



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:42 AM UTC

PDB ID : 2R17 / pdb_00002r17
Title : Functional architecture of the retromer cargo-recognition complex
Authors : Hierro, A.; Rojas, A.L.; Rojas, R.; Murthy, N.; Effantin, G.; Kajava, A.V.;
Steven, A.C.; Bonifacino, J.S.; Hurley, J.H.
Deposited on : 2007-08-22
Resolution : 2.80 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

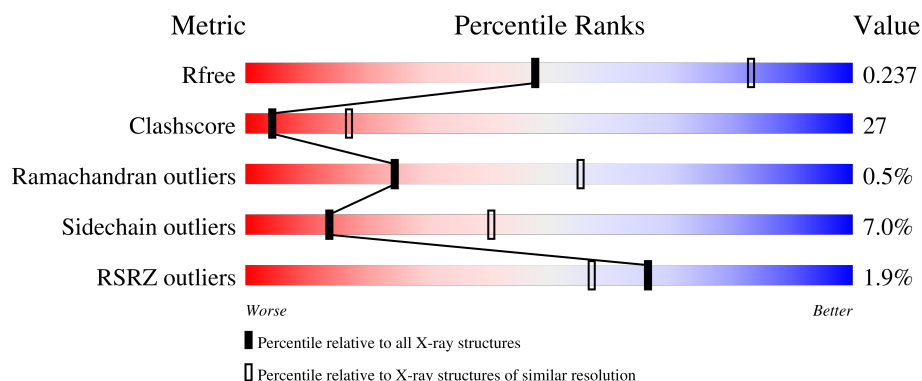
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	183	
1	B	183	
2	C	298	
2	D	298	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7640 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 Vacuolar protein sorting-associated protein 29.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	Se	0	0	0
			1455	941	243	264	3	4			
1	B	183	Total	C	N	O	S	Se	0	0	0
			1455	941	243	264	3	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MSE	-	initiating methionine	UNP Q9UBQ0
B	0	MSE	-	initiating methionine	UNP Q9UBQ0

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 35.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	298	Total	C	N	O	S	Se	0	0	0
			2416	1534	422	450	6	4			
2	D	276	Total	C	N	O	S	Se	0	0	0
			2253	1442	390	411	6	4			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

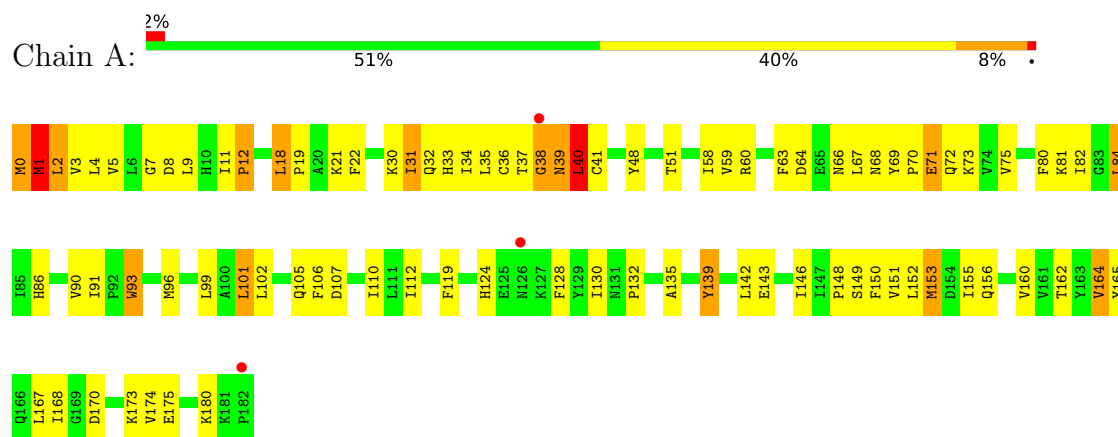
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	10	Total	O	0	0
			10	10		
4	C	17	Total	O	0	0
			17	17		
4	D	14	Total	O	0	0
			14	14		

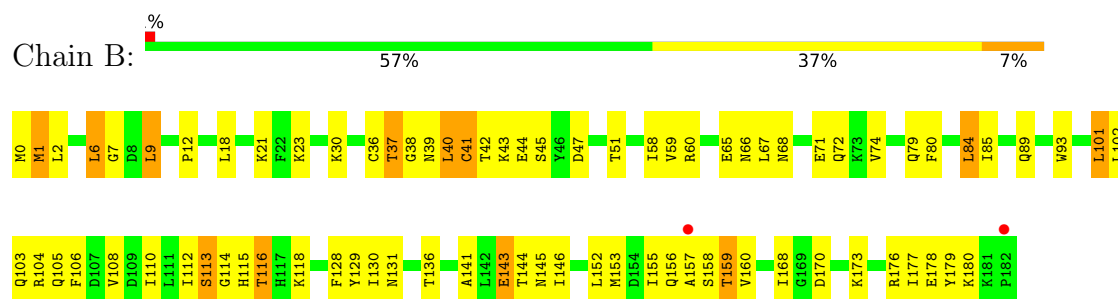
3 Residue-property plots

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.

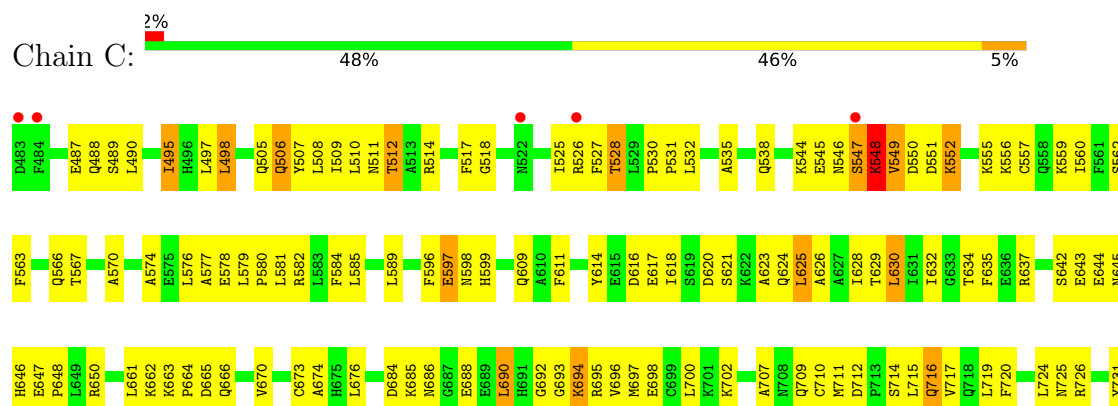
- Molecule 1: Vacuolar protein sorting-associated protein 29

