



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:33 AM EDT

PDB ID : 2PM7 / pdb_00002pm7
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

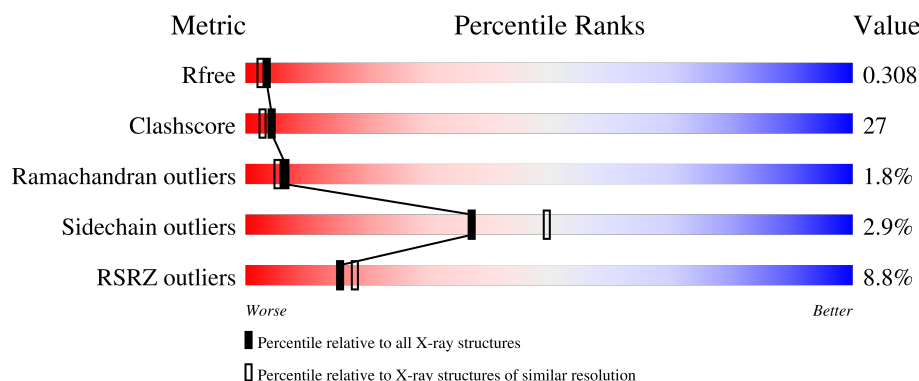
1 Overall quality at a glance

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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

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 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

Continued on next page...

Continued from previous page...

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
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			

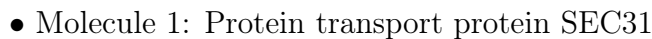
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	MET	modified residue	UNP Q04491
B	11	MSE	LEU	engineered 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	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		

- Molecule 1: Protein transport protein SEC31



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 30.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-2.35) 96.8 (30.00-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.47 (at 2.36Å)	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%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.883	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10195	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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	0.35	0/2764	0.87	3/3712 (0.1%)
1	C	0.41	0/2781	0.88	11/3735 (0.3%)
2	B	0.42	0/2250	0.95	11/3055 (0.4%)
2	D	0.54	0/2318	1.03	11/3146 (0.3%)
All	All	0.43	0/10113	0.93	36/13648 (0.3%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	377	TYR	N-CA-C	7.92	121.79	109.52
2	B	226	SER	N-CA-C	7.41	120.43	109.24
2	D	250	GLU	N-CA-C	7.22	120.01	111.71
1	A	377	TYR	N-CA-C	7.17	119.82	109.14
1	C	533	ASN	N-CA-C	-7.13	99.91	110.46
2	D	226	SER	N-CA-C	7.10	120.20	109.41
1	C	406	ASN	CA-C-N	6.88	128.43	119.84
1	C	406	ASN	C-N-CA	6.88	128.43	119.84
2	B	128	VAL	N-CA-C	6.82	117.71	107.75
2	B	145	ALA	N-CA-C	-6.54	101.73	110.55
1	C	713	THR	N-CA-C	-6.52	104.96	113.17
1	A	608	ILE	N-CA-C	6.33	117.08	110.62
1	C	732	GLU	N-CA-C	-6.11	103.94	111.40
1	C	554	SER	N-CA-C	-5.96	104.91	111.82
2	D	207	VAL	N-CA-C	-5.95	101.04	108.89
2	B	105	VAL	N-CA-C	-5.82	100.67	108.35
2	B	74	SER	N-CA-C	5.66	117.39	108.96
2	D	179	ASP	N-CA-C	-5.61	105.79	113.30
2	B	177	GLY	N-CA-C	5.59	119.36	111.42
2	B	138	PRO	N-CA-C	5.58	119.03	111.22
1	C	536	MSE	N-CA-C	5.46	116.91	111.07
2	D	41	GLU	N-CA-C	-5.42	106.45	112.57
2	D	128	VAL	N-CA-C	5.31	115.77	108.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	110	HIS	N-CA-C	5.29	117.04	111.28
1	C	703	PHE	N-CA-C	-5.21	105.60	111.28
1	C	587	ASN	N-CA-C	5.15	120.42	114.04
2	D	219	ARG	N-CA-C	5.08	117.26	110.35
2	B	290	GLU	CA-C-N	5.08	125.36	119.93
2	B	290	GLU	C-N-CA	5.08	125.36	119.93
1	C	378	GLY	N-CA-C	5.06	122.58	115.30
1	A	638	ALA	N-CA-C	-5.05	106.80	113.17
2	D	109	PRO	N-CA-C	-5.05	103.17	111.15
2	B	182	VAL	N-CA-C	-5.05	101.10	108.17
2	D	206	TRP	N-CA-C	5.05	117.79	110.42
2	D	182	VAL	N-CA-C	-5.04	101.05	108.11
2	B	118	VAL	N-CA-C	5.01	115.92	108.46

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	183	0
1	C	2746	0	2715	158	0
2	B	2196	0	2126	141	0
2	D	2263	0	2191	90	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	531	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 27.

