



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:22 AM UTC

PDB ID : 8R4K / pdb_00008r4k
Title : Plastidial phosphorylase Pho1 trimer from Solanum tuberosum
Authors : Koulas, S.M.; Leonidas, D.D.
Deposited on : 2023-11-13
Resolution : 3.30 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

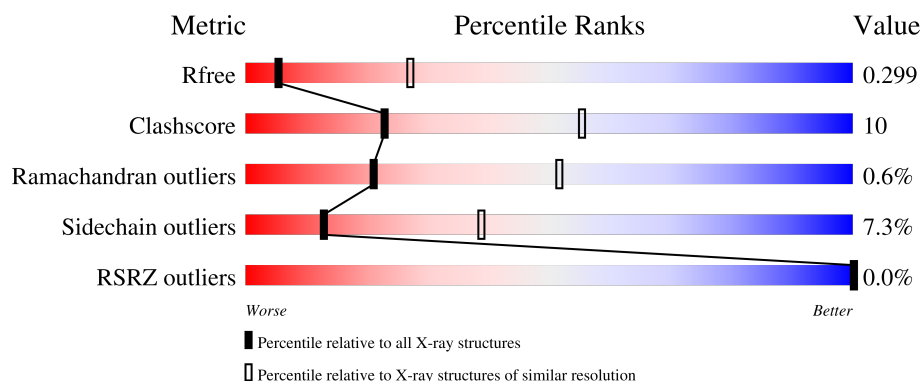
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	916	 64% 25% • 9%
1	B	916	 65% 24% • 9%
1	C	916	 64% 25% • 9%

2 Entry composition [i](#)

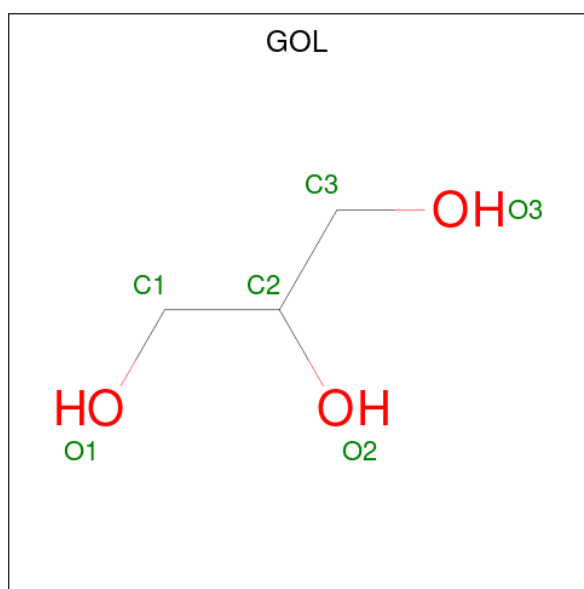
There are 3 unique types of molecules in this entry. The entry contains 20061 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-1,4 glucan phosphorylase L-1 isozyme, chloroplastic/a myloplastic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	830	Total	C	N	O	P	S	0	0	0
			6664	4258	1116	1264	1	25			
1	B	830	Total	C	N	O	P	S	0	0	0
			6664	4258	1116	1264	1	25			
1	C	830	Total	C	N	O	P	S	0	0	0
			6664	4258	1116	1264	1	25			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

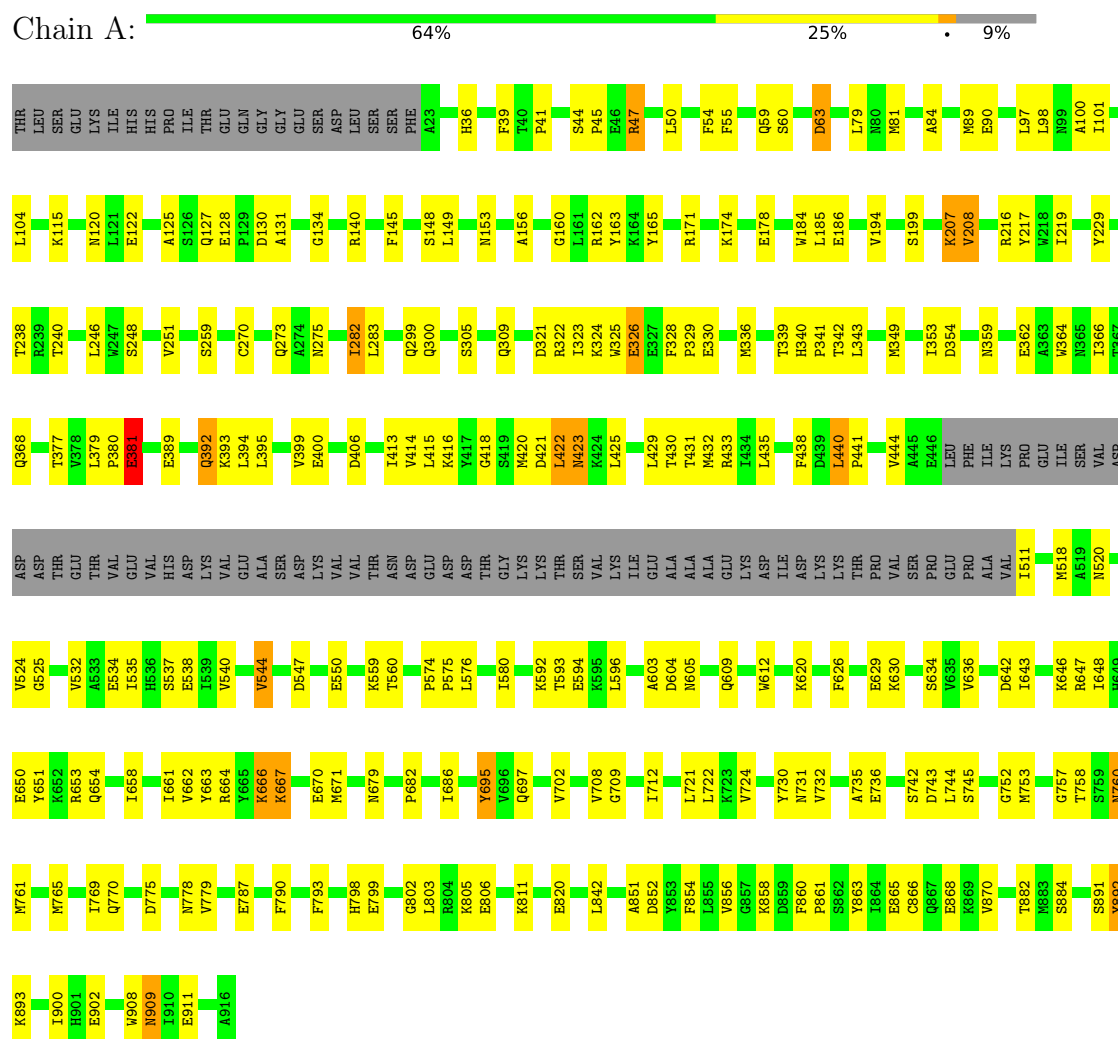
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	19	Total 19	O 19	0	0
3	C	9	Total 9	O 9	0	0