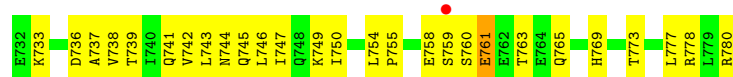


- Molecule 1: Vacuolar protein sorting-associated protein 29

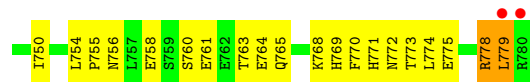
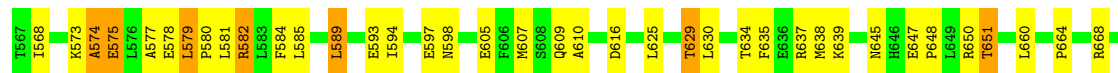


- Molecule 2: Vacuolar protein sorting-associated protein 35





● Molecule 2: Vacuolar protein sorting-associated protein 35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.25Å 128.47Å 140.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.1 (50.00-2.80) 98.8 (50.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.09 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.268 0.226 , 0.237	Depositor DCC
R_{free} test set	1509 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7640	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.43	0/1486	0.96	7/2009 (0.3%)
1	B	0.47	0/1486	0.98	2/2009 (0.1%)
2	C	0.49	1/2459 (0.0%)	0.99	11/3303 (0.3%)
2	D	0.48	0/2293	0.95	7/3078 (0.2%)
All	All	0.47	1/7724 (0.0%)	0.97	27/10399 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	547	SER	CA-C	-5.06	1.45	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	LEU	N-CA-C	-12.31	96.55	111.69
2	C	547	SER	N-CA-C	10.63	126.07	113.20
2	C	761	GLU	N-CA-C	-8.28	102.22	111.82
2	C	617	GLU	N-CA-C	8.20	123.28	113.28
1	A	40	LEU	N-CA-C	-7.63	103.42	112.89
2	D	756	ASN	N-CA-C	7.25	119.40	109.11
1	A	93	TRP	N-CA-C	6.96	122.86	111.37
2	C	714	SER	N-CA-C	6.72	118.26	111.07
2	C	616	ASP	N-CA-C	6.37	118.79	111.02
2	D	574	ALA	N-CA-C	-6.30	105.87	112.93
2	C	733	LYS	N-CA-C	-6.20	105.30	112.92
2	D	616	ASP	N-CA-C	6.19	121.11	113.50
2	D	562	SER	N-CA-C	-6.05	104.60	111.14
1	A	31	ILE	N-CA-C	6.03	117.27	108.58
2	C	562	SER	N-CA-C	-6.00	104.67	112.23
1	A	71	GLU	N-CA-C	-5.71	105.06	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	PHE	N-CA-C	5.71	118.93	109.46
1	A	82	ILE	N-CA-C	5.70	116.10	108.11
1	A	1	MSE	N-CA-C	5.67	118.97	109.95
2	C	506	GLN	N-CA-C	5.65	117.12	111.07
1	B	80	PHE	N-CA-C	5.53	117.98	109.07
2	C	548	LYS	N-CA-C	-5.41	106.54	114.39
2	D	522	ASN	N-CA-C	-5.39	99.32	110.80
2	C	547	SER	CA-C-N	-5.25	113.95	121.98
2	C	547	SER	C-N-CA	-5.25	113.95	121.98
2	D	552	LYS	N-CA-C	-5.14	105.36	113.02
2	D	520	GLY	N-CA-C	5.05	125.15	113.18

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	1455	0	1468	91	0
1	B	1455	0	1468	62	0
2	C	2416	0	2401	136	0
2	D	2253	0	2256	129	0
3	D	12	0	16	0	0
4	A	8	0	0	1	0
4	B	10	0	0	1	0
4	C	17	0	0	2	0
4	D	14	0	0	6	0
All	All	7640	0	7609	406	0

