	595	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	661	LYS	2.1
1	A	728	SER	2.1
1	A	700	ILE	2.0
1	A	532	GLU	2.0
1	C	679	GLU	2.0
2	D	225	VAL	2.0
1	C	521	GLY	2.0
1	A	549	GLU	2.0
1	C	660	LYS	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.