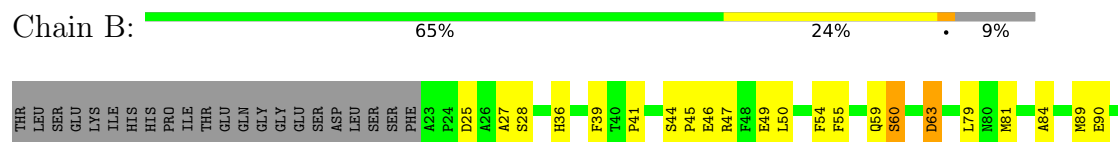
3 Residue-property plots

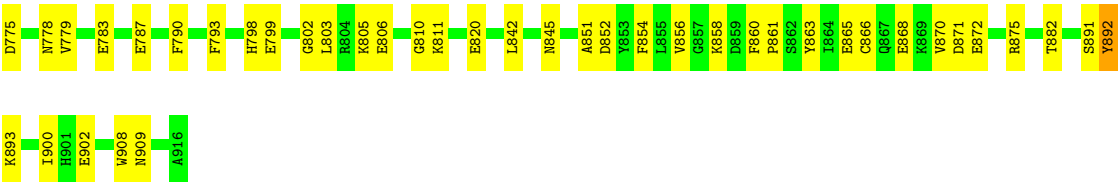
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha-1,4 glucan phosphorylase L-1 isozyme, chloroplastic/amyloplastic



- Molecule 1: Alpha-1,4 glucan phosphorylase L-1 isozyme, chloroplastic/amyloplastic





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.06Å 134.91Å 123.11Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	123.07 – 3.30 123.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (123.07-3.30) 97.7 (123.07-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.254 , 0.300 0.254 , 0.299	Depositor DCC
R_{free} test set	2539 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	93.5	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 8.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20061	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, 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	0.56	0/6790	1.09	2/9188 (0.0%)
1	B	0.55	0/6790	1.09	3/9188 (0.0%)
1	C	0.57	0/6790	1.11	2/9188 (0.0%)
All	All	0.56	0/20370	1.10	7/27564 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	607	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	63	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	63	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	654	GLN	N-CA-C	-5.05	105.90	111.71
1	C	654	GLN	N-CA-C	-5.05	105.90	111.71
1	B	63	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	654	GLN	N-CA-C	-5.00	105.95	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6664	0	6538	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6664	0	6538	137	0
1	C	6664	0	6538	136	0
2	A	6	0	8	0	0
3	A	35	0	0	0	0
3	B	19	0	0	0	0
3	C	9	0	0	1	0
All	All	20061	0	19622	411	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 10.

