



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:26 PM GMT

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 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/ValidationPDFNotes.html>

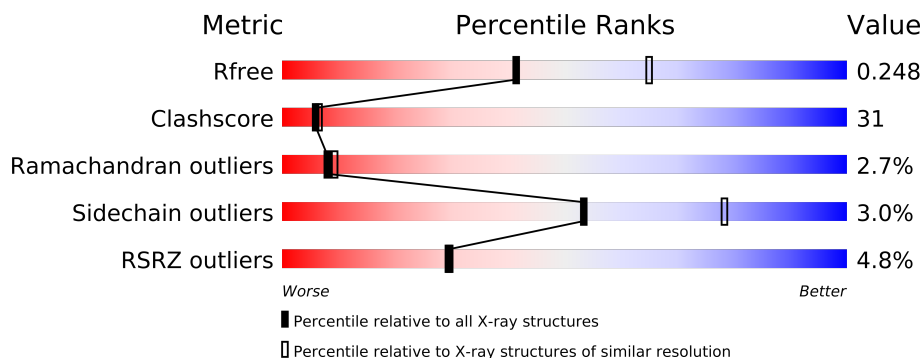
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3566 (2.50-2.42)
Clashscore	79885	4471 (2.50-2.42)
Ramachandran outliers	78287	4383 (2.50-2.42)
Sidechain outliers	78261	4385 (2.50-2.42)
RSRZ outliers	66119	3568 (2.50-2.42)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10195 atoms, of which 0 are hydrogen and 0 are deuterium.

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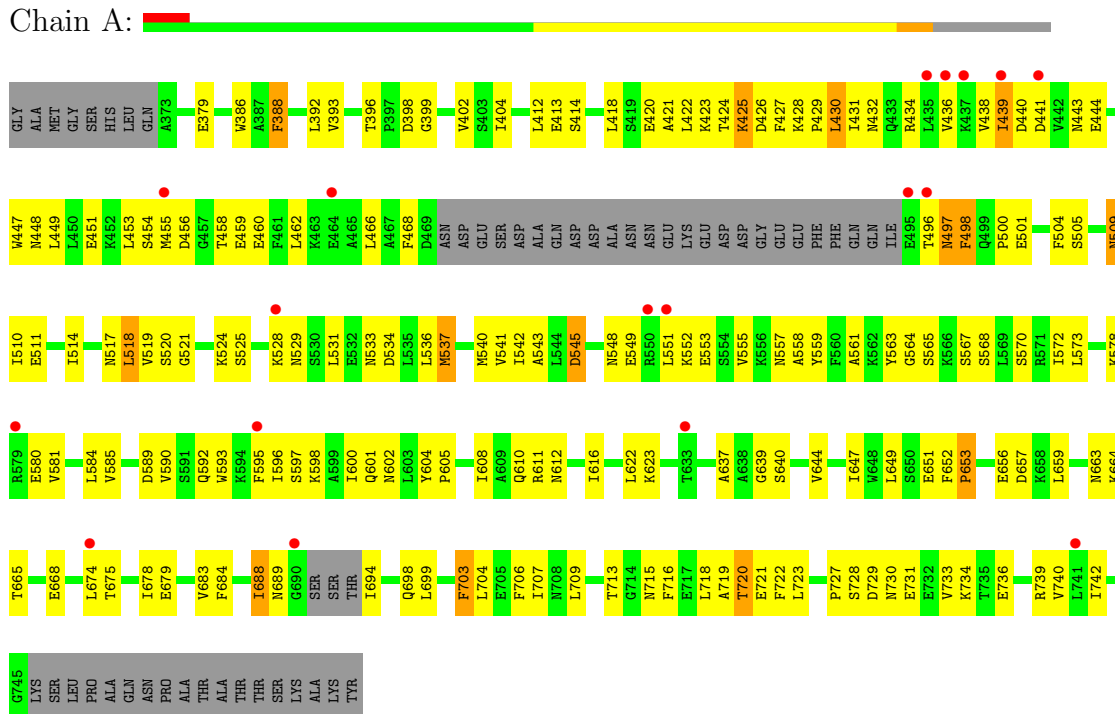
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	61	Total 61	O 61	0	0
3	C	51	Total 51	O 51	0	0
3	D	121	Total 121	O 121	0	0

3 Residue-property plots

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.

