



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:19 PM UTC

PDB ID : 4P19 / pdb_00004p19
Title : Closed, apo inward-facing state of the glutamate transporter homologue GltPh
Authors : Verdon, G.; Boudker, O.
Deposited on : 2014-02-25
Resolution : 3.25 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
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

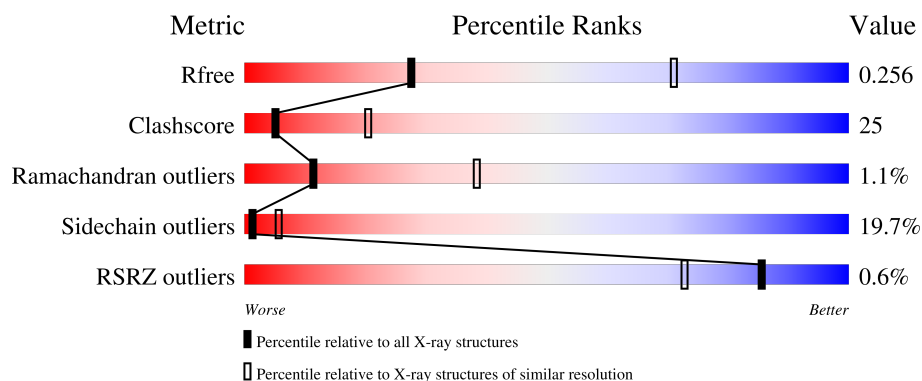
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	422	56%32%9%..
1	B	422	55%31%9%..
1	C	422	56%31%10%..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9124 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 425aa long hypothetical proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3058	2011	493	536	18			
1	B	408	Total	C	N	O	S	0	0	0
			3015	1983	487	527	18			
1	C	413	Total	C	N	O	S	0	0	0
			3048	2003	492	535	18			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	55	CYS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	321	ALA	CYS	engineered mutation	UNP O59010
A	364	CYS	ALA	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	418	THR	-	expression tag	UNP O59010
A	419	LEU	-	expression tag	UNP O59010
A	420	VAL	-	expression tag	UNP O59010
A	421	PRO	-	expression tag	UNP O59010
A	422	ARG	-	expression tag	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	55	CYS	LYS	engineered mutation	UNP O59010
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	321	ALA	CYS	engineered mutation	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	364	CYS	ALA	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
B	418	THR	-	expression tag	UNP O59010
B	419	LEU	-	expression tag	UNP O59010
B	420	VAL	-	expression tag	UNP O59010
B	421	PRO	-	expression tag	UNP O59010
B	422	ARG	-	expression tag	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	55	CYS	LYS	engineered mutation	UNP O59010
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	321	ALA	CYS	engineered mutation	UNP O59010
C	364	CYS	ALA	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	418	THR	-	expression tag	UNP O59010
C	419	LEU	-	expression tag	UNP O59010
C	420	VAL	-	expression tag	UNP O59010
C	421	PRO	-	expression tag	UNP O59010
C	422	ARG	-	expression tag	UNP O59010

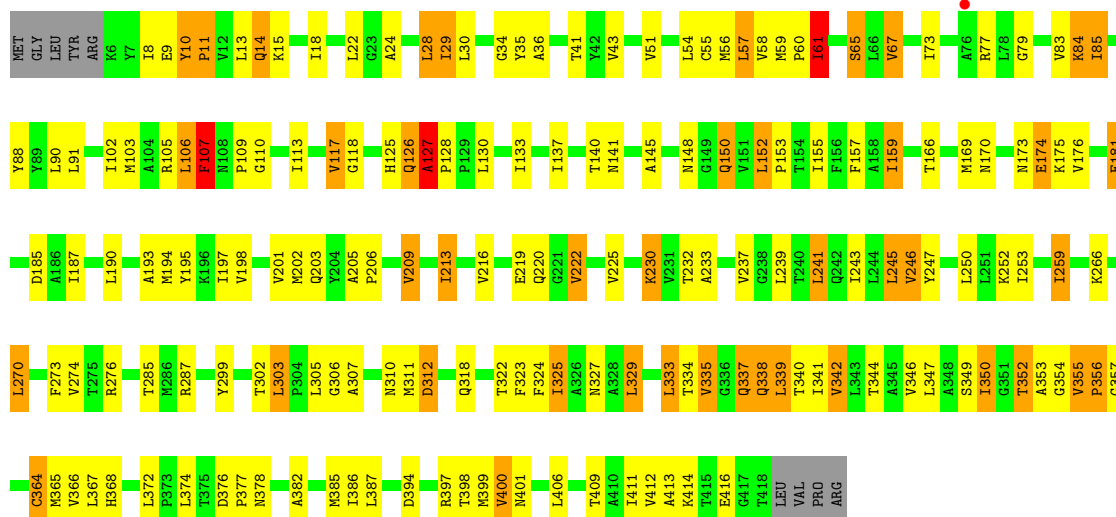
- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Hg 1 1	0	0
2	B	1	Total Hg 1 1	0	0
2	C	1	Total Hg 1 1	0	0



- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain C: 56% 31% 10% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	109.93Å 201.81Å 207.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.25 15.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-3.25) 98.1 (15.00-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.222 , 0.258 0.223 , 0.256	Depositor DCC