All (411) 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)
1:A:36:HIS:HE1	1:A:63:ASP:OD2	1.38	1.07
1:A:36:HIS:CE1	1:A:63:ASP:OD2	2.20	0.93
1:A:328:PHE:HB3	1:A:329:PRO:HD3	1.50	0.92
1:A:666:LYS:HD2	1:A:670:GLU:OE2	1.76	0.85
1:B:25:ASP:OD1	1:B:27:ALA:N	2.16	0.77
1:B:759:SER:HA	1:B:762:LLP:HD2	1.68	0.76
1:C:392:GLN:HA	1:C:399:VAL:HG21	1.67	0.76
1:B:392:GLN:HA	1:B:399:VAL:HG21	1.69	0.74
1:A:392:GLN:HA	1:A:399:VAL:HG21	1.69	0.74
1:B:328:PHE:HB3	1:B:329:PRO:HD3	1.70	0.73
1:A:413:ILE:HG21	1:A:429:LEU:HD23	1.71	0.73
1:C:798:HIS:CE1	1:C:799:GLU:HG3	2.23	0.73
1:A:658:ILE:O	1:A:662:VAL:HG23	1.89	0.72
1:B:658:ILE:O	1:B:662:VAL:HG23	1.90	0.72
1:B:379:LEU:HB3	1:B:381:GLU:OE2	1.90	0.72
1:B:798:HIS:CE1	1:B:799:GLU:HG3	2.25	0.72
1:C:842:LEU:HA	1:C:852:ASP:HB2	1.72	0.71
1:A:842:LEU:HA	1:A:852:ASP:HB2	1.72	0.71
1:B:842:LEU:HA	1:B:852:ASP:HB2	1.72	0.71
1:C:379:LEU:HB3	1:C:381:GLU:OE2	1.90	0.71
1:C:658:ILE:O	1:C:662:VAL:HG23	1.90	0.71
1:A:752:GLY:H	1:A:775:ASP:HB3	1.56	0.70
1:A:798:HIS:CE1	1:A:799:GLU:HG3	2.25	0.70
1:A:50:LEU:HB3	1:A:127:GLN:NE2	2.07	0.69
1:A:328:PHE:HB3	1:A:329:PRO:CD	2.22	0.69
1:A:379:LEU:HB3	1:A:381:GLU:OE2	1.92	0.69
1:B:413:ILE:HG21	1:B:429:LEU:HD23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HB3	1:B:127:GLN:NE2	2.08	0.68
1:B:752:GLY:H	1:B:775:ASP:HB3	1.57	0.68
1:C:50:LEU:HB3	1:C:127:GLN:NE2	2.08	0.68
1:C:535:ILE:H	1:C:535:ILE:HD12	1.58	0.67
1:B:327:GLU:HA	1:B:330:GLU:HG3	1.75	0.67
1:C:36:HIS:NE2	1:C:63:ASP:OD2	2.25	0.66
1:C:413:ILE:HG21	1:C:429:LEU:HD23	1.76	0.66
1:B:36:HIS:NE2	1:B:63:ASP:OD2	2.25	0.66
1:C:752:GLY:H	1:C:775:ASP:HB3	1.59	0.65
1:C:392:GLN:CA	1:C:399:VAL:HG21	2.27	0.65
1:B:535:ILE:HD12	1:B:535:ILE:H	1.62	0.64
1:B:759:SER:HA	1:B:762:LLP:CD	2.26	0.64
1:A:392:GLN:CA	1:A:399:VAL:HG21	2.28	0.63
1:C:98:LEU:HD23	1:C:101:ILE:HD11	1.80	0.63
1:A:421:ASP:O	1:A:423:ASN:N	2.32	0.63
1:B:666:LYS:HE2	1:B:820:GLU:HG2	1.81	0.63
1:B:775:ASP:O	1:B:778:ASN:HB2	2.00	0.62
1:B:392:GLN:CA	1:B:399:VAL:HG21	2.29	0.62
1:A:663:TYR:CE1	1:A:667:LYS:HE3	2.35	0.62
1:B:745:SER:OG	1:B:770:GLN:HG3	2.00	0.62
1:C:663:TYR:CE1	1:C:667:LYS:HE3	2.35	0.61
1:A:643:ILE:HD12	1:A:742:SER:HB3	1.82	0.60
1:C:643:ILE:HD12	1:C:742:SER:HB3	1.83	0.60
1:C:775:ASP:O	1:C:778:ASN:HB2	2.02	0.60
1:A:775:ASP:O	1:A:778:ASN:HB2	2.01	0.60
1:A:666:LYS:CD	1:A:670:GLU:OE2	2.49	0.60
1:C:328:PHE:HB3	1:C:329:PRO:HD3	1.83	0.60
1:A:745:SER:OG	1:A:770:GLN:HG3	2.02	0.60
1:A:757:GLY:O	1:A:761:MET:HE3	2.01	0.60
1:C:745:SER:OG	1:C:770:GLN:HG3	2.02	0.60
1:C:421:ASP:O	1:C:423:ASN:N	2.36	0.59
1:A:321:ASP:O	1:A:323:ILE:HG22	2.02	0.59
1:A:433:ARG:HH22	1:A:438:PHE:HB3	1.67	0.59
1:C:535:ILE:O	1:C:538:GLU:HB2	2.02	0.59
1:C:440:LEU:H	1:C:440:LEU:HD22	1.67	0.59
1:C:321:ASP:O	1:C:323:ILE:HG22	2.02	0.59
1:C:759:SER:OG	1:C:762:LLP:OP2	2.19	0.59
1:B:421:ASP:O	1:B:423:ASN:N	2.36	0.58
1:C:433:ARG:HH22	1:C:438:PHE:HB3	1.68	0.58
1:A:666:LYS:HE3	1:A:820:GLU:HG2	1.85	0.58
1:B:643:ILE:HD12	1:B:742:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:GLY:O	1:B:761:MET:HE3	2.03	0.58
1:B:424:LYS:HE2	1:B:427:GLU:OE1	2.03	0.58
1:A:174:LYS:HB3	1:B:600:GLN:HE22	1.68	0.58
1:C:368:GLN:HA	1:C:525:GLY:O	2.04	0.58
1:C:858:LYS:O	1:C:861:PRO:HD2	2.04	0.58
1:B:353:ILE:HG22	1:B:354:ASP:OD1	2.04	0.57
1:A:760:ASN:OD1	1:A:760:ASN:N	2.38	0.57
1:B:858:LYS:O	1:B:861:PRO:HD2	2.04	0.57
1:A:353:ILE:HG22	1:A:354:ASP:OD1	2.05	0.57
1:A:368:GLN:HA	1:A:525:GLY:O	2.05	0.57
1:A:413:ILE:HG21	1:A:429:LEU:CD2	2.34	0.57
1:B:165:TYR:HB2	1:B:282:ILE:HG22	1.86	0.56
1:B:433:ARG:HH22	1:B:438:PHE:HB3	1.71	0.56
1:A:165:TYR:HB2	1:A:282:ILE:HG22	1.86	0.56
1:A:535:ILE:O	1:A:538:GLU:HB2	2.06	0.56
1:C:666:LYS:HE2	1:C:820:GLU:HG2	1.87	0.56
1:B:535:ILE:O	1:B:538:GLU:HB2	2.05	0.56
1:C:342:THR:HB	1:C:518:MET:HE3	1.86	0.56
1:C:760:ASN:OD1	1:C:760:ASN:N	2.39	0.56
1:A:858:LYS:O	1:A:861:PRO:HD2	2.05	0.56
1:B:368:GLN:HA	1:B:525:GLY:O	2.04	0.56
1:C:432:MET:HE2	1:C:547:ASP:HB3	1.88	0.56
1:A:658:ILE:HD11	1:A:708:VAL:HG11	1.88	0.55
1:C:353:ILE:HG22	1:C:354:ASP:OD1	2.06	0.55
1:C:658:ILE:HD11	1:C:708:VAL:HG11	1.88	0.55
1:B:321:ASP:O	1:B:323:ILE:HG22	2.05	0.55
1:B:342:THR:HB	1:B:518:MET:HE3	1.87	0.55
1:C:165:TYR:HB2	1:C:282:ILE:HG22	1.87	0.55
1:A:666:LYS:HG3	1:A:667:LYS:HE2	1.89	0.55
1:B:171:ARG:HB2	1:B:171:ARG:CZ	2.35	0.55
1:B:760:ASN:OD1	1:B:760:ASN:N	2.39	0.55
1:B:440:LEU:HD22	1:B:440:LEU:H	1.72	0.55
1:A:432:MET:HE2	1:A:547:ASP:HB3	1.89	0.55