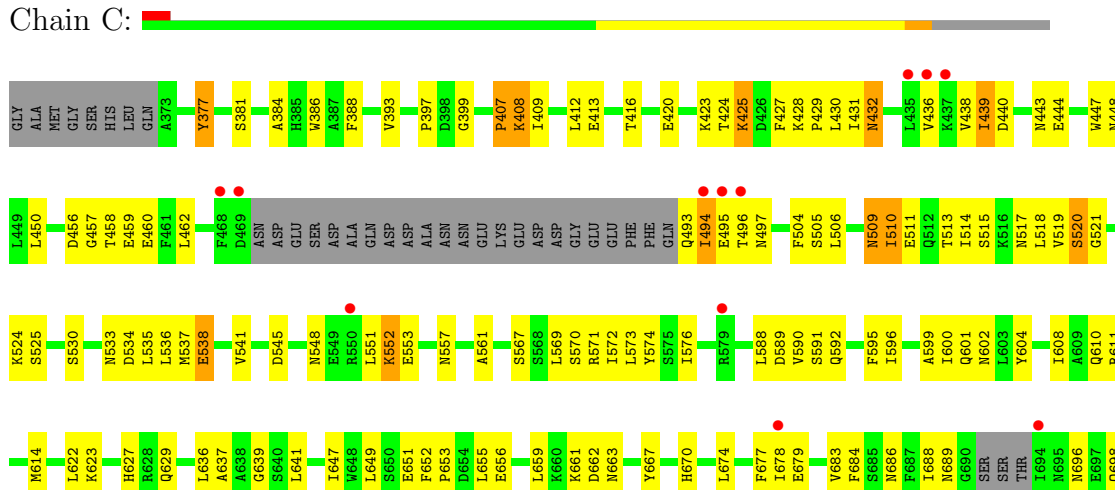
• Molecule 1: Protein transport protein SEC31

Chain A:



• Molecule 1: Protein transport protein SEC31

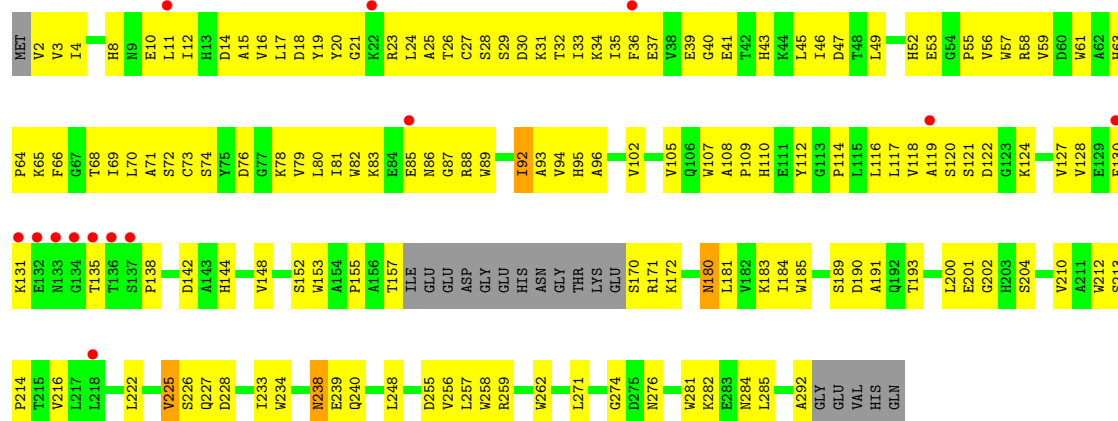
Chain C:





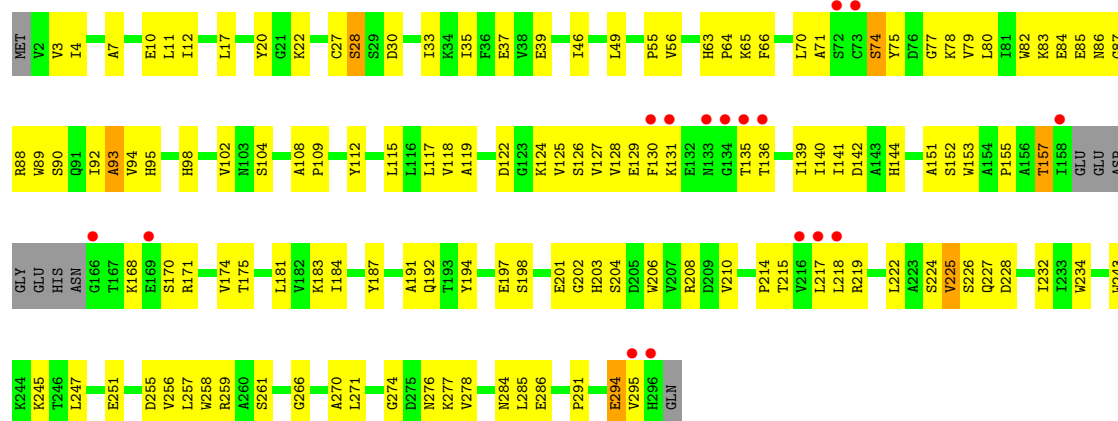
• Molecule 2: Protein transport protein SEC13

Chain B:



• Molecule 2: Protein transport protein SEC13

Chain D:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.44Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.301 0.256 , 0.248	Depositor DCC
R_{free} test set	2783 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.8	EDS
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 59182 reflections	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (612) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:688:ILE:HG13	1:C:689:ASN:H	1.21	1.04
1:C:408:LYS:H	1:C:408:LYS:HD3	1.22	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:HD3	1:C:425:LYS:O	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:703:PHE:O	1:C:707:ILE:HG12	1.78	0.84
1:C:524:LYS:HG3	1:C:525:SER:H	1.43	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:152:SER:HB2	3:D:407:HOH:O	1.80	0.79
1:C:408:LYS:N	1:C:408:LYS:HD3	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:510:ILE:HD12	1:C:510:ILE:H	1.55	0.72
1:C:428:LYS:HB2	1:C:429:PRO:HD3	1.69	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
1:C:444:GLU:HG2	1:C:448:ASN:ND2	2.08	0.68
2:B:24:LEU:HB3	2:B:36:PHE:HB2	1.76	0.68
2:B:144:HIS:CE1	2:B:183:LYS:HD2	2.28	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:233:ILE:HD11	2:B:248:LEU:HD13	1.76	0.68
1:A:736:GLU:O	1:A:740:VAL:HG23	1.93	0.67
1:A:528:LYS:HG3	1:C:493:GLN:HE22	1.58	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:C:535:LEU:HB3	1:C:538:GLU:CG	2.23	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:A:557:ASN:HB3	1:C:496:THR:HG23	1.77	0.65
2:D:184:ILE:HD11	2:D:222:LEU:HD11	1.78	0.65
1:C:590:VAL:HG13	1:C:622:LEU:CD2	2.25	0.65
2:B:157:THR:OG1	2:B:170:SER:HB2	1.95	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
1:A:414:SER:OG	1:A:715:ASN:HB2	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
2:D:49:LEU:HB3	2:D:82:TRP:CZ3	2.32	0.65
1:A:519:VAL:HG13	1:C:599:ALA:HA	1.79	0.65
1:A:427:PHE:CD2	1:A:683:VAL:HG22	2.31	0.65
1:C:408:LYS:CD	1:C:408:LYS:H	2.05	0.64
1:A:608:ILE:HB	1:A:611:ARG:HH12	1.62	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:274:GLY:C	2:B:276:ASN:H	2.00	0.63
2:B:102:VAL:CG2	3:B:353:HOH:O	2.45	0.63
2:B:18:ASP:HB2	3:B:317:HOH:O	1.97	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
2:D:174:VAL:HG23	2:D:183:LYS:O	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:B:66:PHE:HE2	2:B:114:PRO:HD3	1.65	0.62
1:A:703:PHE:HA	3:A:200:HOH:O	2.00	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:592:GLN:O	1:A:592:GLN:HG3	1.99	0.61
2:B:157:THR:HG22	2:B:157:THR:O	2.00	0.61
2:B:102:VAL:HG23	3:B:353:HOH:O	2.00	0.61
1:A:517:ASN:ND2	1:A:529:ASN:HD22	1.98	0.61
1:A:458:THR:HG23	1:A:459:GLU:H	1.66	0.61
1:A:392:LEU:HD13	3:A:219:HOH:O	2.00	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
1:C:553:GLU:HG2	1:C:557:ASN:HD21	1.66	0.60
2:B:4:ILE:HG13	2:B:43:HIS:ND1	2.16	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
1:C:377:TYR:HB3	3:C:113:HOH:O	2.02	0.59
2:B:29:SER:HA	2:B:55:PRO:HB3	1.84	0.59
2:D:291:PRO:CB	2:D:295:VAL:HG22	2.32	0.59
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:D:49:LEU:HD13	2:D:82:TRP:CD2	2.37	0.59
1:A:386:TRP:HA	3:A:219:HOH:O	2.01	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:730:ASN:O	1:A:733:VAL:HB	2.03	0.59
1:A:674:LEU:O	1:A:678:ILE:HG12	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:C:592:GLN:HG3	1:C:595:PHE:CB	2.33	0.58
1:A:584:LEU:HD12	1:A:584:LEU:N	2.18	0.58
1:A:496:THR:HG23	1:C:557:ASN:CB	2.31	0.58
2:B:68:THR:C	2:B:69:ILE:HD12	2.23	0.58
1:A:511:GLU:HG3	3:A:107:HOH:O	2.03	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
2:B:24:LEU:HG	2:B:25:ALA:N	2.19	0.58