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 (406) 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:520:GLY:HA3	2:D:524:ARG:HD3	1.15	1.14
2:D:525:ILE:HA	2:D:528:THR:HG22	1.28	1.14
1:A:8:ASP:H	1:A:38:GLY:HA3	1.15	1.10
2:D:635:PHE:HA	2:D:638:MSE:HE2	1.37	1.02
2:C:712:ASP:O	2:C:716:GLN:HB2	1.63	0.98
2:D:520:GLY:HA3	2:D:524:ARG:CD	1.94	0.97
2:C:544:LYS:O	2:C:547:SER:CB	2.13	0.96
2:D:758:GLU:O	2:D:763:THR:HG21	1.68	0.94
2:D:625:LEU:O	2:D:629:THR:HG22	1.66	0.94
2:C:517:PHE:HB3	2:C:528:THR:HG21	1.48	0.93
2:C:760:SER:H	2:C:763:THR:HG22	1.33	0.92
2:C:498:LEU:HD11	2:C:510:LEU:HG	1.52	0.91
2:C:544:LYS:O	2:C:547:SER:HB2	1.70	0.91
2:C:614:TYR:O	2:C:618:ILE:HG22	1.70	0.91
2:C:550:ASP:OD1	2:C:551:ASP:N	2.05	0.90
2:D:520:GLY:CA	2:D:524:ARG:HD3	2.02	0.89
2:D:497:LEU:H	2:D:497:LEU:HD23	1.38	0.87
2:D:589:LEU:HD13	2:D:634:THR:HG23	1.57	0.87
1:A:40:LEU:CD2	1:A:40:LEU:H	1.89	0.86
1:B:143:GLU:HB3	1:B:146:ILE:HD11	1.58	0.85
2:C:584:PHE:CZ	2:C:609:GLN:HG2	2.11	0.84
2:D:543:TYR:CE2	2:D:560:ILE:HD11	2.13	0.84
2:D:697:MSE:HE3	2:D:739:THR:HG22	1.60	0.83
1:A:38:GLY:HA2	1:A:86:HIS:CD2	2.14	0.83
2:C:694:LYS:H	2:C:694:LYS:HD3	1.43	0.82
1:B:42:THR:HG22	1:B:44:GLU:H	1.44	0.82
1:A:3:VAL:HG22	1:A:33:HIS:HB2	1.61	0.81
2:C:621:SER:HB2	2:C:661:LEU:HD22	1.62	0.81
2:D:779:LEU:N	2:D:779:LEU:HD12	1.95	0.81
2:D:525:ILE:HA	2:D:528:THR:CG2	2.08	0.81
2:D:695:ARG:HG3	2:D:696:VAL:N	1.95	0.80
1:B:42:THR:HB	4:B:186:HOH:O	1.81	0.80
2:D:635:PHE:HA	2:D:638:MSE:CE	2.11	0.79
2:C:711:MSE:HA	2:C:711:MSE:HE2	1.63	0.78
1:A:151:VAL:HG22	1:A:164:VAL:HA	1.64	0.78
1:B:101:LEU:HD13	2:D:725:ASN:HB3	1.66	0.78
2:C:760:SER:H	2:C:763:THR:CG2	1.97	0.78
2:D:700:LEU:HD21	2:D:726:ARG:HG2	1.67	0.77
2:C:544:LYS:O	2:C:547:SER:HB3	1.84	0.77
2:C:579:LEU:HB3	2:C:580:PRO:HD3	1.66	0.76
1:B:1:MSE:HG2	1:B:155:ILE:HB	1.66	0.76
2:D:715:LEU:O	2:D:719:LEU:HD13	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD13	2:C:725:ASN:HB3	1.69	0.75
1:B:112:ILE:HD13	1:B:130:ILE:HB	1.67	0.74
2:D:497:LEU:HD23	2:D:497:LEU:N	2.02	0.74
2:C:724:LEU:HD12	2:C:773:THR:HG21	1.68	0.73
2:D:695:ARG:HG2	2:D:695:ARG:HH11	1.53	0.73
2:D:543:TYR:HE2	2:D:560:ILE:HD11	1.54	0.73
2:D:719:LEU:O	2:D:723:ILE:HG13	1.88	0.73
1:A:40:LEU:H	1:A:40:LEU:HD23	1.54	0.72
2:D:589:LEU:CD1	2:D:634:THR:HG23	2.19	0.71
1:A:105:GLN:HA	2:C:769:HIS:CD2	2.26	0.70
2:C:517:PHE:HB3	2:C:528:THR:CG2	2.22	0.70
2:D:645:ASN:O	2:D:648:PRO:HD2	1.91	0.70
2:C:712:ASP:OD2	2:C:715:LEU:HD13	1.92	0.70
2:D:494:PHE:CZ	2:D:498:LEU:HD13	2.26	0.70
2:C:550:ASP:OD1	2:C:552:LYS:N	2.22	0.70
2:D:635:PHE:HD2	2:D:638:MSE:HE3	1.57	0.70
1:A:18:LEU:HD12	1:A:18:LEU:H	1.56	0.70
2:C:550:ASP:OD1	2:C:550:ASP:C	2.35	0.69
2:C:578:GLU:O	2:C:582:ARG:HD2	1.91	0.69
2:C:709:GLN:O	2:C:711:MSE:HG2	1.93	0.69
1:A:39:ASN:HD22	1:A:63:PHE:H	1.41	0.69
1:A:38:GLY:HA2	1:A:86:HIS:HD2	1.58	0.68
2:C:707:ALA:HA	2:C:719:LEU:HD23	1.75	0.68
1:A:9:LEU:CD2	1:A:135:ALA:HB3	2.24	0.67
2:D:647:GLU:O	2:D:651:THR:HG23	1.95	0.67
2:C:495:ILE:HD11	2:C:535:ALA:HB2	1.77	0.67
2:C:626:ALA:O	2:C:629:THR:HG22	1.93	0.67
2:C:761:GLU:O	2:C:765:GLN:HG3	1.95	0.67
2:C:598:ASN:HA	4:C:794:HOH:O	1.94	0.66
1:A:112:ILE:HD13	1:A:130:ILE:HB	1.76	0.66
2:C:700:LEU:HD21	2:C:726:ARG:HG2	1.77	0.66
2:D:562:SER:O	2:D:566:GLN:HG3	1.96	0.66
2:D:493:ARG:O	2:D:497:LEU:HD23	1.96	0.66
2:D:584:PHE:CZ	2:D:609:GLN:HG2	2.30	0.65
2:C:760:SER:HB2	2:C:763:THR:H	1.61	0.65
2:C:618:ILE:HD11	2:C:623:ALA:HB1	1.78	0.65
1:A:4:LEU:HB3	1:A:34:ILE:HG12	1.79	0.65
2:D:761:GLU:HA	2:D:764:GLU:OE1	1.96	0.65
2:D:760:SER:O	2:D:764:GLU:HG3	1.96	0.65
2:D:607:MSE:SE	2:D:638:MSE:HE1	2.47	0.64
1:A:164:VAL:CG1	1:A:175:GLU:HB3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:694:LYS:H	2:C:694:LYS:CD	2.10	0.64
1:B:0:MSE:SE	1:B:156:GLN:CD	2.91	0.63
2:C:662:LYS:HB3	2:C:664:PRO:HD2	1.81	0.63
2:D:697:MSE:HB2	4:D:789:HOH:O	1.97	0.63
2:D:543:TYR:CD2	2:D:560:ILE:HD11	2.33	0.63
1:A:0:MSE:CG	1:A:0:MSE:O	2.46	0.63
1:B:40:LEU:HD11	1:B:58:ILE:HD13	1.80	0.63
1:B:72:GLN:HB3	1:B:85:ILE:HD12	1.79	0.63
2:D:579:LEU:HB3	2:D:580:PRO:HD3	1.80	0.63
2:D:695:ARG:HG2	4:D:789:HOH:O	1.99	0.63
2:D:754:LEU:HB3	2:D:755:PRO:HD3	1.80	0.62
2:D:514:ARG:HG3	2:D:514:ARG:HH11	1.63	0.62
1:A:19:PRO:HG2	1:A:22:PHE:HB2	1.81	0.62
2:D:525:ILE:CA	2:D:528:THR:HG22	2.19	0.62
1:A:36:CYS:HB3	1:A:58:ILE:HG12	1.82	0.62
1:B:79:GLN:OE1	1:B:158:SER:HB2	2.01	0.61