R_{free} test set	1803 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	109.9	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9124	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: HG

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	0.72	0/3117	1.20	11/4254 (0.3%)
1	B	0.76	0/3074	1.22	14/4195 (0.3%)
1	C	0.76	1/3107 (0.0%)	1.19	16/4240 (0.4%)
All	All	0.74	1/9298 (0.0%)	1.21	41/12689 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	416	GLU	CA-C	5.23	1.55	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	TYR	N-CA-C	-18.09	91.94	108.22
1	C	342	VAL	N-CA-C	9.92	119.85	110.53
1	A	9	GLU	N-CA-C	-8.40	92.93	107.20
1	C	190	LEU	N-CA-C	-7.14	103.42	111.14
1	B	309	ILE	N-CA-C	6.83	119.60	112.83
1	C	364	CYS	N-CA-C	-6.76	103.60	110.97
1	B	61	ILE	N-CA-CB	6.71	118.40	110.55
1	B	246	VAL	CB-CA-C	-6.66	106.05	111.71
1	B	246	VAL	N-CA-C	6.64	117.72	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	ILE	N-CA-CB	6.61	118.28	110.55
1	C	246	VAL	CB-CA-C	-6.59	106.11	111.71
1	A	8	ILE	CA-C-N	6.33	130.20	121.33
1	A	8	ILE	C-N-CA	6.33	130.20	121.33
1	B	245	LEU	N-CA-C	6.25	119.07	111.82
1	A	309	ILE	N-CA-C	6.12	118.05	112.29
1	A	127	ALA	N-CA-C	-6.00	94.21	111.00
1	C	67	VAL	N-CA-C	-5.99	104.67	110.42
1	B	29	ILE	N-CA-CB	5.99	118.23	110.57
1	C	245	LEU	N-CA-C	5.93	118.70	111.82
1	B	372	LEU	N-CA-C	5.87	122.78	109.81
1	A	117	VAL	N-CA-C	5.73	117.66	111.58
1	A	61	ILE	N-CA-CB	5.53	117.02	110.55
1	B	66	LEU	N-CA-C	5.49	117.27	111.28
1	B	149	GLY	N-CA-C	5.47	126.14	113.18
1	C	117	VAL	N-CA-C	5.47	116.13	110.82
1	B	10	TYR	N-CA-C	-5.46	100.03	108.55
1	B	155	ILE	N-CA-CB	5.38	116.27	110.62
1	C	107	PHE	N-CA-C	-5.38	102.52	110.48
1	C	246	VAL	N-CA-CB	5.38	116.90	111.57
1	A	210	PHE	N-CA-C	-5.25	105.45	111.07
1	C	376	ASP	CA-C-N	5.24	126.39	119.84
1	C	376	ASP	C-N-CA	5.24	126.39	119.84
1	B	257	ASP	CA-C-N	5.22	124.85	119.05
1	B	257	ASP	C-N-CA	5.22	124.85	119.05
1	C	125	HIS	CA-C-N	-5.17	115.71	123.00
1	C	125	HIS	C-N-CA	-5.17	115.71	123.00
1	A	126	GLN	N-CA-C	-5.13	101.95	109.81
1	A	125	HIS	N-CA-C	-5.11	100.40	108.73
1	B	29	ILE	CB-CA-C	-5.08	105.36	112.02
1	C	29	ILE	N-CA-CB	5.05	117.79	110.52
1	C	127	ALA	N-CA-C	5.01	120.88	109.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	126	GLN	Peptide

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	3058	0	3227	157	0
1	B	3015	0	3180	175	0
1	C	3048	0	3209	140	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	9124	0	9616	463	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 25.