1:A:612:ASN:O	1:A:616:ILE:HG12	2.03	0.58
2:B:108:ALA:HB1	2:B:109:PRO:CD	2.34	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:731:GLU:O	1:A:734:LYS:HB3	2.04	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
2:D:79:VAL:HB	2:D:95:HIS:HB3	1.86	0.57
1:A:468:PHE:CE1	1:A:598:LYS:HE3	2.40	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
2:B:4:ILE:HG13	2:B:43:HIS:CG	2.40	0.56
1:C:462:LEU:HD22	1:C:637:ALA:HB2	1.87	0.56
2:B:189:SER:C	2:B:191:ALA:H	2.09	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:616:ILE:HD11	1:A:640:SER:HB2	1.88	0.56
1:C:509:ASN:N	1:C:509:ASN:ND2	2.51	0.56
1:A:584:LEU:H	1:A:584:LEU:HD12	1.71	0.56
1:C:431:ILE:HD11	1:C:683:VAL:HG11	1.88	0.56
2:B:4:ILE:N	2:B:4:ILE:HD12	2.20	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:730:ASN:HB3	1:A:733:VAL:CG2	2.36	0.55
2:B:180:ASN:ND2	2:B:180:ASN:N	2.53	0.55
1:A:509:ASN:ND2	1:A:509:ASN:N	2.54	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:56:VAL:HA	2:B:74:SER:HB2	1.88	0.55
2:B:8:HIS:ND1	2:B:30:ASP:OD2	2.39	0.55
2:D:210:VAL:O	2:D:210:VAL:HG23	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:N	2:D:4:ILE:HD12	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
2:D:226:SER:HB3	2:D:228:ASP:OD1	2.07	0.54
1:C:733:VAL:O	1:C:737:LYS:HG3	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:C:590:VAL:HG13	1:C:622:LEU:HD23	1.90	0.54
1:A:517:ASN:HD21	1:A:529:ASN:ND2	2.04	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
1:C:423:LYS:CG	1:C:424:THR:N	2.71	0.54
2:B:45:LEU:O	2:B:46:ILE:HD13	2.08	0.54
2:D:86:ASN:O	2:D:88:ARG:N	2.40	0.54
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
1:A:418:LEU:HD23	1:A:718:LEU:HD21	1.89	0.53
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:104:SER:OG	2:D:119:ALA:HB3	2.08	0.53
2:D:10:GLU:HG3	2:D:30:ASP:HB3	1.90	0.53
1:C:707:ILE:O	1:C:710:THR:HB	2.09	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: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
2:D:225:VAL:CG2	2:D:271:LEU:HD11	2.38	0.53
1:A:649:LEU:HB3	1:A:698:GLN:OE1	2.09	0.53
2:D:232:ILE:HD13	2:D:247:LEU:HD23	1.91	0.53
2:D:83:LYS:HB3	2:D:92:ILE:HG21	1.90	0.52
1:C:494:ILE:HG13	1:C:495:GLU:N	2.18	0.52
2:B:25:ALA:HB2	2:B:61:TRP:CZ2	2.44	0.52
1:A:531:LEU:C	1:A:533:ASN:H	2.13	0.52
2:D:294:GLU:O	2:D:294:GLU:HG3	2.09	0.52
2:D:22:LYS:HE2	2:D:39:GLU:OE1	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:117:LEU:HD12	3:B:340:HOH:O	2.08	0.52
2:B:33:ILE:CD1	2:B:56:VAL:HG11	2.39	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:C:519:VAL:C	1:C:521:GLY:N	2.63	0.51
1:C:377:TYR:HA	3:C:113:HOH:O	2.11	0.51
1:A:551:LEU:C	1:A:553:GLU:H	2.11	0.51
2:B:95:HIS:CE1	2:B:128:VAL:HG21	2.46	0.51
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:126:SER:HA	2:D:139:ILE:O	2.11	0.51
2:D:84:GLU:HB2	2:D:89:TRP:CE2	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:B:238:ASN:HD22	2:B:240:GLN:N	2.07	0.50
1:A:524:LYS:HG3	1:A:525:SER:N	2.26	0.50
2:D:115:LEU:HD11	2:D:127:VAL:HG12	1.93	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:C:494:ILE:HG23	1:C:495:GLU:N	2.26	0.50
2:B:33:ILE:HB	2:B:49:LEU:HB2	1.92	0.50
2:B:4:ILE:HG22	2:B:4:ILE:O	2.11	0.50
1:A:567:SER:HB3	1:A:570:SER:HB2	1.93	0.50
2:B:255:ASP:CG	2:B:256:VAL:H	2.14	0.50
1:A:664:LYS:HA	1:A:668:GLU:OE1	2.11	0.50
1:C:397:PRO:HA	2:D:276:ASN:HD21	1.77	0.50
2:B:259:ARG:HG3	2:B:259:ARG:HH11	1.77	0.50
2:B:26:THR:O	2:B:33:ILE:HG23	2.12	0.50
1:A:608:ILE:HB	1:A:611:ARG:NH1	2.27	0.50
2:D:215:THR:O	2:D:215:THR:HG23	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
2:B:105:VAL:CG2	2:B:116:LEU:HD21	2.41	0.49
1:A:402:VAL:HG11	2:B:24:LEU:CD2	2.42	0.49
2:D:33:ILE:HB	2:D:49:LEU:HB2	1.94	0.49