2:C:526:ARG:CZ	2:C:576:LEU:HD21	2.30	0.61
2:C:552:LYS:N	2:C:552:LYS:HD2	2.16	0.61
2:D:695:ARG:HG3	2:D:696:VAL:H	1.64	0.61
2:C:508:LEU:O	2:C:512:THR:HG23	1.99	0.61
1:A:150:PHE:HE1	1:A:152:LEU:HD22	1.65	0.60
1:A:48:TYR:O	1:A:51:THR:HB	2.00	0.60
2:D:645:ASN:C	2:D:648:PRO:HD2	2.26	0.60
2:D:779:LEU:HD12	2:D:779:LEU:H	1.67	0.60
2:D:544:LYS:O	2:D:547:SER:HB2	2.00	0.60
1:A:39:ASN:HD22	1:A:63:PHE:N	2.00	0.60
1:A:1:MSE:H	1:A:1:MSE:SE	2.35	0.60
2:C:620:ASP:O	2:C:624:GLN:HG3	2.02	0.59
1:B:116:THR:HG22	1:B:118:LYS:H	1.66	0.59
2:D:664:PRO:HA	2:D:719:LEU:HD21	1.84	0.59
2:C:645:ASN:C	2:C:648:PRO:HD2	2.27	0.59
2:C:739:THR:OG1	2:C:742:VAL:HG23	2.01	0.59
1:A:148:PRO:O	1:A:149:SER:HB3	2.01	0.59
2:D:525:ILE:HD11	2:D:574:ALA:HB2	1.85	0.59
1:A:8:ASP:N	1:A:38:GLY:HA3	2.00	0.59
2:D:543:TYR:CE1	2:D:556:LYS:HD3	2.37	0.59
2:D:724:LEU:HD22	2:D:773:THR:HG21	1.84	0.59
1:A:4:LEU:HB2	1:A:31:ILE:HD13	1.85	0.59
1:A:18:LEU:HD12	1:A:18:LEU:N	2.18	0.59
1:B:128:PHE:CZ	1:B:130:ILE:HD11	2.38	0.58
1:B:101:LEU:HD12	1:B:101:LEU:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:530:PRO:HB2	2:D:531:PRO:HD3	1.86	0.58
1:B:116:THR:CG2	1:B:118:LYS:H	2.17	0.58
2:C:744:ASN:HA	2:C:747:ILE:CD1	2.34	0.58
2:D:647:GLU:HB3	2:D:648:PRO:HD3	1.86	0.58
1:A:139:TYR:CD2	2:C:538:GLN:HG3	2.38	0.58
2:C:526:ARG:NH2	2:C:576:LEU:HD21	2.17	0.58
2:C:645:ASN:O	2:C:648:PRO:HD2	2.04	0.58
2:C:584:PHE:CE2	2:C:609:GLN:HG2	2.37	0.58
2:D:508:LEU:O	2:D:512:THR:HG23	2.04	0.58
1:B:110:ILE:HA	1:B:128:PHE:O	2.04	0.57
1:B:168:ILE:HD12	1:B:173:LYS:HD2	1.86	0.57
2:D:520:GLY:HA3	2:D:524:ARG:CG	2.34	0.57
1:A:71:GLU:HB3	1:A:72:GLN:OE1	2.04	0.57
2:C:577:ALA:C	2:C:580:PRO:HD2	2.30	0.57
1:B:38:GLY:O	1:B:39:ASN:HB2	2.04	0.57
1:B:176:ARG:O	1:B:177:ILE:HD13	2.04	0.57
2:C:495:ILE:CD1	2:C:535:ALA:HB2	2.34	0.57
2:C:650:ARG:NH1	2:C:695:ARG:HH12	2.03	0.57
2:D:577:ALA:C	2:D:580:PRO:HD2	2.29	0.57
2:C:745:GLN:O	2:C:749:LYS:HG3	2.05	0.56
2:C:582:ARG:HG2	2:C:582:ARG:HH11	1.70	0.56
2:C:760:SER:N	2:C:763:THR:HG22	2.11	0.56
1:A:152:LEU:HD21	1:A:165:TYR:CE2	2.40	0.56
2:C:577:ALA:O	2:C:580:PRO:HD2	2.06	0.56
2:D:695:ARG:HG2	2:D:695:ARG:NH1	2.17	0.56
1:B:40:LEU:HB3	1:B:45:SER:HB2	1.87	0.56
2:C:489:SER:HB3	4:C:782:HOH:O	2.04	0.56
1:A:40:LEU:H	1:A:40:LEU:HD22	1.69	0.56
1:A:67:LEU:HD23	1:A:67:LEU:O	2.05	0.56
1:A:152:LEU:HD21	1:A:165:TYR:HE2	1.71	0.56
1:B:41:CYS:O	1:B:65:GLU:HG3	2.06	0.56
1:A:2:LEU:HD11	1:A:152:LEU:HD12	1.87	0.56
1:A:130:ILE:HG13	1:A:153:MSE:HE3	1.88	0.55
1:A:0:MSE:O	1:A:0:MSE:HG3	2.03	0.55
2:D:494:PHE:CE1	2:D:498:LEU:HD13	2.41	0.55
1:A:2:LEU:HD23	1:A:2:LEU:O	2.07	0.55
2:C:760:SER:N	2:C:763:THR:CG2	2.69	0.55
2:D:503:PRO:HG3	2:D:542:ARG:HG3	1.88	0.55
2:C:744:ASN:HA	2:C:747:ILE:HD11	1.89	0.55
2:C:666:GLN:O	2:C:670:VAL:HG23	2.07	0.55
2:C:663:LYS:N	2:C:664:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:487:GLU:O	2:C:490:LEU:HB3	2.07	0.55
2:D:487:GLU:O	2:D:490:LEU:HB3	2.07	0.55
2:C:549:VAL:O	2:C:549:VAL:CG1	2.56	0.54
2:D:719:LEU:N	2:D:719:LEU:HD12	2.22	0.54
2:C:698:GLU:O	2:C:702:LYS:HG3	2.07	0.54
2:D:779:LEU:N	2:D:779:LEU:CD1	2.68	0.54
1:B:21:LYS:NZ	1:B:170:ASP:O	2.33	0.53
1:B:159:THR:OG1	1:B:180:LYS:HG2	2.09	0.53
1:B:72:GLN:HB3	1:B:85:ILE:CD1	2.39	0.53
1:A:164:VAL:HG13	1:A:175:GLU:HB3	1.91	0.53
1:A:21:LYS:HZ2	1:A:170:ASP:C	2.17	0.53
1:B:60:ARG:HD3	1:B:67:LEU:HD12	1.91	0.53
2:D:713:PRO:O	2:D:717:VAL:HG23	2.08	0.53
1:A:9:LEU:HD22	1:A:135:ALA:HB3	1.91	0.52
2:D:560:ILE:O	2:D:563:PHE:HB3	2.09	0.52
2:D:635:PHE:HD2	2:D:638:MSE:CE	2.22	0.52
1:A:39:ASN:HA	1:A:64:ASP:OD2	2.10	0.52
1:A:174:VAL:HG12	1:A:175:GLU:N	2.24	0.52
1:B:47:ASP:O	1:B:51:THR:HG23	2.09	0.52
2:C:557:CYS:HA	2:C:560:ILE:HG22	1.91	0.52
1:A:0:MSE:HB2	1:A:156:GLN:HA	1.91	0.52
1:A:3:VAL:HG22	1:A:33:HIS:CB	2.37	0.52
2:D:702:LYS:O	2:D:706:ILE:HG13	2.10	0.52
1:A:101:LEU:O	1:A:101:LEU:HD12	2.09	0.51
1:B:101:LEU:HD12	1:B:101:LEU:C	2.35	0.51
2:C:488:GLN:OE1	2:C:527:PHE:HB3	2.10	0.51
2:D:639:LYS:HA	4:D:793:HOH:O	2.09	0.51
1:A:35:LEU:HD21	1:A:75:VAL:HG11	1.92	0.51
2:C:497:LEU:N	2:C:497:LEU:HD23	2.25	0.51
2:C:643:GLU:HB2	2:C:684:ASP:OD2	2.11	0.51
2:C:505:GLN:O	2:C:509:ILE:HG13	2.10	0.51
2:C:552:LYS:N	2:C:552:LYS:CD	2.74	0.51
2:C:618:ILE:HG23	2:C:618:ILE:O	2.09	0.51
2:C:557:CYS:O	2:C:560:ILE:HG22	2.11	0.51
2:C:694:LYS:O	2:C:698:GLU:HG3	2.11	0.51
1:A:168:ILE:HD12	1:A:173:LYS:HD2	1.93	0.51
1:B:6:LEU:CD1	1:B:6:LEU:C	2.83	0.51