1:A:535:ILE:HD12	1:A:535:ILE:H	1.72	0.54
1:B:98:LEU:HD23	1:B:101:ILE:HD11	1.89	0.54
1:B:563:VAL:HG11	1:B:762:LLP:HG2	1.88	0.54
1:C:23:ALA:N	1:C:24:PRO:HD3	2.23	0.54
1:A:380:PRO:HG3	1:A:544:VAL:HG13	1.89	0.54
1:B:732:VAL:O	1:B:736:GLU:HG3	2.08	0.54
1:A:440:LEU:HD22	1:A:440:LEU:H	1.72	0.54
1:B:413:ILE:HG21	1:B:429:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:732:VAL:O	1:C:736:GLU:HG3	2.08	0.54
1:C:413:ILE:HG21	1:C:429:LEU:CD2	2.37	0.54
1:C:765:MET:HG2	1:C:891:SER:HB3	1.90	0.54
1:B:25:ASP:OD1	1:B:28:SER:N	2.33	0.53
1:A:342:THR:HB	1:A:518:MET:HE3	1.89	0.53
1:B:658:ILE:HD11	1:B:708:VAL:HG11	1.91	0.53
1:C:532:VAL:O	1:C:560:THR:HA	2.09	0.53
1:A:520:ASN:O	1:A:524:VAL:HG23	2.10	0.52
1:B:806:GLU:HG2	1:B:811:LYS:HB2	1.91	0.52
1:A:650:GLU:OE2	1:A:697:GLN:HG2	2.10	0.52
1:B:532:VAL:O	1:B:560:THR:HA	2.09	0.52
1:B:36:HIS:HB3	1:B:59:GLN:HE21	1.74	0.52
1:C:520:ASN:O	1:C:524:VAL:HG23	2.10	0.52
1:C:47:ARG:HB2	1:C:47:ARG:CZ	2.38	0.52
1:A:47:ARG:HB2	1:A:47:ARG:CZ	2.38	0.52
1:A:532:VAL:O	1:A:560:THR:HA	2.09	0.52
1:A:732:VAL:O	1:A:736:GLU:HG3	2.09	0.52
1:C:359:ASN:ND2	1:C:362:GLU:OE1	2.43	0.51
1:C:865:GLU:O	1:C:868:GLU:HB2	2.10	0.51
1:B:50:LEU:HB3	1:B:127:GLN:HE21	1.75	0.51
1:B:650:GLU:OE2	1:B:697:GLN:HG2	2.11	0.51
1:C:336:MET:HB3	1:C:341:PRO:HG2	1.92	0.51
1:C:642:ASP:OD1	1:C:744:LEU:HD23	2.10	0.51
1:B:324:LYS:C	1:B:326:GLU:H	2.19	0.51
1:A:574:PRO:N	1:A:575:PRO:HD2	2.25	0.51
1:A:642:ASP:OD1	1:A:744:LEU:HD23	2.11	0.51
1:B:642:ASP:OD1	1:B:744:LEU:HD23	2.10	0.51
1:C:50:LEU:HB3	1:C:127:GLN:HE21	1.75	0.51
1:A:50:LEU:HB3	1:A:127:GLN:HE21	1.76	0.51
1:B:324:LYS:C	1:B:326:GLU:N	2.68	0.51
1:C:36:HIS:HB3	1:C:59:GLN:HE21	1.74	0.51
1:C:594:GLU:HA	1:C:892:TYR:CD2	2.45	0.51
1:A:36:HIS:HB3	1:A:59:GLN:HE21	1.75	0.50
1:A:98:LEU:HD23	1:A:101:ILE:HD11	1.93	0.50
1:B:520:ASN:O	1:B:524:VAL:HG23	2.11	0.50
1:A:594:GLU:HA	1:A:892:TYR:CD2	2.47	0.50
1:B:392:GLN:HG3	1:B:399:VAL:HG11	1.94	0.50
1:C:650:GLU:OE2	1:C:697:GLN:HG2	2.12	0.50
1:A:100:ALA:O	1:A:104:LEU:HG	2.12	0.50
1:B:574:PRO:N	1:B:575:PRO:HD2	2.27	0.50
1:A:336:MET:HB3	1:A:341:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ASN:ND2	1:B:362:GLU:OE1	2.45	0.50
1:C:574:PRO:N	1:C:575:PRO:HD2	2.26	0.50
1:A:145:PHE:CG	1:A:900:ILE:HD11	2.47	0.49
1:B:145:PHE:CG	1:B:900:ILE:HD11	2.47	0.49
1:C:339:THR:O	1:C:342:THR:OG1	2.30	0.49
1:A:765:MET:HG2	1:A:891:SER:HB3	1.94	0.49
1:A:359:ASN:ND2	1:A:362:GLU:OE1	2.45	0.49
1:A:865:GLU:O	1:A:868:GLU:HB2	2.13	0.49
1:B:336:MET:HB3	1:B:341:PRO:HG2	1.94	0.49
1:C:84:ALA:O	1:C:156:ALA:HA	2.13	0.49
1:B:432:MET:HE2	1:B:547:ASP:HB3	1.95	0.49
1:B:594:GLU:HA	1:B:892:TYR:CD2	2.47	0.49
1:B:865:GLU:O	1:B:868:GLU:HB2	2.13	0.49
1:C:325:TRP:CD1	1:C:358:LEU:HD21	2.48	0.49
1:B:765:MET:HG2	1:B:891:SER:HB3	1.95	0.48
1:C:54:PHE:HA	1:C:124:VAL:HG13	1.94	0.48
1:C:806:GLU:HG2	1:C:811:LYS:HB2	1.95	0.48
1:B:90:GLU:HB2	1:B:134:GLY:HA2	1.95	0.48
1:B:576:LEU:O	1:B:580:ILE:HG13	2.13	0.48
1:B:908:TRP:O	1:B:909:ASN:HB3	2.14	0.48
1:A:695:TYR:CD1	1:A:695:TYR:C	2.92	0.48
1:B:695:TYR:CD1	1:B:695:TYR:C	2.90	0.48
1:B:171:ARG:HG2	1:B:171:ARG:HH11	1.79	0.48
1:C:145:PHE:CG	1:C:900:ILE:HD11	2.48	0.48
1:A:416:LYS:C	1:A:418:GLY:H	2.21	0.48
1:C:695:TYR:CD1	1:C:695:TYR:C	2.91	0.48
1:C:90:GLU:HB2	1:C:134:GLY:HA2	1.95	0.48
1:C:416:LYS:C	1:C:418:GLY:H	2.21	0.48
1:A:90:GLU:HB2	1:A:134:GLY:HA2	1.94	0.48
1:A:305:SER:O	1:A:309:GLN:HG3	2.14	0.48
1:A:806:GLU:HG2	1:A:811:LYS:HB2	1.95	0.48
1:A:153:ASN:HA	1:A:240:THR:HG21	1.96	0.47
1:C:89:MET:HE1	1:C:299:GLN:HB3	1.96	0.47
1:C:908:TRP:O	1:C:909:ASN:HB3	2.14	0.47
1:A:576:LEU:O	1:A:580:ILE:HG13	2.14	0.47
1:C:100:ALA:O	1:C:104:LEU:HG	2.14	0.47
1:A:326:GLU:H	1:A:326:GLU:HG3	1.49	0.47
1:B:695:TYR:C	1:B:695:TYR:HD1	2.23	0.47
1:B:339:THR:O	1:B:342:THR:OG1	2.33	0.47
1:B:620:LYS:NZ	1:B:743:ASP:OD2	2.40	0.47
1:C:120:ASN:HD21	1:C:122:GLU:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:LEU:O	1:C:580:ILE:HG13	2.13	0.47
1:A:84:ALA:O	1:A:156:ALA:HA	2.15	0.47
1:A:744:LEU:HA	1:A:769:ILE:O	2.15	0.47
1:B:911:GLU:O	1:B:912:ALA:C	2.56	0.47
1:C:44:SER:HB3	1:C:45:PRO:HD2	1.97	0.47
1:B:84:ALA:O	1:B:156:ALA:HA	2.14	0.47
1:C:112:GLU:O	1:C:115:LYS:HB2	2.14	0.47
1:A:163:TYR:CZ	1:A:283:LEU:HD13	2.49	0.47
1:A:908:TRP:O	1:A:909:ASN:HB3	2.15	0.47
1:B:153:ASN:HA	1:B:240:THR:HG21	1.96	0.47
1:A:574:PRO:HD2	1:A:575:PRO:HD2	1.97	0.47
1:A:752:GLY:H	1:A:775:ASP:CB	2.26	0.47
1:A:793:PHE:CE2	1:A:863:TYR:HB2	2.50	0.47