2:B:200:LEU:HD13	2:B:234:TRP:CE3	2.47	0.49
2:D:10:GLU:CG	2:D:30:ASP:HB3	2.42	0.49
2:B:95:HIS:HE1	2:B:138:PRO:HG3	1.77	0.49
1:C:551:LEU:C	1:C:551:LEU:HD23	2.33	0.49
2:D:203:HIS:CE1	2:D:232:ILE:HG12	2.48	0.49
1:A:663:ASN:HA	2:B:285:LEU:HD11	1.94	0.49
1:A:432:ASN:O	1:A:436:VAL:HG23	2.11	0.49
2:B:63:HIS:CD2	3:B:334:HOH:O	2.65	0.49
2:D:261:SER:HA	3:D:351:HOH:O	2.13	0.49
2:B:148:VAL:O	3:B:338:HOH:O	2.20	0.49
1:C:530:SER:O	1:C:533:ASN:O	2.31	0.49
2:D:222:LEU:HG	2:D:243:TRP:CZ3	2.48	0.49
1:A:585:VAL:HA	1:A:596:ILE:HG21	1.95	0.49
1:A:731:GLU:HA	1:A:734:LYS:HB3	1.93	0.49
1:A:430:LEU:HD23	1:A:430:LEU:O	2.13	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:70:LEU:HG	2:D:71:ALA:N	2.28	0.49
2:B:184:ILE:N	2:B:184:ILE:HD12	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:536:LEU:HD23	1:C:537:MET:HE3	1.94	0.48
1:A:466:LEU:O	1:A:598:LYS:HE2	2.13	0.48
2:D:94:VAL:HG13	2:D:94:VAL:O	2.11	0.48
1:A:644:VAL:HG11	1:A:684:PHE:CE2	2.48	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
2:D:10:GLU:HB2	2:D:28:SER:OG	2.14	0.48
1:C:733:VAL:HG12	1:C:737:LYS:HE3	1.95	0.48
1:C:728:SER:HB3	1:C:737:LYS:NZ	2.29	0.48
1:C:388:PHE:CE1	1:C:739:ARG:HD3	2.49	0.48
2:B:212:TRP:CD2	2:B:222:LEU:HD21	2.49	0.48
2:B:29:SER:C	2:B:31:LYS:H	2.16	0.48
2:D:227:GLN:HG2	3:D:409:HOH:O	2.13	0.48
1:C:514:ILE:HA	1:C:517:ASN:HD22	1.79	0.48
2:B:59:VAL:HA	2:B:71:ALA:O	2.14	0.48
2:D:90:SER:O	2:D:92:ILE:HG23	2.14	0.48
1:C:439:ILE:HG13	1:C:440:ASP:N	2.27	0.48
2:B:69:ILE:CG2	2:B:70:LEU:N	2.77	0.48
1:A:514:ILE:HA	1:A:517:ASN:ND2	2.28	0.48
2:B:15:ALA:HA	2:B:25:ALA:O	2.14	0.47
2:B:8:HIS:CE1	2:B:34:LYS:HE2	2.48	0.47
1:C:727:PRO:C	1:C:729:ASP:N	2.67	0.47
1:C:456:ASP:O	1:C:460:GLU:HB2	2.14	0.47
2:B:93:ALA:HB1	3:B:344:HOH:O	2.14	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
1:A:412:LEU:C	1:A:412:LEU:HD23	2.35	0.47
2:B:172:LYS:HA	2:B:185:TRP:O	2.14	0.47
2:B:72:SER:O	2:B:79:VAL:HG13	2.14	0.47
1:C:408:LYS:CE	2:D:294:GLU:HG2	2.36	0.47
2:B:119:ALA:HB1	2:B:148:VAL:HG12	1.96	0.47
1:C:424:THR:O	1:C:425:LYS:CB	2.62	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:438:VAL:HG21	1:C:444:GLU:HA	1.97	0.47
2:B:34:LYS:HB3	2:B:36:PHE:HE1	1.80	0.47
2:D:276:ASN:ND2	3:D:310:HOH:O	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:386:TRP:NE1	2:D:270:ALA:HB2	2.30	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
2:D:92:ILE:O	2:D:93:ALA:HB2	2.15	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
1:A:652:PHE:HB3	1:A:653:PRO:CD	2.44	0.47
1:A:392:LEU:CD1	3:A:219:HOH:O	2.61	0.47
1:C:641:LEU:HD12	1:C:684:PHE:HE2	1.80	0.47
2:B:233:ILE:CD1	2:B:248:LEU:HD13	2.43	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:D:35:ILE:HG13	2:D:89:TRP:CE2	2.50	0.47
1:C:412:LEU:CD2	1:C:713:THR:HG22	2.45	0.47
1:A:572:ILE:CD1	1:C:504:PHE:HE1	2.28	0.47
1:C:731:GLU:HA	1:C:734:LYS:HB3	1.97	0.47
2:D:108:ALA:HB2	2:D:153:TRP:CE2	2.50	0.47
1:C:553:GLU:HG2	1:C:557:ASN:ND2	2.28	0.46
1:A:536:LEU:HD23	1:C:537:MET:CE	2.46	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:D:222:LEU:HB2	2:D:234:TRP:HB2	1.97	0.46
2:B:259:ARG:HG3	2:B:259:ARG:NH1	2.30	0.46
1:C:438:VAL:HG23	1:C:443:ASN:ND2	2.30	0.46
2:D:274:GLY:C	2:D:276:ASN:N	2.69	0.46
1:A:462:LEU:HD13	1:A:637:ALA:HB2	1.97	0.46
2:D:141:ILE:HG22	3:D:322:HOH:O	2.14	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
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:C:386:TRP:HZ3	3:C:214:HOH:O	1.98	0.46
2:B:200:LEU:HB3	2:B:234:TRP:CH2	2.50	0.46
1:A:441:ASP:HA	3:A:212:HOH:O	2.15	0.46
2:D:98:HIS:ND1	2:D:122:ASP:OD2	2.49	0.46
2:B:124:LYS:HE2	2:B:142:ASP:OD1	2.15	0.46
1:A:739:ARG:HD2	2:B:19:TYR:CZ	2.50	0.46
1:A:727:PRO:C	1:A:729:ASP:N	2.69	0.46