1:B:130:ILE:HG13	1:B:153:MSE:HE3	1.92	0.51
2:D:702:LYS:HG3	2:D:706:ILE:HD11	1.93	0.51
1:B:101:LEU:HD13	2:D:725:ASN:CB	2.39	0.51
2:C:618:ILE:HD11	2:C:623:ALA:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:581:LEU:C	2:C:581:LEU:HD23	2.36	0.50
2:D:525:ILE:HB	2:D:529:LEU:CD1	2.42	0.50
1:A:40:LEU:HD23	1:A:40:LEU:N	2.24	0.50
1:B:6:LEU:C	1:B:6:LEU:HD12	2.35	0.50
1:B:66:ASN:OD1	1:B:68:ASN:HB2	2.12	0.50
1:B:128:PHE:CE2	1:B:130:ILE:HD11	2.46	0.50
2:D:597:GLU:HA	4:D:782:HOH:O	2.12	0.50
2:D:581:LEU:CD1	2:D:610:ALA:HB1	2.42	0.50
2:D:704:LEU:HD21	2:D:746:LEU:HD21	1.93	0.49
2:D:719:LEU:H	2:D:719:LEU:CD1	2.26	0.49
2:D:525:ILE:HB	2:D:529:LEU:HD12	1.94	0.49
2:D:720:PHE:HB3	2:D:750:ILE:HD11	1.95	0.49
2:D:724:LEU:HD23	2:D:724:LEU:C	2.37	0.49
2:C:744:ASN:O	2:C:747:ILE:HG12	2.13	0.49
1:B:18:LEU:HA	1:B:136:THR:HG22	1.94	0.49
1:B:130:ILE:HG13	1:B:153:MSE:CE	2.43	0.49
2:C:585:LEU:CD1	2:C:630:LEU:HD12	2.42	0.49
2:D:720:PHE:HB3	2:D:750:ILE:CD1	2.43	0.49
1:A:101:LEU:HD13	2:C:725:ASN:CB	2.42	0.49
2:D:584:PHE:CE1	2:D:609:GLN:HG2	2.48	0.48
1:A:37:THR:CG2	1:A:112:ILE:HG22	2.43	0.48
1:A:90:VAL:C	1:A:91:ILE:HD12	2.38	0.48
2:C:532:LEU:O	2:C:535:ALA:HB3	2.13	0.48
2:C:684:ASP:C	2:C:686:ASN:H	2.21	0.48
2:D:740:ILE:O	2:D:740:ILE:HG22	2.14	0.48
2:C:731:TYR:HB2	2:C:738:VAL:HG11	1.94	0.48
2:D:497:LEU:N	2:D:497:LEU:CD2	2.73	0.48
1:A:112:ILE:CD1	1:A:130:ILE:HB	2.43	0.48
2:D:502:ASP:HB3	2:D:505:GLN:HB3	1.95	0.48
1:A:70:PRO:HG2	1:A:73:LYS:HE3	1.95	0.48
1:A:22:PHE:CE1	1:A:167:LEU:HB2	2.48	0.48
2:D:668:ARG:O	2:D:672:THR:HG23	2.14	0.48
2:D:704:LEU:HD21	2:D:746:LEU:CD2	2.44	0.48
2:D:746:LEU:HD13	2:D:746:LEU:C	2.38	0.48
2:C:525:ILE:HD11	2:C:574:ALA:HB2	1.96	0.48
1:B:40:LEU:O	1:B:41:CYS:HB2	2.13	0.48
2:D:719:LEU:N	2:D:719:LEU:CD1	2.77	0.48
2:D:516:HIS:HB3	4:D:781:HOH:O	2.13	0.47
2:D:573:LYS:C	2:D:575:GLU:H	2.21	0.47
2:C:777:LEU:O	2:C:778:ARG:HB2	2.13	0.47
2:C:596:PHE:O	2:C:599:HIS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:688:GLU:OE1	2:C:688:GLU:HA	2.14	0.47
1:B:113:SER:O	1:B:131:ASN:HA	2.15	0.47
1:A:180:LYS:HB2	4:A:188:HOH:O	2.15	0.47
2:C:736:ASP:OD1	2:C:737:ALA:N	2.47	0.47
1:B:104:ARG:NH1	2:D:725:ASN:OD1	2.47	0.47
2:C:746:LEU:O	2:C:750:ILE:HG13	2.14	0.47
2:C:685:LYS:NZ	2:C:690:LEU:O	2.48	0.47
2:D:607:MSE:O	2:D:610:ALA:HB3	2.15	0.47
1:B:59:VAL:HG13	1:B:84:LEU:HD13	1.97	0.47
2:C:759:SER:HA	2:C:763:THR:HG21	1.97	0.47
1:B:152:LEU:HD12	1:B:152:LEU:O	2.16	0.46
2:C:744:ASN:HA	2:C:747:ILE:HG12	1.97	0.46
1:A:96:MSE:HE3	1:A:124:HIS:CE1	2.49	0.46
1:B:18:LEU:HD23	1:B:136:THR:HG23	1.97	0.46
1:B:40:LEU:HB3	1:B:45:SER:CB	2.45	0.46
1:B:42:THR:CG2	1:B:43:LYS:N	2.77	0.46
2:C:495:ILE:HD13	2:C:495:ILE:HA	1.65	0.46
2:D:493:ARG:O	2:D:497:LEU:CD2	2.61	0.46
2:D:545:GLU:C	2:D:547:SER:H	2.24	0.46
1:A:119:PHE:CE2	1:A:164:VAL:HB	2.50	0.46
1:B:129:TYR:O	1:B:130:ILE:HD13	2.16	0.46
2:C:694:LYS:HG2	2:C:695:ARG:H	1.80	0.46
2:C:754:LEU:N	2:C:755:PRO:CD	2.78	0.46
1:A:60:ARG:HB2	1:A:69:TYR:HB2	1.97	0.46
2:C:530:PRO:HB2	2:C:531:PRO:HD3	1.97	0.46
1:A:155:ILE:HG13	1:A:160:VAL:HG23	1.97	0.45
2:C:514:ARG:O	2:C:518:GLY:N	2.44	0.45
2:D:768:LYS:HE2	2:D:772:ASN:OD1	2.16	0.45
1:B:42:THR:HG22	1:B:43:LYS:N	2.32	0.45
2:C:674:ALA:HB1	2:C:696:VAL:HG13	1.98	0.45
2:D:484:PHE:CD2	2:D:485:ALA:N	2.83	0.45
1:A:91:ILE:HD12	1:A:91:ILE:N	2.31	0.45
1:A:143:GLU:HG3	1:A:146:ILE:HD13	1.99	0.45
2:C:717:VAL:O	2:C:720:PHE:HB2	2.16	0.45
1:B:105:GLN:HA	2:D:769:HIS:ND1	2.32	0.45
2:C:589:LEU:HG	2:C:634:THR:HG23	1.99	0.45
2:D:609:GLN:HG3	4:D:785:HOH:O	2.16	0.45
1:A:2:LEU:CD1	1:A:152:LEU:HD12	2.47	0.45
1:A:81:LYS:HD3	1:A:107:ASP:O	2.17	0.45
1:B:141:ALA:O	2:D:593:GLU:HG2	2.17	0.45
2:D:585:LEU:HB3	2:D:634:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:637:ARG:HA	2:D:637:ARG:NE	2.32	0.45
2:D:544:LYS:HD2	2:D:594:ILE:HG23	1.98	0.45
2:C:621:SER:HB2	2:C:661:LEU:CD2	2.42	0.45
2:C:673:CYS:O	2:C:674:ALA:C	2.59	0.45
1:A:150:PHE:CE1	1:A:152:LEU:HD22	2.50	0.44
2:D:625:LEU:HD23	2:D:660:LEU:HD13	1.99	0.44
2:C:697:MSE:HG3	2:C:737:ALA:HB1	1.98	0.44
2:D:724:LEU:O	2:D:728:ILE:HG13	2.18	0.44
2:C:526:ARG:HG2	2:C:576:LEU:HD11	2.00	0.44
2:C:545:GLU:O	2:C:545:GLU:HG2	2.18	0.44
2:D:498:LEU:HD23	2:D:498:LEU:O	2.17	0.44
1:A:150:PHE:O	1:A:151:VAL:HG23	2.18	0.44
1:A:153:MSE:HE2	1:A:162:THR:CG2	2.47	0.44
1:B:59:VAL:CG2	1:B:84:LEU:HD22	2.47	0.44
2:C:741:GLN:O	2:C:745:GLN:HG3	2.18	0.44