All (463) 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:B:355:VAL:CG1	1:B:358:ALA:HB2	1.72	1.18
1:B:349:SER:O	1:B:352:THR:HG23	1.43	1.17
1:A:155:ILE:HD11	1:A:365:MET:HE2	1.22	1.16
1:A:355:VAL:CG1	1:A:358:ALA:HB2	1.75	1.14
1:A:155:ILE:HD11	1:A:365:MET:CE	1.85	1.06
1:B:355:VAL:HG11	1:B:358:ALA:HB2	1.30	1.06
1:B:105:ARG:NH2	1:B:335:VAL:HA	1.70	1.05
1:A:355:VAL:HG11	1:A:358:ALA:HB2	1.11	1.04
1:B:333:LEU:HD13	1:B:337:GLN:HG3	1.38	1.03
1:A:311:MET:HE3	1:A:346:VAL:HG12	1.38	1.02
1:A:333:LEU:HD11	1:A:337:GLN:HB3	1.42	1.02
1:A:61:ILE:O	1:A:65:SER:HB2	1.62	1.00
1:C:333:LEU:CD1	1:C:337:GLN:HB3	1.93	0.98
1:C:333:LEU:HD11	1:C:337:GLN:HB3	1.46	0.97
1:C:61:ILE:O	1:C:65:SER:HB2	1.63	0.96
1:B:333:LEU:CD1	1:B:337:GLN:HG3	1.94	0.96
1:B:155:ILE:HD11	1:B:365:MET:CE	1.97	0.94
1:B:368:HIS:CE1	1:B:374:LEU:HB2	2.03	0.93
1:A:349:SER:O	1:A:352:THR:HG23	1.69	0.92
1:B:105:ARG:HH22	1:B:334:THR:C	1.79	0.90
1:B:57:LEU:O	1:B:61:ILE:HG12	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:MET:HE3	1:B:346:VAL:HG12	1.55	0.89
1:B:368:HIS:HE1	1:B:374:LEU:HB2	1.35	0.89
1:A:57:LEU:O	1:A:61:ILE:HG12	1.73	0.88
1:B:155:ILE:HD11	1:B:365:MET:HE2	1.54	0.87
1:B:145:ALA:HA	1:B:150:GLN:HG3	1.56	0.87
1:A:355:VAL:HG12	1:A:355:VAL:O	1.73	0.86
1:A:105:ARG:HH22	1:A:334:THR:C	1.83	0.86
1:A:10:TYR:HE2	1:A:14:GLN:HB3	1.40	0.86
1:B:355:VAL:HG12	1:B:355:VAL:O	1.75	0.86
1:C:57:LEU:O	1:C:61:ILE:HG12	1.75	0.85
1:B:339:LEU:HD11	1:B:343:LEU:HD11	1.59	0.85
1:C:84:LYS:HD3	1:C:412:VAL:HG23	1.57	0.85
1:C:354:GLY:HA2	1:C:355:VAL:HB	1.58	0.84
1:B:61:ILE:O	1:B:65:SER:HB2	1.76	0.84
1:A:307:ALA:O	1:A:353:ALA:HB3	1.77	0.84
1:C:105:ARG:HH22	1:C:334:THR:C	1.83	0.84
1:A:355:VAL:HG11	1:A:358:ALA:CB	2.04	0.83
1:A:10:TYR:CE2	1:A:14:GLN:HB3	2.14	0.83
1:C:10:TYR:HE2	1:C:14:GLN:HB3	1.39	0.83
1:A:9:GLU:CD	1:A:9:GLU:C	2.47	0.82
1:C:166:THR:HA	1:C:169:MET:HE2	1.61	0.81
1:B:323:PHE:O	1:B:327:ASN:HB2	1.80	0.81
1:A:198:VAL:HG11	1:A:356:PRO:HG2	1.63	0.81
1:A:311:MET:HE3	1:A:346:VAL:CG1	2.10	0.80
1:C:30:LEU:O	1:C:34:GLY:HA3	1.80	0.80
1:B:10:TYR:CG	1:B:11:PRO:HD2	2.18	0.79
1:C:306:GLY:O	1:C:310:ASN:HB2	1.82	0.79
1:B:105:ARG:HH22	1:B:335:VAL:N	1.80	0.78
1:B:355:VAL:HG13	1:B:358:ALA:HB2	1.63	0.78
1:C:349:SER:O	1:C:352:THR:HG23	1.81	0.78