2:D:65:LYS:HE2	2:D:66:PHE:CZ	2.50	0.46
1:C:641:LEU:HD12	1:C:684:PHE:CE2	2.51	0.46
2:B:31:LYS:O	3:B:321:HOH:O	2.20	0.46
1:A:718:LEU:O	1:A:722:PHE:HD1	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:117:LEU:HB2	2:B:153:TRP:NE1	2.31	0.46
2:B:25:ALA:HB2	2:B:61:TRP:HZ2	1.81	0.46
1:A:663:ASN:CA	2:B:285:LEU:HD11	2.46	0.46
1:A:436:VAL:HG12	1:A:436:VAL:O	2.16	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:412:LEU:CD2	1:A:713:THR:HG22	2.38	0.45
1:A:392:LEU:HA	3:A:219:HOH:O	2.16	0.45
1:C:458:THR:HG23	1:C:459:GLU:N	2.30	0.45
2:B:121:SER:HA	3:B:338:HOH:O	2.15	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:C:639:GLY:HA2	1:C:688:ILE:CD1	2.47	0.45
1:C:431:ILE:HD13	1:C:447:TRP:HZ3	1.82	0.45
1:A:601:GLN:HE22	1:A:611:ARG:HD3	1.82	0.45
1:A:543:ALA:C	1:A:545:ASP:H	2.19	0.45
2:B:284:ASN:HB2	3:B:352:HOH:O	2.16	0.45
2:D:37:GLU:HB2	2:D:46:ILE:HD11	1.98	0.45
1:C:524:LYS:CG	1:C:525:SER:H	2.24	0.45
2:B:274:GLY:C	2:B:276:ASN:N	2.69	0.45
1:A:559:TYR:CE2	1:C:541:VAL:HG21	2.52	0.45
2:D:30:ASP:OD1	2:D:30:ASP:C	2.54	0.45
1:C:590:VAL:O	1:C:590:VAL:CG1	2.64	0.45
2:B:66:PHE:CD2	2:B:114:PRO:HB3	2.51	0.45
1:C:674:LEU:O	1:C:678:ILE:HD13	2.15	0.45
2:B:191:ALA:HB1	2:B:193:THR:HG22	1.99	0.45
2:D:83:LYS:CB	2:D:92:ILE:HG21	2.47	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
2:D:139:ILE:O	2:D:140:ILE:HD13	2.16	0.45
1:A:564:GLY:HA2	1:A:570:SER:OG	2.16	0.45
1:C:399:GLY:O	2:D:11:LEU:HD12	2.17	0.45
2:B:35:ILE:HG13	2:B:89:TRP:CE2	2.51	0.45
2:B:30:ASP:OD1	2:B:32:THR:HG23	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:652:PHE:HB3	1:C:653:PRO:CD	2.42	0.44
2:B:14:ASP:HB3	2:B:27:CYS:SG	2.58	0.44
1:A:573:LEU:HD23	1:C:518:LEU:CD1	2.47	0.44
2:D:142:ASP:HB3	3:D:366:HOH:O	2.17	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
1:A:379:GLU:HG2	2:B:258:TRP:CZ2	2.53	0.44
2:D:187:TYR:HB2	2:D:194:TYR:CE2	2.53	0.44
1:A:504:PHE:CZ	1:C:588:LEU:HD13	2.52	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
2:D:184:ILE:O	2:D:197:GLU:HB2	2.17	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:B:102:VAL:HG22	3:B:353:HOH:O	2.13	0.44
1:A:551:LEU:C	1:A:553:GLU:N	2.71	0.44
2:B:213:SER:HB2	2:B:262:TRP:CE2	2.53	0.44
2:D:108:ALA:HB1	2:D:109:PRO:CD	2.48	0.43
2:D:63:HIS:ND1	2:D:64:PRO:HD2	2.32	0.43
2:D:10:GLU:HB2	2:D:28:SER:HG	1.83	0.43
1:A:639:GLY:HA2	1:A:688:ILE:CD1	2.35	0.43
2:B:112:TYR:N	2:B:112:TYR:CD2	2.86	0.43
2:B:63:HIS:CE1	2:B:65:LYS:HB3	2.53	0.43
1:C:614:MET:HA	1:C:614:MET:HE2	1.99	0.43
1:C:571:ARG:O	1:C:574:TYR:HB3	2.18	0.43
1:C:420:GLU:HA	1:C:423:LYS:HD3	2.01	0.43
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:636:LEU:HD12	1:C:688:ILE:CD1	2.48	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:A:519:VAL:C	1:A:521:GLY:N	2.71	0.43
1:C:661:LYS:C	1:C:663:ASN:N	2.72	0.43
1:A:422:LEU:CD2	1:A:721:GLU:HG2	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:C:439:ILE:CG2	1:C:659:LEU:HD21	2.39	0.43
2:B:74:SER:C	2:B:76:ASP:N	2.71	0.43
1:C:519:VAL:O	1:C:521:GLY:N	2.51	0.43
2:B:87:GLY:C	2:B:88:ARG:HG3	2.39	0.43
1:A:496:THR:CG2	1:A:497:ASN:N	2.81	0.43
1:A:388:PHE:CE2	1:A:716:PHE:HE2	2.37	0.43
2:B:18:ASP:CG	2:B:23:ARG:HB3	2.39	0.43
1:C:412:LEU:HD21	1:C:713:THR:HG22	2.01	0.43
1:A:504:PHE:CE1	1:C:588:LEU:HD13	2.53	0.43
2:B:107:TRP:CH2	2:B:130:PHE:HE1	2.37	0.43
2:B:64:PRO:HD2	3:B:334:HOH:O	2.18	0.43
2:B:46:ILE:HG22	2:B:46:ILE:O	2.19	0.43
1:C:590:VAL:HG13	1:C:622:LEU:HD22	1.99	0.42
1:A:608:ILE:HA	1:A:611:ARG:NH1	2.34	0.42
1:A:438:VAL:CG2	1:A:439:ILE:N	2.81	0.42
2:B:225:VAL:CG2	2:B:271:LEU:HD11	2.50	0.42
1:A:511:GLU:HG2	1:C:569:LEU:HB2	1.99	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