2:C:692:GLY:HA2	2:C:694:LYS:CE	2.47	0.44
2:D:724:LEU:CD2	2:D:728:ILE:HD11	2.47	0.44
2:D:771:HIS:O	2:D:775:GLU:HG2	2.17	0.44
2:C:578:GLU:O	2:C:582:ARG:CD	2.65	0.43
2:C:628:ILE:O	2:C:632:ILE:HG13	2.18	0.43
2:D:717:VAL:O	2:D:721:ILE:HG13	2.18	0.43
1:A:37:THR:OG1	1:A:38:GLY:N	2.50	0.43
2:D:563:PHE:CD1	2:D:563:PHE:C	2.96	0.43
2:D:564:ALA:O	2:D:568:ILE:HG13	2.18	0.43
1:A:66:ASN:OD1	1:A:68:ASN:HB2	2.18	0.43
1:A:128:PHE:CE1	1:A:130:ILE:HD11	2.53	0.43
2:C:618:ILE:HD11	2:C:623:ALA:C	2.44	0.43
1:A:11:ILE:O	1:A:41:CYS:HB2	2.18	0.43
1:B:18:LEU:HD23	1:B:136:THR:CG2	2.49	0.43
1:B:114:GLY:O	1:B:115:HIS:HB3	2.19	0.43
2:D:500:SER:CB	2:D:505:GLN:HG2	2.49	0.43
1:B:144:THR:HG23	1:B:145:ASN:N	2.33	0.43
2:C:635:PHE:CD1	2:C:676:LEU:HD22	2.53	0.43
2:D:728:ILE:O	2:D:732:GLU:HG3	2.17	0.43
1:A:101:LEU:HD12	1:A:101:LEU:C	2.43	0.43
2:D:704:LEU:O	2:D:707:ALA:HB3	2.17	0.43
1:A:59:VAL:HG13	1:A:84:LEU:HD13	1.99	0.43
1:A:90:VAL:O	1:A:93:TRP:HA	2.18	0.43
2:C:625:LEU:O	2:C:629:THR:HB	2.17	0.43
2:D:516:HIS:CD2	2:D:516:HIS:C	2.96	0.43
2:D:529:LEU:N	2:D:530:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PHE:O	1:A:107:ASP:HB3	2.19	0.43
1:A:142:LEU:HD21	2:C:589:LEU:HD22	2.00	0.43
2:C:498:LEU:HD22	2:C:506:GLN:OE1	2.18	0.43
1:B:9:LEU:HD23	1:B:9:LEU:N	2.34	0.43
2:C:544:LYS:C	2:C:546:ASN:N	2.77	0.43
2:C:642:SER:OG	2:C:644:GLU:HG2	2.19	0.43
2:D:578:GLU:OE2	2:D:582:ARG:NH2	2.52	0.43
1:A:30:LYS:O	1:A:32:GLN:NE2	2.51	0.42
2:D:581:LEU:HD12	2:D:610:ALA:HB1	1.99	0.42
1:B:103:GLN:NE2	1:B:108:VAL:O	2.48	0.42
1:A:18:LEU:H	1:A:18:LEU:CD1	2.29	0.42
1:A:99:LEU:O	1:A:102:LEU:HB3	2.19	0.42
2:D:517:PHE:O	2:D:528:THR:HG21	2.19	0.42
2:D:746:LEU:O	2:D:750:ILE:HG12	2.19	0.42
1:B:36:CYS:SG	1:B:40:LEU:HD21	2.59	0.42
1:B:89:GLN:OE1	1:B:89:GLN:N	2.47	0.42
2:C:548:LYS:HZ3	2:C:548:LYS:HG2	1.59	0.42
2:D:504:ASP:O	2:D:508:LEU:HD23	2.19	0.42
1:A:22:PHE:CE2	1:A:150:PHE:HD2	2.38	0.42
2:C:551:ASP:C	2:C:552:LYS:HD2	2.44	0.42
2:C:663:LYS:HB2	2:C:664:PRO:HD3	2.02	0.42
2:D:529:LEU:O	2:D:530:PRO:C	2.61	0.42
1:B:59:VAL:HG21	1:B:84:LEU:HD22	2.01	0.42
2:D:724:LEU:HD21	2:D:728:ILE:HD11	2.02	0.42
2:C:517:PHE:CB	2:C:528:THR:HG21	2.34	0.42
2:D:761:GLU:O	2:D:765:GLN:HG3	2.20	0.42
1:A:93:TRP:CE3	2:C:637:ARG:HG3	2.55	0.41
1:A:149:SER:HA	1:A:165:TYR:O	2.19	0.41
2:D:597:GLU:O	2:D:598:ASN:CB	2.68	0.41
2:C:567:THR:O	2:C:570:ALA:HB3	2.20	0.41
2:C:576:LEU:HD23	2:C:576:LEU:HA	1.95	0.41
2:D:579:LEU:CB	2:D:580:PRO:HD3	2.49	0.41
1:A:5:VAL:HG12	1:A:132:PRO:HB3	2.03	0.41
1:A:19:PRO:HG2	1:A:22:PHE:CG	2.55	0.41
1:B:2:LEU:CD2	1:B:30:LYS:HG2	2.49	0.41
2:C:597:GLU:O	2:C:598:ASN:CB	2.67	0.41
1:B:2:LEU:HD23	1:B:30:LYS:HG2	2.02	0.41
2:C:507:TYR:CE2	2:C:559:LYS:HD3	2.55	0.41
2:C:743:LEU:O	2:C:747:ILE:HG23	2.20	0.41
2:C:550:ASP:OD2	2:C:556:LYS:HE2	2.21	0.41
2:C:597:GLU:O	2:C:598:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:724:LEU:HA	2:C:746:LEU:HD23	2.02	0.41
2:C:758:GLU:O	2:C:759:SER:C	2.64	0.41
1:A:39:ASN:HA	1:A:64:ASP:CG	2.46	0.41
1:A:110:ILE:HG12	1:A:128:PHE:HB3	2.03	0.41
2:C:694:LYS:HD3	2:C:694:LYS:N	2.21	0.41
2:C:744:ASN:HA	2:C:747:ILE:CG1	2.51	0.41
2:D:503:PRO:HG3	2:D:542:ARG:CG	2.50	0.41
2:D:579:LEU:HB3	2:D:580:PRO:CD	2.50	0.41
2:D:721:ILE:HD13	2:D:770:PHE:HB2	2.01	0.41
2:C:646:HIS:O	2:C:650:ARG:HB2	2.21	0.41
2:D:746:LEU:HD13	2:D:746:LEU:O	2.20	0.41
1:A:11:ILE:HA	1:A:12:PRO:HA	1.88	0.41
1:A:152:LEU:H	1:A:152:LEU:HD23	1.84	0.41
2:C:514:ARG:NH2	2:C:566:GLN:HG2	2.36	0.41
2:C:643:GLU:CB	2:C:684:ASP:OD2	2.69	0.41
2:C:690:LEU:H	2:C:690:LEU:HD12	1.86	0.41
1:A:1:MSE:SE	1:A:1:MSE:N	3.03	0.41
1:B:18:LEU:HB2	1:B:23:LYS:HG3	2.03	0.41
2:C:692:GLY:O	2:C:693:GLY:C	2.62	0.41
1:A:7:GLY:HA3	1:A:38:GLY:H	1.86	0.40
1:A:22:PHE:CD2	1:A:150:PHE:HD2	2.40	0.40
1:A:58:ILE:O	1:A:70:PRO:HD2	2.21	0.40
2:C:665:ASP:OD1	2:C:665:ASP:N	2.54	0.40
2:D:775:GLU:HA	2:D:778:ARG:HH11	1.86	0.40
1:A:35:LEU:CD2	1:A:75:VAL:HG11	2.52	0.40
1:B:7:GLY:HA3	1:B:37:THR:HG22	2.03	0.40
2:C:724:LEU:C	2:C:724:LEU:HD13	2.46	0.40
2:D:556:LYS:O	2:D:560:ILE:HG13	2.20	0.40
1:B:93:TRP:CE3	2:D:637:ARG:HG3	2.56	0.40
1:B:160:VAL:HG13	1:B:179:TYR:HB3	2.03	0.40
2:C:780:ARG:HH11	2:C:780:ARG:HG2	1.86	0.40
1:B:102:LEU:HD11	1:B:106:PHE:CE1	2.56	0.40
2:D:647:GLU:HA	2:D:650:ARG:CZ	2.52	0.40
2:C:544:LYS:C	2:C:546:ASN:H	2.29	0.40
2:C:563:PHE:CD1	2:C:563:PHE:C	2.99	0.40
2:D:520:GLY:HA3	2:D:524:ARG:HG2	2.04	0.40