All (531) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:274:GLY:C	2:B:276:ASN:H	1.94	0.74
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:3:VAL:C	2:D:4:ILE:HD12	2.15	0.71
2:D:33:ILE:HD11	2:D:56:VAL:HG11	1.73	0.71
1:A:519:VAL:C	1:A:521:GLY:H	1.98	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
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:531:LEU:C	1:A:533:ASN:H	2.01	0.68
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:674:MSE:O	1:C:678:ILE:HD12	1.95	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: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
2:D:274:GLY:C	2:D:276:ASN:H	2.04	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
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
1:C:659:LEU:HD22	1:C:664:LYS:HZ2	1.65	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:THR:HG23	1:A:459:GLU:H	1.64	0.61
1:C:661:LYS:C	1:C:663:ASN:H	2.07	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
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
2:D:285:LEU:C	2:D:287:GLY:H	2.10	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:LEU:HD21	3:C:246:HOH:O	2.01	0.58
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
2:B:189:SER:C	2:B:191:ALA:H	2.12	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
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:A:551:LEU:C	1:A:551:LEU:HD23	2.30	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:519:VAL:C	1:A:521:GLY:N	2.64	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:663:ASN:C	2:D:285:LEU:HD11	2.32	0.54
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: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: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
1:C:519:VAL:C	1:C:521:GLY:H	2.15	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
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:659:LEU:HD22	1:C:664:LYS:NZ	2.23	0.52
2:D:251:GLU:H	2:D:251:GLU:CD	2.17	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:85:GLU:O	2:B:86:ASN:HB2	2.09	0.52
2:B:49:LEU:HD13	2:B:82:TRP:CD2	2.45	0.51
1:A:412:LEU:C	1:A:412:LEU:HD23	2.36	0.51
1:C:430:LEU:C	1:C:430:LEU:HD23	2.35	0.51
1:C:688:ILE:HG13	1:C:689:ASN:H	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:728:SER:HB3	1:C:737:LYS:NZ	2.25	0.51
2:D:30:ASP:OD1	2:D:30:ASP:C	2.54	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
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
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:274:GLY:C	2:B:276:ASN:N	2.62	0.50
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:D:293:GLY:O	2:D:294:GLU:C	2.55	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:551:LEU:HD23	1:C:551:LEU:C	2.36	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
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:D:274:GLY:C	2:D:276:ASN:N	2.70	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
1:A:551:LEU:C	1:A:553:GLU:H	2.20	0.49
2:B:29:SER:C	2:B:31:LYS:H	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:30:ASP:OD1	2:B:30:ASP:C	2.55	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
1:C:509:ASN:N	1:C:509:ASN:ND2	2.58	0.48
2:D:53:GLU:HG3	3:D:378:HOH:O	2.13	0.48
2:D:285:LEU:C	2:D:287:GLY:N	2.71	0.48
1:A:537:MSE:HA	1:A:540:MSE:HE3	1.96	0.48
1:A:545:ASP:CG	1:C:556:LYS:HZ3	2.21	0.48
1:A:616:ILE:HD11	1:A:640:SER:CB	2.43	0.48
1:A:727:PRO:C	1:A:729:ASP:H	2.20	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:661:LYS:C	1:C:663:ASN:N	2.73	0.47
2:D:191:ALA:O	2:D:192:GLN:HB2	2.15	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:227:GLN:C	2:D:229:ARG:H	2.22	0.47
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
2:B:189:SER:C	2:B:191:ALA:N	2.73	0.46
1:A:531:LEU:C	1:A:533:ASN:N	2.70	0.46
2:B:214:PRO:O	2:B:215:THR:C	2.59	0.46
1:A:388:PHE:CD1	1:A:739:ARG:CZ	2.99	0.46
1:A:661:LYS:C	1:A:663:ASN:H	2.23	0.46
2:B:29:SER:C	2:B:31:LYS:N	2.73	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: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
1:A:592:GLN:HG3	1:A:592:GLN:O	2.16	0.45
1:C:728:SER:HB3	1:C:737:LYS:HZ1	1.80	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:29:SER:C	3:D:417:HOH:O	2.59	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: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
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
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
2:D:217:LEU:O	2:D:218:LEU:C	2.60	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
2:D:28:SER:OG	2:D:29:SER:N	2.49	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
1:A:710:THR:O	1:A:713:THR:OG1	2.32	0.43
2:B:10:GLU:O	2:B:11:MSE:C	2.61	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:416:THR:O	1:A:417:THR:C	2.61	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
1:A:551:LEU:C	1:A:553:GLU:N	2.77	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
2:D:122:ASP:CG	3:D:409:HOH:O	2.62	0.42
1:A:649:LEU:HB3	1:A:698:GLN:OE1	2.20	0.42
2:B:121:SER:N	3:B:337:HOH:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:519:VAL:C	1:C:521:GLY:N	2.76	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
2:B:180:ASN:N	2:B:180:ASN:ND2	2.65	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: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
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:577:SER:C	1:A:579:ARG:H	2.28	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
2:B:120:SER:C	2:B:122:ASP:H	2.26	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:B:30:ASP:C	2:B:31:LYS:HG3	2.45	0.42
2:D:295:VAL:HG12	2:D:296:HIS:H	1.85	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
2:B:216:VAL:O	2:B:216:VAL:HG12	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
1:C:543:ALA:C	1:C:545:ASP:H	2.28	0.41
1:C:723:LEU:HD21	1:C:736:GLU:CG	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:387:ALA:O	1:A:388:PHE:C	2.64	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
1:A:388:PHE:CD1	1:A:739:ARG:NH2	2.89	0.41
1:A:438:VAL:HG22	1:A:439:ILE:N	2.35	0.41
1:A:511:GLU:HG3	3:A:107:HOH:O	2.21	0.41
1:C:661:LYS:O	1:C:663:ASN:N	2.53	0.41
1:A:430:LEU:HD23	1:A:430:LEU:C	2.46	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: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
1:C:446:ASP:CG	1:C:628:ARG:HH12	2.29	0.41
2:D:105:VAL:O	2:D:105:VAL:HG23	2.21	0.41
1:A:581:VAL:O	1:A:582:ASP:C	2.63	0.40
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: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%)	4	3
1	C	341/399 (86%)	315 (92%)	22 (6%)	4 (1%)	10	9
2	B	275/297 (93%)	246 (90%)	26 (10%)	3 (1%)	11	11
2	D	284/297 (96%)	258 (91%)	19 (7%)	7 (2%)	4	3
All	All	1239/1392 (89%)	1111 (90%)	106 (9%)	22 (2%)	6	5