1:C:744:LEU:HA	1:C:769:ILE:O	2.14	0.47
1:B:131:ALA:HA	1:B:184:TRP:CE3	2.50	0.47
1:B:163:TYR:CZ	1:B:283:LEU:HD13	2.49	0.47
1:B:194:VAL:HG22	1:B:229:TYR:CE2	2.50	0.47
1:C:380:PRO:HG3	1:C:544:VAL:HG13	1.96	0.47
1:B:416:LYS:C	1:B:418:GLY:H	2.23	0.47
1:B:744:LEU:HA	1:B:769:ILE:O	2.15	0.46
1:C:327:GLU:O	1:C:328:PHE:C	2.57	0.46
1:C:753:MET:HE1	1:C:854:PHE:HE1	1.81	0.46
1:B:340:HIS:HB2	1:B:341:PRO:HD3	1.97	0.46
1:B:39:PHE:C	1:B:41:PRO:HD3	2.40	0.46
1:B:574:PRO:HD2	1:B:575:PRO:HD2	1.97	0.46
1:A:339:THR:O	1:A:342:THR:OG1	2.33	0.46
1:A:540:VAL:HA	1:A:544:VAL:HG23	1.98	0.46
1:B:148:SER:O	1:B:149:LEU:C	2.58	0.46
1:C:163:TYR:CZ	1:C:283:LEU:HD13	2.50	0.46
1:C:97:LEU:HD23	1:C:125:ALA:HA	1.97	0.46
1:C:752:GLY:H	1:C:775:ASP:CB	2.27	0.46
1:B:793:PHE:CE2	1:B:863:TYR:HB2	2.50	0.46
1:C:537:SER:O	1:C:540:VAL:HG22	2.16	0.46
1:C:793:PHE:CE2	1:C:863:TYR:HB2	2.50	0.46
1:C:153:ASN:HA	1:C:240:THR:HG21	1.98	0.46
1:A:535:ILE:HD11	1:A:779:VAL:HG11	1.98	0.45
1:A:620:LYS:NZ	1:A:743:ASP:OD2	2.41	0.45
1:C:389:GLU:OE1	1:C:389:GLU:N	2.38	0.45
1:A:148:SER:O	1:A:149:LEU:C	2.58	0.45
1:A:753:MET:HE1	1:A:854:PHE:HE1	1.81	0.45
1:B:97:LEU:HD23	1:B:125:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLU:OE2	1:C:138:LEU:HB3	2.15	0.45
1:A:803:LEU:HD13	1:A:858:LYS:HG2	1.98	0.45
1:B:682:PRO:HA	1:B:721:LEU:O	2.17	0.45
1:B:803:LEU:HD13	1:B:858:LYS:HG2	1.99	0.45
1:C:648:ILE:HG21	1:C:702:VAL:HG23	1.97	0.45
1:A:392:GLN:HG3	1:A:399:VAL:HG11	1.99	0.45
1:A:194:VAL:HG22	1:A:229:TYR:CE2	2.51	0.45
1:B:648:ILE:HG21	1:B:702:VAL:HG23	1.98	0.45
1:C:148:SER:O	1:C:149:LEU:C	2.59	0.45
1:C:325:TRP:HD1	1:C:358:LEU:HD21	1.80	0.45
1:C:646:LYS:HB3	1:C:646:LYS:HE2	1.73	0.45
1:A:325:TRP:O	1:A:366:ILE:CD1	2.65	0.45
1:A:709:GLY:HA2	1:A:724:VAL:HB	1.98	0.45
1:A:802:GLY:O	1:A:805:LYS:HB3	2.15	0.45
1:B:305:SER:O	1:B:309:GLN:HG3	2.15	0.45
1:A:131:ALA:HA	1:A:184:TRP:CE3	2.52	0.45
1:A:682:PRO:HA	1:A:721:LEU:O	2.16	0.45
1:B:380:PRO:HG3	1:B:544:VAL:HG13	1.99	0.45
1:C:54:PHE:CZ	1:C:128:GLU:HB2	2.52	0.45
1:C:305:SER:O	1:C:309:GLN:HG3	2.15	0.45
1:C:682:PRO:HA	1:C:721:LEU:O	2.16	0.45
1:B:416:LYS:O	1:B:418:GLY:N	2.47	0.45
1:B:588:ASP:HB3	1:B:592:LYS:HD2	1.97	0.45
1:A:603:ALA:HB1	1:A:882:THR:HG23	1.98	0.44
1:C:574:PRO:HD2	1:C:575:PRO:HD2	1.97	0.44
1:C:695:TYR:C	1:C:695:TYR:HD1	2.25	0.44
1:A:178:GLU:OE1	1:B:601:LYS:HE2	2.17	0.44
1:A:537:SER:O	1:A:540:VAL:HG22	2.17	0.44
1:A:574:PRO:CD	1:A:575:PRO:HD2	2.47	0.44
1:C:300:GLN:NE2	1:C:340:HIS:O	2.50	0.44
1:A:300:GLN:NE2	1:A:340:HIS:O	2.50	0.44
1:A:790:PHE:C	1:A:790:PHE:CD1	2.95	0.44
1:B:752:GLY:H	1:B:775:ASP:CB	2.27	0.44
1:C:392:GLN:HG3	1:C:399:VAL:HG11	1.99	0.44
1:B:236:TYR:CE1	1:B:237:LYS:HG3	2.51	0.44
1:B:790:PHE:CD1	1:B:790:PHE:C	2.94	0.44
1:C:803:LEU:HD13	1:C:858:LYS:HG2	1.99	0.44
1:A:39:PHE:C	1:A:41:PRO:HD3	2.41	0.44
1:A:851:ALA:O	1:A:852:ASP:C	2.60	0.44
1:B:160:GLY:O	1:B:246:LEU:HA	2.17	0.44
1:B:540:VAL:HA	1:B:544:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:VAL:HA	1:C:217:TYR:O	2.18	0.44
1:A:658:ILE:HA	1:A:661:ILE:HD12	1.99	0.44
1:B:730:TYR:CE1	1:B:735:ALA:HB2	2.53	0.44
1:B:753:MET:HE2	1:B:753:MET:HB3	1.74	0.44
1:C:574:PRO:CD	1:C:575:PRO:HD2	2.48	0.44
1:A:425:LEU:O	1:A:429:LEU:HG	2.18	0.44
1:C:160:GLY:O	1:C:246:LEU:HA	2.18	0.44
1:C:759:SER:CB	1:C:762:LLP:OP2	2.66	0.44
1:A:120:ASN:HD21	1:A:122:GLU:HG2	1.83	0.44
1:C:39:PHE:C	1:C:41:PRO:HD3	2.43	0.44
1:C:603:ALA:HB1	1:C:882:THR:HG23	1.99	0.44
1:C:709:GLY:HA2	1:C:724:VAL:HB	1.99	0.44
1:A:44:SER:HB3	1:A:45:PRO:HD2	1.98	0.44
1:B:574:PRO:CD	1:B:575:PRO:HD2	2.48	0.44
1:B:709:GLY:HA2	1:B:724:VAL:HB	2.00	0.44
1:C:790:PHE:CD1	1:C:790:PHE:C	2.95	0.44
1:A:860:PHE:HB3	1:A:861:PRO:HD3	1.99	0.43
1:A:695:TYR:C	1:A:695:TYR:HD1	2.25	0.43
1:C:666:LYS:HE3	1:C:820:GLU:OE2	2.18	0.43
1:C:851:ALA:O	1:C:852:ASP:C	2.61	0.43
1:A:97:LEU:HD23	1:A:125:ALA:HA	1.99	0.43
1:C:559:LYS:HE3	1:C:902:GLU:C	2.43	0.43
1:C:802:GLY:O	1:C:805:LYS:HB3	2.18	0.43
1:A:406:ASP:OD2	1:A:435:LEU:HG	2.18	0.43
1:A:664:ARG:HG3	1:A:664:ARG:HH11	1.82	0.43
1:B:171:ARG:CZ	1:B:171:ARG:CB	2.96	0.43
1:B:851:ALA:O	1:B:852:ASP:C	2.61	0.43
1:C:540:VAL:HA	1:C:544:VAL:HG23	2.00	0.43
1:A:184:TRP:CE2	1:A:185:LEU:HG	2.54	0.43
1:C:131:ALA:HA	1:C:184:TRP:CE3	2.52	0.43
1:A:648:ILE:HG21	1:A:702:VAL:HG23	1.99	0.43
1:C:425:LEU:O	1:C:429:LEU:HG	2.19	0.43
1:C:589:TRP:O	1:C:593:THR:HA	2.18	0.43
1:A:646:LYS:HB3	1:A:646:LYS:HE2	1.73	0.43
1:B:300:GLN:NE2	1:B:340:HIS:O	2.51	0.43