There are no symmetry-related clashes.

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	181/183 (99%)	158 (87%)	22 (12%)	1 (1%)	21	51
1	B	181/183 (99%)	172 (95%)	7 (4%)	2 (1%)	11	36
2	C	296/298 (99%)	277 (94%)	18 (6%)	1 (0%)	36	66
2	D	270/298 (91%)	248 (92%)	21 (8%)	1 (0%)	30	60
All	All	928/962 (96%)	855 (92%)	68 (7%)	5 (0%)	24	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	710	CYS
2	D	520	GLY
1	A	38	GLY
1	B	41	CYS
1	B	157	ALA

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	161/157 (102%)	149 (92%)	12 (8%)	12	37
1	B	161/157 (102%)	147 (91%)	14 (9%)	9	30
2	C	259/255 (102%)	242 (93%)	17 (7%)	15	43
2	D	242/255 (95%)	227 (94%)	15 (6%)	16	45
All	All	823/824 (100%)	765 (93%)	58 (7%)	14	40

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MSE
1	A	1	MSE
1	A	2	LEU
1	A	12	PRO
1	A	18	LEU
1	A	39	ASN
1	A	40	LEU
1	A	84	LEU
1	A	101	LEU
1	A	139	TYR
1	A	153	MSE
1	A	164	VAL
1	B	1	MSE
1	B	6	LEU
1	B	9	LEU
1	B	12	PRO
1	B	37	THR
1	B	71	GLU
1	B	74	VAL
1	B	84	LEU
1	B	101	LEU
1	B	113	SER
1	B	116	THR
1	B	143	GLU
1	B	159	THR
1	B	178	GLU
2	C	495	ILE
2	C	498	LEU
2	C	511	ASN
2	C	512	THR
2	C	528	THR
2	C	548	LYS
2	C	549	VAL
2	C	552	LYS
2	C	555	LYS
2	C	597	GLU
2	C	611	PHE
2	C	625	LEU
2	C	630	LEU
2	C	647	GLU
2	C	690	LEU
2	C	694	LYS