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	299 (98%)	7 (2%)	44	58
1	C	308/340 (91%)	297 (96%)	11 (4%)	31	41
2	B	237/245 (97%)	233 (98%)	4 (2%)	53	68
2	D	244/245 (100%)	234 (96%)	10 (4%)	27	36
All	All	1095/1170 (94%)	1063 (97%)	32 (3%)	37	49

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	404	ILE
1	A	439	ILE
1	A	449	MSE
1	A	509	ASN
1	A	534	ASP
1	A	545	ASP
1	A	729	ASP
2	B	50	THR
2	B	112	TYR
2	B	152	SER
2	B	225	VAL
1	C	408	LYS
1	C	432	ASN
1	C	509	ASN
1	C	510	ILE
1	C	534	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	538	GLU
1	C	590	VAL
1	C	624	GLU
1	C	655	LEU
1	C	657	ASP
1	C	688	ILE
2	D	28	SER
2	D	85	GLU
2	D	92	ILE
2	D	115	MSE
2	D	157	THR
2	D	198	SER
2	D	204	SER
2	D	225	VAL
2	D	251	GLU
2	D	295	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	GLN
1	A	406	ASN
1	A	433	GLN
1	A	443	ASN
1	A	448	ASN
1	A	509	ASN
1	A	529	ASN
1	A	547	ASN
1	A	592	GLN
1	A	670	HIS
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	433	GLN
1	C	443	ASN
1	C	448	ASN
1	C	509	ASN
1	C	529	ASN
1	C	606	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	612	ASN
1	C	670	HIS
1	C	686	ASN
1	C	689	ASN
2	D	103	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 oligosaccharides 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