1:B:311:MET:CE	1:B:346:VAL:HG12	2.13	0.78
1:C:198:VAL:HG11	1:C:356:PRO:HG2	1.67	0.77
1:A:420:VAL:HG12	1:A:420:VAL:O	1.84	0.76
1:B:105:ARG:NH2	1:B:335:VAL:CA	2.49	0.76
1:A:333:LEU:HD11	1:A:337:GLN:CB	2.16	0.76
1:B:10:TYR:CE2	1:B:11:PRO:HG2	2.21	0.76
1:B:355:VAL:CG1	1:B:355:VAL:O	2.33	0.75
1:A:155:ILE:CD1	1:A:365:MET:HE2	2.10	0.75
1:C:55:CYS:O	1:C:58:VAL:HG12	1.85	0.75
1:A:299:TYR:HB2	1:A:303:LEU:HD22	1.69	0.75
1:C:145:ALA:HA	1:C:150:GLN:HG3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:HD11	1:B:343:LEU:CD1	2.15	0.74
1:B:355:VAL:CG1	1:B:358:ALA:CB	2.62	0.73
1:B:355:VAL:HG11	1:B:358:ALA:CB	2.14	0.73
1:B:310:ASN:ND2	1:B:401:ASN:HA	2.02	0.73
1:B:370:VAL:HG12	1:B:370:VAL:O	1.88	0.73
1:C:333:LEU:HD13	1:C:337:GLN:HB3	1.71	0.73
1:B:105:ARG:HH22	1:B:335:VAL:HA	1.54	0.73
1:A:323:PHE:O	1:A:327:ASN:HB2	1.89	0.73
1:A:355:VAL:CG1	1:A:355:VAL:O	2.36	0.73
1:A:333:LEU:CD1	1:A:337:GLN:HB3	2.19	0.72
1:B:337:GLN:O	1:B:341:ILE:HG22	1.89	0.71
1:A:107:PHE:HD1	1:A:107:PHE:H	1.35	0.71
1:A:418:THR:O	1:A:419:LEU:HD22	1.91	0.71
1:B:352:THR:O	1:B:355:VAL:HG11	1.91	0.71
1:C:299:TYR:HB2	1:C:303:LEU:HD22	1.70	0.71
1:C:241:LEU:O	1:C:245:LEU:HB2	1.90	0.70
1:B:10:TYR:O	1:B:15:LYS:HE3	1.91	0.70
1:C:57:LEU:HD13	1:C:198:VAL:HG22	1.73	0.70
1:B:85:ILE:HD13	1:B:302:THR:HB	1.72	0.70
1:C:155:ILE:HD11	1:C:365:MET:HE2	1.71	0.70
1:B:198:VAL:HG11	1:B:356:PRO:HG2	1.74	0.70
1:C:198:VAL:HG11	1:C:356:PRO:CG	2.21	0.70
1:B:239:LEU:HG	1:B:400:VAL:HG21	1.72	0.70
1:C:239:LEU:HG	1:C:400:VAL:CG2	2.22	0.70
1:B:354:GLY:HA2	1:B:355:VAL:HG12	1.73	0.70
1:C:10:TYR:CE2	1:C:11:PRO:HG2	2.27	0.70
1:A:105:ARG:HH21	1:A:338:GLN:HG3	1.56	0.69
1:A:333:LEU:CD1	1:A:337:GLN:CB	2.70	0.69
1:B:337:GLN:O	1:B:341:ILE:CG2	2.41	0.69
1:C:198:VAL:CG1	1:C:356:PRO:HG3	2.22	0.69
1:B:56:MET:HE3	1:C:157:PHE:HD1	1.58	0.69
1:B:241:LEU:O	1:B:245:LEU:HB2	1.93	0.69
1:A:54:LEU:HD23	1:A:387:LEU:HD11	1.74	0.69
1:C:155:ILE:HD11	1:C:365:MET:CE	2.23	0.68
1:B:107:PHE:HB3	1:B:230:LYS:HD3	1.75	0.68
1:C:85:ILE:HD13	1:C:302:THR:HB	1.75	0.68
1:B:363:LEU:O	1:B:366:VAL:HG12	1.92	0.68
1:B:250:LEU:O	1:B:253:ILE:HG22	1.93	0.68
1:C:10:TYR:CE2	1:C:14:GLN:HB3	2.26	0.68
1:C:110:GLY:O	1:C:113:ILE:HG22	1.94	0.68