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:414:SER:HG	1:A:715:ASN:HB2	1.82	0.42
1:A:706:PHE:HB2	3:A:200:HOH:O	2.19	0.42
1:A:610:GLN:HA	1:A:610:GLN:OE1	2.20	0.42
1:A:404:ILE:HD12	1:A:404:ILE:N	2.35	0.42
2:B:16:VAL:HG12	2:B:61:TRP:HD1	1.84	0.42
1:C:420:GLU:HA	1:C:423:LYS:CD	2.50	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
1:C:536:LEU:O	1:C:537:MET:C	2.57	0.42
2:D:225:VAL:HG22	2:D:257:LEU:HB2	2.00	0.42
2:B:155:PRO:CG	2:B:214:PRO:HA	2.49	0.42
1:A:584:LEU:CD1	1:A:584:LEU:N	2.81	0.42
2:D:157:THR:HG21	2:D:170:SER:HB2	2.00	0.42
1:A:497:ASN:OD1	1:A:498:PHE:N	2.53	0.42
1:A:428:LYS:HB2	1:A:429:PRO:CD	2.38	0.42
2:B:52:HIS:CD2	2:B:56:VAL:HG22	2.55	0.42
2:B:63:HIS:CD2	2:B:110:HIS:HB3	2.54	0.42
1:C:655:LEU:HD12	1:C:655:LEU:HA	1.78	0.42
2:B:281:TRP:N	2:B:281:TRP:CD1	2.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:500:PRO:O	1:A:501:GLU:HG2	2.20	0.42
1:A:431:ILE:HG21	1:A:451:GLU:HA	2.02	0.42
1:C:408:LYS:HG3	2:D:294:GLU:OE1	2.19	0.42
1:A:447:TRP:O	1:A:451:GLU:N	2.53	0.42
1:A:429:PRO:HD2	3:A:159:HOH:O	2.18	0.42
1:C:493:GLN:HG3	1:C:494:ILE:N	2.35	0.42
1:A:458:THR:CG2	1:A:459:GLU:N	2.81	0.42
1:C:589:ASP:C	1:C:591:SER:H	2.23	0.42
2:B:233:ILE:HD12	2:B:233:ILE:N	2.35	0.42
2:D:118:VAL:HB	2:D:126:SER:OG	2.20	0.42
2:D:118:VAL:O	2:D:125:VAL:HA	2.20	0.42
1:A:549:GLU:HA	1:A:552:LYS:HB3	2.01	0.42
1:A:644:VAL:HG21	1:A:684:PHE:CZ	2.55	0.41
2:B:225:VAL:CG1	2:B:257:LEU:O	2.68	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: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:C:424:THR:O	1:C:425:LYS:HB3	2.19	0.41
1:A:412:LEU:HD23	1:A:413:GLU:N	2.36	0.41
2:D:277:LYS:HG3	2:D:278:VAL:H	1.86	0.41
2:B:213:SER:HB2	2:B:262:TRP:CD2	2.55	0.41
2:D:7:ALA:HB3	2:D:12:ILE:HD11	2.01	0.41
1:A:517:ASN:ND2	1:A:529:ASN:ND2	2.63	0.41
1:C:447:TRP:CE3	1:C:450:LEU:HD12	2.55	0.41
2:B:17:LEU:HB3	2:B:21:GLY:HA2	2.03	0.41
1:A:653:PRO:O	1:A:656:GLU:N	2.54	0.41
2:B:238:ASN:HB2	3:B:327:HOH:O	2.20	0.41
2:B:2:VAL:HG13	2:B:41:GLU:HA	2.03	0.41
2:D:191:ALA:O	2:D:192:GLN:HB2	2.20	0.41
2:B:152:SER:OG	2:B:210:VAL:O	2.33	0.41
1:A:434:ARG:HG3	1:A:447:TRP:CH2	2.55	0.41
1:A:420:GLU:O	1:A:423:LYS:HG2	2.20	0.41
2:B:212:TRP:HA	2:B:222:LEU:HD23	2.03	0.41
1:A:578:LYS:HD3	1:A:580:GLU:OE2	2.21	0.41
2:D:203:HIS:NE2	2:D:232:ILE:HG12	2.35	0.41
1:A:551:LEU:HD23	1:A:551:LEU:C	2.41	0.41
2:D:181:LEU:CD2	2:D:201:GLU:HG2	2.50	0.41
1:C:438:VAL:HG21	1:C:444:GLU:CA	2.50	0.41
1:A:694:ILE:HG23	1:A:699:LEU:HD23	2.02	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:444:GLU:HG2	1:A:448:ASN:ND2	2.36	0.41
1:C:497:ASN:CG	1:C:497:ASN:O	2.59	0.41
1:A:704:LEU:O	1:A:707:ILE:HB	2.21	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:C:649:LEU:CD2	1:C:698:GLN:HG2	2.38	0.40
1:C:438:VAL:HG22	1:C:439:ILE:N	2.36	0.40
2:D:33:ILE:HB	2:D:49:LEU:HD12	2.03	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:A:439:ILE:HG13	1:A:440:ASP:H	1.85	0.40
1:C:551:LEU:O	1:C:553:GLU:N	2.54	0.40
1:A:598:LYS:O	1:A:602:ASN:HB2	2.20	0.40
1:A:563:TYR:C	1:A:565:SER:H	2.24	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:C:652:PHE:CE2	1:C:702:LYS:HE2	2.56	0.40
1:C:572:ILE:HG22	1:C:573:LEU:N	2.35	0.40
1:A:456:ASP:O	1:A:460:GLU:HB2	2.22	0.40
1:C:535:LEU:CD2	1:C:538:GLU:HG3	2.52	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: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	Distance(Å)	Clash(Å)
3:A:118:HOH:O	3:D:311:HOH:O[1_644]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	6	7
1	C	341/399 (86%)	298 (87%)	34 (10%)	9 (3%)	8	10
2	B	275/297 (93%)	241 (88%)	30 (11%)	4 (2%)	15	23
2	D	284/297 (96%)	255 (90%)	20 (7%)	9 (3%)	6	7
All	All	1239/1392 (89%)	1079 (87%)	127 (10%)	33 (3%)	8	9