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	336/399 (84%)	1.21	47 (13%) 6 7	52, 87, 110, 119	0
1	C	338/399 (84%)	0.72	23 (6%) 23 26	35, 67, 99, 117	0
2	B	273/297 (91%)	0.84	27 (9%) 13 14	28, 64, 105, 120	0
2	D	282/297 (94%)	0.27	11 (3%) 43 49	27, 49, 90, 113	0
All	All	1229/1392 (88%)	0.78	108 (8%) 15 18	27, 70, 106, 120	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	741	LEU	4.8
1	A	738	ALA	4.4
1	C	533	ASN	4.2
2	B	114	PRO	3.9
2	B	216	VAL	3.7
1	C	570	SER	3.7
1	A	424	THR	3.7
1	C	745	GLY	3.5
1	A	576	ILE	3.5
2	B	134	GLY	3.4
2	B	139	ILE	3.3
1	A	520	SER	3.2
1	A	432	ASN	3.2
1	A	416	THR	3.1
2	D	136	THR	3.1
1	A	725	SER	3.0
1	A	522	ASN	3.0
2	D	217	LEU	3.0
2	D	135	THR	3.0
1	A	373	ALA	2.9
1	A	558	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	91	GLN	2.9
1	A	666	ILE	2.9
2	B	28	SER	2.9
1	A	519	VAL	2.9
2	B	2	VAL	2.9
1	A	521	GLY	2.8
1	C	438	VAL	2.8
1	C	426	ASP	2.8
1	A	579	ARG	2.8
2	D	169	GLU	2.8
1	A	729	ASP	2.8
2	B	18	ASP	2.8
1	A	554	SER	2.7
1	C	498	PHE	2.7
1	A	596	ILE	2.7
1	A	724	ASN	2.7
1	A	745	GLY	2.7
1	A	575	SER	2.7
1	A	557	ASN	2.7
2	B	137	SER	2.7
1	C	546	SER	2.6
2	B	138	PRO	2.6
2	B	135	THR	2.6
2	B	42	THR	2.6
1	A	551	LEU	2.5
1	C	494	ILE	2.5
1	A	402	VAL	2.5
1	C	678	ILE	2.5
2	B	38	VAL	2.5
1	C	709	LEU	2.5
1	A	620	ASP	2.5
2	B	25	ALA	2.5
1	A	407	PRO	2.5
1	A	375	THR	2.4
2	D	239	GLU	2.4
2	D	216	VAL	2.4
2	B	66	PHE	2.4
1	A	387	ALA	2.4
2	D	130	PHE	2.4
1	C	423	LYS	2.4
2	B	16	VAL	2.4
2	D	218	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	463	LYS	2.3
1	A	403	SER	2.3
1	A	439	ILE	2.3
1	A	415	ASN	2.3
1	A	642	ASP	2.3
1	C	521	GLY	2.3
1	A	694	ILE	2.3
1	A	442	VAL	2.3
1	C	453	LEU	2.3
2	B	92	ILE	2.3
2	B	130	PHE	2.3
1	A	690	GLY	2.3
2	B	46	ILE	2.3
1	A	453	LEU	2.2
2	B	133	ASN	2.2
2	B	89	TRP	2.2
1	A	404	ILE	2.2
1	A	412	LEU	2.2
1	C	519	VAL	2.2
1	A	448	ASN	2.2
1	C	545	ASP	2.2
1	A	592	GLN	2.2
1	C	454	SER	2.2
1	A	716	PHE	2.2
1	A	710	THR	2.2
2	D	134	GLY	2.2
1	A	600	ILE	2.1
1	C	517	ASN	2.1
1	C	541	VAL	2.1
2	B	88	ARG	2.1
1	C	464	GLU	2.1
2	B	187	TYR	2.1
1	A	438	VAL	2.1
2	B	68	THR	2.1
2	B	131	LYS	2.1
1	A	608	ILE	2.1
1	A	626	GLY	2.1
2	D	40	GLY	2.1
1	C	526	ALA	2.0
2	B	45	LEU	2.0
2	D	238	ASN	2.0
1	C	688	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	550	ARG	2.0
1	C	468	PHE	2.0
2	B	4	ILE	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 oligosaccharides 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.