1:B:731:ASN:OD1	1:B:731:ASN:C	2.62	0.43
1:A:207:LYS:HD3	1:A:207:LYS:HA	1.64	0.43
1:A:349:MET:SD	1:A:364:TRP:HA	2.59	0.43
1:B:535:ILE:HD11	1:B:779:VAL:HG11	2.00	0.43
1:B:603:ALA:HB1	1:B:882:THR:HG23	2.00	0.43
1:B:646:LYS:HE2	1:B:646:LYS:HB3	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:VAL:HA	1:B:217:TYR:O	2.19	0.43
1:B:537:SER:O	1:B:540:VAL:HG22	2.19	0.43
1:A:89:MET:HE1	1:A:299:GLN:HB3	2.01	0.43
1:C:207:LYS:HD2	1:C:207:LYS:HA	1.77	0.43
1:C:349:MET:SD	1:C:364:TRP:HA	2.59	0.43
1:C:730:TYR:CE1	1:C:735:ALA:HB2	2.54	0.42
1:A:160:GLY:O	1:A:246:LEU:HA	2.18	0.42
1:A:534:GLU:HB2	1:A:535:ILE:HD12	2.00	0.42
1:A:559:LYS:HE3	1:A:902:GLU:C	2.44	0.42
1:A:730:TYR:CE1	1:A:735:ALA:HB2	2.54	0.42
1:B:658:ILE:HA	1:B:661:ILE:HD12	2.01	0.42
1:C:140:ARG:HA	1:C:140:ARG:HD2	1.76	0.42
1:C:194:VAL:HG22	1:C:229:TYR:CE2	2.54	0.42
1:C:340:HIS:HB2	1:C:341:PRO:HD3	2.00	0.42
1:C:598:GLU:O	1:C:601:LYS:HG2	2.20	0.42
1:B:120:ASN:HD21	1:B:122:GLU:HG2	1.84	0.42
1:B:207:LYS:HD3	1:B:207:LYS:HA	1.85	0.42
1:C:626:PHE:CE1	1:C:630:LYS:HG3	2.54	0.42
1:C:731:ASN:OD1	1:C:731:ASN:C	2.62	0.42
1:B:171:ARG:HH11	1:B:171:ARG:CG	2.32	0.42
1:B:860:PHE:HB3	1:B:861:PRO:HD3	2.00	0.42
1:C:184:TRP:CE2	1:C:185:LEU:HG	2.54	0.42
1:A:605:ASN:O	1:A:609:GLN:HG3	2.20	0.42
1:A:208:VAL:HA	1:A:217:TYR:O	2.20	0.42
1:A:392:GLN:HA	1:A:399:VAL:CG2	2.46	0.42
1:B:184:TRP:CE2	1:B:185:LEU:HG	2.54	0.42
1:B:604:ASP:O	1:B:605:ASN:C	2.63	0.42
1:C:604:ASP:O	1:C:605:ASN:C	2.63	0.42
1:C:872:GLU:O	1:C:875:ARG:HB2	2.20	0.42
1:B:44:SER:HB3	1:B:45:PRO:HD2	2.01	0.42
1:B:653:ARG:HG2	1:B:856:VAL:HG22	2.02	0.42
1:C:23:ALA:N	1:C:24:PRO:CD	2.83	0.42
1:C:593:THR:HG22	1:C:593:THR:O	2.19	0.42
1:C:860:PHE:HB3	1:C:861:PRO:HD3	2.00	0.42
1:A:140:ARG:HD2	1:A:140:ARG:HA	1.76	0.42
1:B:54:PHE:CZ	1:B:128:GLU:HB2	2.55	0.42
1:B:392:GLN:CG	1:B:399:VAL:HG11	2.50	0.42
1:B:425:LEU:O	1:B:429:LEU:HG	2.20	0.42
1:B:583:TRP:CD1	1:B:608:LEU:HD13	2.55	0.42
1:C:866:CYS:O	1:C:870:VAL:HG23	2.20	0.42
1:B:349:MET:SD	1:B:364:TRP:HA	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:GLU:OE1	1:B:389:GLU:N	2.37	0.41
1:A:394:LEU:HD23	1:A:395:LEU:HG	2.02	0.41
1:B:216:ARG:HH21	1:B:400:GLU:CD	2.28	0.41
1:B:866:CYS:O	1:B:870:VAL:HG23	2.20	0.41
1:A:626:PHE:CE1	1:A:630:LYS:HG3	2.55	0.41
1:A:216:ARG:HH21	1:A:400:GLU:CD	2.28	0.41
1:A:671:MET:CE	1:A:679:ASN:HD22	2.34	0.41
1:B:559:LYS:HE3	1:B:902:GLU:C	2.44	0.41
1:B:605:ASN:C	1:B:605:ASN:OD1	2.63	0.41
1:A:343:LEU:HD23	1:A:343:LEU:HA	1.91	0.41
1:A:593:THR:HG22	1:A:593:THR:O	2.21	0.41
1:B:872:GLU:O	1:B:875:ARG:HB2	2.20	0.41
1:C:658:ILE:HA	1:C:661:ILE:HD12	2.02	0.41
1:A:54:PHE:CZ	1:A:128:GLU:HB2	2.56	0.41
1:C:699:LYS:NZ	3:C:1101:HOH:O	2.53	0.41
1:B:593:THR:O	1:B:593:THR:HG22	2.20	0.41
1:A:612:TRP:NE1	1:A:884:SER:OG	2.47	0.41
1:A:653:ARG:HG2	1:A:856:VAL:HG22	2.02	0.41
1:A:798:HIS:ND1	1:A:799:GLU:HG3	2.36	0.41
1:A:891:SER:O	1:A:893:LYS:N	2.54	0.41
1:B:60:SER:O	1:B:63:ASP:HB2	2.20	0.41
1:B:534:GLU:HB2	1:B:535:ILE:HD12	2.03	0.41
1:B:664:ARG:HG3	1:B:664:ARG:HH11	1.85	0.41
1:B:891:SER:O	1:B:893:LYS:N	2.54	0.41
1:C:324:LYS:C	1:C:326:GLU:N	2.78	0.41
1:C:392:GLN:HA	1:C:399:VAL:CG2	2.45	0.41
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.90	0.41
1:A:731:ASN:OD1	1:A:731:ASN:C	2.61	0.41
1:A:866:CYS:O	1:A:870:VAL:HG23	2.21	0.41
1:B:731:ASN:O	1:B:732:VAL:C	2.64	0.41
1:C:605:ASN:O	1:C:609:GLN:HG3	2.21	0.41
1:C:653:ARG:HG2	1:C:856:VAL:HG22	2.03	0.41
1:C:810:GLY:HA2	1:C:845:ASN:ND2	2.36	0.41
1:A:328:PHE:CB	1:A:329:PRO:HD3	2.35	0.40
1:A:340:HIS:HB2	1:A:341:PRO:HD3	2.03	0.40
1:A:712:ILE:HG21	1:A:722:LEU:HD23	2.03	0.40
1:B:89:MET:HE1	1:B:299:GLN:HB3	2.04	0.40
1:B:598:GLU:O	1:B:601:LYS:HG2	2.21	0.40
1:C:417:TYR:CD1	1:C:417:TYR:N	2.89	0.40
1:A:162:ARG:HB2	1:A:246:LEU:HB3	2.03	0.40
1:A:643:ILE:HA	1:A:686:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:MET:O	1:A:765:MET:HG3	2.20	0.40
1:A:892:TYR:N	1:A:892:TYR:CD1	2.90	0.40
1:B:140:ARG:HG2	1:B:762:LLP:NZ	2.36	0.40
1:C:535:ILE:HD11	1:C:779:VAL:HG11	2.04	0.40
1:C:731:ASN:O	1:C:732:VAL:C	2.64	0.40
1:A:731:ASN:O	1:A:732:VAL:C	2.64	0.40
1:C:199:SER:HA	1:C:226:ALA:O	2.22	0.40
1:C:394:LEU:HD23	1:C:395:LEU:HG	2.03	0.40
1:C:406:ASP:OD2	1:C:435:LEU:HG	2.22	0.40
1:C:681:VAL:HG13	1:C:871:ASP:OD1	2.22	0.40
1:C:891:SER:O	1:C:893:LYS:N	2.55	0.40
1:A:389:GLU:OE1	1:A:389:GLU:N	2.39	0.40
1:A:604:ASP:O	1:A:605:ASN:C	2.63	0.40
1:B:626:PHE:CE1	1:B:630:LYS:HG3	2.56	0.40
1:C:56:ALA:O	1:C:60:SER:HB2	2.21	0.40