1:B:24:ALA:O	1:B:28:LEU:HB2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:HH22	1:B:335:VAL:CA	2.05	0.67
1:C:323:PHE:O	1:C:327:ASN:HB2	1.94	0.67
1:B:105:ARG:HH21	1:B:338:GLN:HG3	1.60	0.67
1:C:406:LEU:HA	1:C:409:THR:HG22	1.77	0.67
1:A:73:ILE:HD12	1:A:350:ILE:HD12	1.76	0.67
1:A:107:PHE:CD1	1:A:107:PHE:N	2.63	0.66
1:B:54:LEU:HD23	1:B:387:LEU:HD11	1.77	0.66
1:A:217:MET:SD	1:A:224:VAL:CG2	2.84	0.66
1:A:107:PHE:O	1:A:109:PRO:HD3	1.95	0.66
1:A:107:PHE:HZ	1:A:237:VAL:HG21	1.59	0.66
1:B:339:LEU:CD1	1:B:343:LEU:CD1	2.74	0.66
1:B:84:LYS:HD3	1:B:412:VAL:HG23	1.78	0.65
1:C:105:ARG:HH21	1:C:338:GLN:HG3	1.60	0.65
1:C:107:PHE:HD1	1:C:107:PHE:H	1.45	0.65
1:A:57:LEU:HB3	1:A:194:MET:CE	2.26	0.65
1:A:198:VAL:HG11	1:A:356:PRO:CG	2.27	0.65
1:B:174:GLU:OE1	1:B:174:GLU:HA	1.97	0.65
1:B:60:PRO:HB2	1:B:194:MET:HG3	1.79	0.65
1:B:354:GLY:HA2	1:B:355:VAL:CB	2.27	0.64
1:A:10:TYR:HE2	1:A:14:GLN:CB	2.08	0.64
1:B:126:GLN:HB2	1:B:127:ALA:HB2	1.78	0.64
1:A:85:ILE:HD13	1:A:302:THR:HB	1.78	0.64
1:A:20:LEU:HD12	1:A:213:ILE:HG12	1.80	0.63
1:C:364:CYS:SG	1:C:368:HIS:CD2	2.91	0.63
1:C:174:GLU:HA	1:C:174:GLU:OE1	1.98	0.63
1:B:310:ASN:HD21	1:B:401:ASN:HA	1.62	0.63
1:B:10:TYR:HE2	1:B:14:GLN:HB3	1.64	0.63
1:A:150:GLN:HG2	1:A:153:PRO:HG2	1.80	0.63
1:C:202:MET:HE2	1:C:276:ARG:HH22	1.63	0.62
1:A:311:MET:CE	1:A:346:VAL:HG12	2.25	0.62
1:A:10:TYR:CE2	1:A:14:GLN:CB	2.81	0.62
1:C:10:TYR:O	1:C:15:LYS:HE3	1.99	0.62
1:A:217:MET:SD	1:A:224:VAL:HG23	2.40	0.62
1:C:333:LEU:HD13	1:C:337:GLN:CB	2.29	0.62
1:C:239:LEU:HG	1:C:400:VAL:HG21	1.80	0.61
1:B:74:SER:HB3	1:B:166:THR:HG21	1.82	0.61
1:B:107:PHE:HD1	1:B:107:PHE:H	1.48	0.61
1:C:10:TYR:CG	1:C:11:PRO:HD2	2.35	0.61
1:B:107:PHE:O	1:B:109:PRO:HD3	2.01	0.61
1:A:310:ASN:ND2	1:A:401:ASN:HA	2.16	0.61
1:B:237:VAL:O	1:B:241:LEU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:PHE:CZ	1:A:237:VAL:HG21	2.35	0.61
1:B:339:LEU:CD1	1:B:343:LEU:HG	2.31	0.61
1:A:406:LEU:HA	1:A:409:THR:HG22	1.81	0.61
1:A:354:GLY:HA2	1:A:355:VAL:O	2.01	0.61
1:C:85:ILE:O	1:C:88:TYR:HB3	2.00	0.61
1:C:307:ALA:O	1:C:353:ALA:HB3	2.01	0.61
1:A:337:GLN:O	1:A:341:ILE:HD12	2.00	0.60
1:C:198:VAL:HB	1:C:356:PRO:HG3	1.83	0.60
1:C:30:LEU:O	1:C:34:GLY:CA	2.49	0.60
1:C:24:ALA:O	1:C:28:LEU:HB2	2.02	0.60
1:C:51:VAL:O	1:C:55:CYS:SG	2.58	0.60
1:C:117:VAL:CG2	1:C:377:PRO:HB2	2.32	0.60