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
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 ⓘ

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%)	55	79
1	C	308/350 (88%)	297 (96%)	11 (4%)	47	71
2	B	237/252 (94%)	232 (98%)	5 (2%)	66	87
2	D	244/252 (97%)	236 (97%)	8 (3%)	50	74
All	All	1095/1204 (91%)	1062 (97%)	33 (3%)	53	78

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
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

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Mol	Chain	Res	Type
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

Some 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
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 chains 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, 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	345/399 (86%)	0.41	18 (5%)	26 26	49, 83, 114, 130	0
1	C	347/399 (86%)	0.16	12 (3%)	42 42	30, 66, 103, 130	0
2	B	279/297 (93%)	0.35	14 (5%)	28 28	15, 62, 110, 142	0
2	D	288/297 (96%)	0.13	16 (5%)	24 23	16, 47, 96, 135	0
All	All	1259/1392 (90%)	0.27	60 (4%)	29 30	15, 68, 109, 142	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	THR	7.8
2	B	133	ASN	7.0
2	B	136	THR	7.0
2	D	295	VAL	6.7
2	B	134	GLY	6.5
2	D	296	HIS	6.5
2	B	135	THR	6.1
2	D	135	THR	5.5
2	D	133	ASN	5.4
2	D	216	VAL	5.2
1	C	496	THR	4.6
2	D	158	ILE	4.4
2	B	137	SER	4.2
2	B	131	LYS	4.2
2	D	134	GLY	4.2
1	A	595	PHE	4.0
1	C	494	ILE	4.0
1	A	436	VAL	3.8
1	C	436	VAL	3.8
2	D	136	THR	3.7
2	D	166	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	469	ASP	3.5
2	B	218	LEU	3.5
1	A	550	ARG	3.4
1	A	741	LEU	3.3
1	A	435	LEU	3.0
1	C	694	ILE	3.0
1	A	551	LEU	2.9
2	B	132	GLU	2.8
1	A	495	GLU	2.7
2	D	72	SER	2.7
2	D	130	PHE	2.7
1	A	690	GLY	2.6
2	D	218	LEU	2.5
1	A	455	MET	2.5
1	A	633	THR	2.5
1	C	550	ARG	2.4
1	C	435	LEU	2.4
2	D	169	GLU	2.4
1	A	579	ARG	2.4
2	B	22	LYS	2.4
2	D	217	LEU	2.3
1	A	437	LYS	2.3
1	C	468	PHE	2.3
2	D	73	CYS	2.3
1	C	437	LYS	2.2
1	C	678	ILE	2.2
1	A	439	ILE	2.2
1	C	579	ARG	2.2
2	B	11	LEU	2.2
1	A	528	LYS	2.2
1	A	441	ASP	2.2
1	C	495	GLU	2.2
1	A	464	GLU	2.1
1	A	674	LEU	2.1
2	B	130	PHE	2.1
2	B	36	PHE	2.1
2	B	119	ALA	2.1
2	B	85	GLU	2.1
2	D	131	LYS	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.