There are no symmetry-related clashes.

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	825/916 (90%)	761 (92%)	59 (7%)	5 (1%)	21	52
1	B	825/916 (90%)	762 (92%)	57 (7%)	6 (1%)	18	49
1	C	825/916 (90%)	765 (93%)	55 (7%)	5 (1%)	21	52
All	All	2475/2748 (90%)	2288 (92%)	171 (7%)	16 (1%)	21	52

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	GLU
1	A	422	LEU

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Mol	Chain	Res	Type
1	B	381	GLU
1	B	422	LEU
1	C	381	GLU
1	C	422	LEU
1	B	322	ARG
1	A	322	ARG
1	B	49	GLU
1	C	322	ARG
1	A	441	PRO
1	A	909	ASN
1	B	441	PRO
1	B	909	ASN
1	C	47	ARG
1	C	441	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	707/786 (90%)	652 (92%)	55 (8%)	11	36
1	B	707/786 (90%)	656 (93%)	51 (7%)	13	40
1	C	707/786 (90%)	658 (93%)	49 (7%)	14	41
All	All	2121/2358 (90%)	1966 (93%)	155 (7%)	13	39

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	55	PHE
1	A	60	SER
1	A	79	LEU
1	A	81	MET
1	A	115	LYS
1	A	130	ASP
1	A	171	ARG