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Mol	Chain	Res	Type
2	C	716	GLN
2	D	486	ASP
2	D	497	LEU
2	D	523	GLN
2	D	575	GLU
2	D	579	LEU
2	D	582	ARG
2	D	589	LEU
2	D	605	GLU
2	D	629	THR
2	D	630	LEU
2	D	651	THR
2	D	726	ARG
2	D	774	LEU
2	D	778	ARG
2	D	779	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
2	C	709	GLN
2	C	765	GLN
2	D	511	ASN
2	D	522	ASN
2	D	566	GLN
2	D	652	GLN
2	D	709	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	D	2	-	5,5,5	0.38	0	5,5,5	0.34	0
3	GOL	D	1	-	5,5,5	0.40	0	5,5,5	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	2	-	-	0/4/4/4	-
3	GOL	D	1	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	179/183 (97%)	0.16	3 (1%) 69 60	24, 62, 91, 105	0
1	B	179/183 (97%)	-0.11	2 (1%) 78 70	24, 46, 65, 75	0
2	C	294/298 (98%)	0.05	6 (2%) 65 56	26, 55, 89, 104	0
2	D	272/298 (91%)	-0.10	7 (2%) 57 47	21, 48, 86, 100	0
All	All	924/962 (96%)	-0.00	18 (1%) 66 57	21, 52, 86, 105	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	739	THR	4.4
2	D	740	ILE	3.5
2	C	547	SER	3.5
2	D	484	PHE	3.1
2	D	779	LEU	3.0
1	B	157	ALA	2.5
1	A	38	GLY	2.3
2	D	485	ALA	2.2
2	D	498	LEU	2.2
2	C	526	ARG	2.1
2	C	484	PHE	2.1
2	D	780	ARG	2.1
1	A	182	PRO	2.1
2	C	483	ASP	2.1
1	A	126	ASN	2.1
2	C	522	ASN	2.1
1	B	182	PRO	2.1
2	C	759	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	2	6/6	0.76	0.19	68,72,73,73	0
3	GOL	D	1	6/6	0.83	0.15	78,79,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.