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Mol	Chain	Res	Type
1	A	186	GLU
1	A	199	SER
1	A	207	LYS
1	A	208	VAL
1	A	219	ILE
1	A	238	THR
1	A	248	SER
1	A	251	VAL
1	A	259	SER
1	A	270	CYS
1	A	273	GLN
1	A	275	ASN
1	A	282	ILE
1	A	324	LYS
1	A	326	GLU
1	A	330	GLU
1	A	377	THR
1	A	381	GLU
1	A	392	GLN
1	A	393	LYS
1	A	414	VAL
1	A	415	LEU
1	A	420	MET
1	A	422	LEU
1	A	423	ASN
1	A	430	THR
1	A	431	THR
1	A	440	LEU
1	A	444	VAL
1	A	511	ILE
1	A	544	VAL
1	A	550	GLU
1	A	592	LYS
1	A	596	LEU
1	A	629	GLU
1	A	634	SER
1	A	636	VAL
1	A	647	ARG
1	A	651	TYR
1	A	666	LYS
1	A	667	LYS
1	A	695	TYR

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Mol	Chain	Res	Type
1	A	758	THR
1	A	760	ASN
1	A	787	GLU
1	A	892	TYR
1	A	911	GLU
1	B	46	GLU
1	B	47	ARG
1	B	55	PHE
1	B	60	SER
1	B	79	LEU
1	B	81	MET
1	B	115	LYS
1	B	130	ASP
1	B	171	ARG
1	B	186	GLU
1	B	207	LYS
1	B	208	VAL
1	B	219	ILE
1	B	238	THR
1	B	248	SER
1	B	251	VAL
1	B	259	SER
1	B	270	CYS
1	B	273	GLN
1	B	275	ASN
1	B	282	ILE
1	B	321	ASP
1	B	326	GLU
1	B	330	GLU
1	B	377	THR
1	B	381	GLU
1	B	392	GLN
1	B	414	VAL
1	B	415	LEU
1	B	422	LEU
1	B	424	LYS
1	B	426	GLU
1	B	430	THR
1	B	431	THR
1	B	440	LEU
1	B	444	VAL
1	B	544	VAL

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Mol	Chain	Res	Type
1	B	592	LYS
1	B	596	LEU
1	B	629	GLU
1	B	636	VAL
1	B	647	ARG
1	B	651	TYR
1	B	667	LYS
1	B	695	TYR
1	B	758	THR
1	B	760	ASN
1	B	787	GLU
1	B	805	LYS
1	B	892	TYR
1	B	911	GLU
1	C	47	ARG
1	C	55	PHE
1	C	79	LEU
1	C	81	MET
1	C	115	LYS
1	C	130	ASP
1	C	171	ARG
1	C	186	GLU
1	C	207	LYS
1	C	208	VAL
1	C	212	SER
1	C	219	ILE
1	C	238	THR
1	C	248	SER
1	C	251	VAL
1	C	259	SER
1	C	270	CYS
1	C	273	GLN
1	C	275	ASN
1	C	282	ILE
1	C	326	GLU
1	C	330	GLU
1	C	377	THR
1	C	381	GLU
1	C	392	GLN
1	C	393	LYS
1	C	414	VAL
1	C	415	LEU

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Mol	Chain	Res	Type
1	C	422	LEU
1	C	425	LEU
1	C	430	THR
1	C	431	THR
1	C	440	LEU
1	C	444	VAL
1	C	511	ILE
1	C	527	HIS
1	C	544	VAL
1	C	596	LEU
1	C	629	GLU
1	C	636	VAL
1	C	647	ARG
1	C	651	TYR
1	C	667	LYS
1	C	695	TYR
1	C	758	THR
1	C	760	ASN
1	C	783	GLU
1	C	787	GLU
1	C	892	TYR

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

Mol	Chain	Res	Type
1	A	36	HIS
1	A	59	GLN
1	A	127	GLN
1	A	300	GLN
1	A	361	ASN
1	A	411	HIS
1	A	546	ASN
1	A	747	HIS
1	B	59	GLN
1	B	127	GLN
1	B	300	GLN
1	B	340	HIS
1	B	361	ASN
1	B	546	ASN
1	B	561	ASN
1	B	600	GLN
1	B	747	HIS

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Mol	Chain	Res	Type
1	C	59	GLN
1	C	127	GLN
1	C	273	GLN
1	C	300	GLN
1	C	361	ASN
1	C	411	HIS
1	C	546	ASN
1	C	714	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	A	762	1	23,24,25	0.69	0	25,32,34	0.51	0
1	LLP	B	762	1	23,24,25	0.66	0	25,32,34	0.74	1 (4%)
1	LLP	C	762	1	23,24,25	0.62	0	25,32,34	0.62	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
1	LLP	A	762	1	-	4/16/17/19	0/1/1/1
1	LLP	B	762	1	-	8/16/17/19	0/1/1/1
1	LLP	C	762	1	-	0/16/17/19	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	762	LLP	OP3-P-OP2	2.48	117.09	107.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	762	LLP	C5'-OP4-P-OP1
1	A	762	LLP	C5'-OP4-P-OP2
1	A	762	LLP	C5'-OP4-P-OP3
1	B	762	LLP	C4-C4'-NZ-CE
1	B	762	LLP	C5'-OP4-P-OP1
1	B	762	LLP	C5'-OP4-P-OP2
1	B	762	LLP	C5'-OP4-P-OP3
1	B	762	LLP	CG-CD-CE-NZ
1	B	762	LLP	CD-CE-NZ-C4'
1	B	762	LLP	CE-CD-CG-CB
1	B	762	LLP	CA-CB-CG-CD
1	A	762	LLP	C6-C5-C5'-OP4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	762	LLP	4	0
1	C	762	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
2	GOL	A	1001	-	5,5,5	0.21	0	5,5,5	0.58	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
2	GOL	A	1001	-	-	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	829/916 (90%)	-0.38	0	100	100	36, 36, 36, 36	0
1	B	829/916 (90%)	-0.45	0	100	100	36, 36, 36, 36	0
1	C	829/916 (90%)	-0.32	1 (0%)	92	90	36, 36, 36, 36	0
All	All	2487/2748 (90%)	-0.38	1 (0%)	100	100	36, 36, 36, 36	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	674	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	LLP	B	762	24/25	0.93	0.09	36,36,36,36	0
1	LLP	A	762	24/25	0.95	0.09	36,36,36,36	0
1	LLP	C	762	24/25	0.96	0.06	36,36,36,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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
2	GOL	A	1001	6/6	0.75	0.13	20,20,20,20	0

6.5 Other polymers

There are no such residues in this entry.