1:A:30:LEU:O	1:A:34:GLY:HA3	2.01	0.60
1:A:311:MET:CE	1:A:346:VAL:CG1	2.80	0.60
1:B:202:MET:HE2	1:B:276:ARG:HH12	1.67	0.60
1:B:310:ASN:HD22	1:B:401:ASN:CG	2.09	0.60
1:A:202:MET:HE2	1:A:276:ARG:HH22	1.67	0.60
1:B:307:ALA:O	1:B:353:ALA:HB3	2.01	0.59
1:C:84:LYS:HD3	1:C:412:VAL:CG2	2.29	0.59
1:C:198:VAL:CG1	1:C:356:PRO:CG	2.79	0.59
1:A:14:GLN:O	1:A:18:ILE:HG12	2.02	0.59
1:B:217:MET:SD	1:B:224:VAL:HG21	2.41	0.59
1:B:312:ASP:N	1:B:312:ASP:OD2	2.26	0.59
1:C:79:GLY:O	1:C:83:VAL:HG23	2.02	0.59
1:A:51:VAL:O	1:A:55:CYS:SG	2.60	0.59
1:A:98:THR:HG22	1:A:102:ILE:HD12	1.85	0.59
1:A:312:ASP:OD2	1:A:312:ASP:N	2.33	0.59
1:B:239:LEU:HG	1:B:400:VAL:CG2	2.32	0.59
1:B:354:GLY:HA2	1:B:355:VAL:O	2.03	0.59
1:A:103:MET:HA	1:A:103:MET:HE2	1.84	0.58
1:A:364:CYS:SG	1:A:368:HIS:CD2	2.97	0.58
1:C:107:PHE:CD1	1:C:107:PHE:N	2.70	0.58
1:A:336:GLY:HA2	1:A:339:LEU:HD11	1.85	0.58
1:B:354:GLY:HA2	1:B:355:VAL:CG1	2.33	0.58
1:A:266:LYS:HA	1:A:269:MET:HE2	1.85	0.58
1:A:105:ARG:NH2	1:A:338:GLN:HG3	2.19	0.58
1:C:312:ASP:OD2	1:C:312:ASP:N	2.35	0.57
1:A:217:MET:SD	1:A:224:VAL:HG21	2.43	0.57
1:B:14:GLN:O	1:B:18:ILE:HG12	2.04	0.57
1:B:193:ALA:O	1:B:197:ILE:HG13	2.05	0.57
1:A:174:GLU:HA	1:A:174:GLU:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HD13	1:B:198:VAL:HG22	1.87	0.57
1:A:250:LEU:O	1:A:253:ILE:HG22	2.05	0.56
1:B:79:GLY:O	1:B:83:VAL:HG23	2.05	0.56
1:C:14:GLN:O	1:C:18:ILE:HG12	2.05	0.56
1:A:24:ALA:O	1:A:28:LEU:HB2	2.05	0.56
1:B:166:THR:HA	1:B:169:MET:HE2	1.86	0.56
1:A:141:ASN:OD1	1:A:141:ASN:C	2.48	0.56
1:C:216:VAL:O	1:C:220:GLN:HB2	2.06	0.56
1:B:54:LEU:CD2	1:B:387:LEU:HD11	2.36	0.56
1:B:25:ILE:O	1:B:29:ILE:HG12	2.05	0.56
1:B:339:LEU:HD13	1:B:343:LEU:HG	1.86	0.56
1:A:198:VAL:HB	1:A:356:PRO:HG3	1.87	0.55
1:B:318:GLN:O	1:B:322:THR:HB	2.05	0.55
1:A:243:ILE:HA	1:A:247:TYR:CD2	2.42	0.55
1:B:155:ILE:HD11	1:B:365:MET:HE3	1.86	0.55
1:B:212:LEU:HD11	1:B:387:LEU:HD23	1.88	0.55
1:B:266:LYS:HA	1:B:269:MET:HE2	1.88	0.55
1:B:61:ILE:HG23	1:B:194:MET:HB3	1.88	0.55
1:B:212:LEU:HD22	1:B:384:ALA:HB1	1.88	0.55
1:C:61:ILE:O	1:C:65:SER:CB	2.47	0.55
1:A:241:LEU:O	1:A:245:LEU:HB2	2.07	0.55
1:A:115:LEU:HD23	1:A:328:ALA:O	2.05	0.55
1:C:354:GLY:CA	1:C:355:VAL:HB	2.32	0.55
1:C:354:GLY:HA2	1:C:355:VAL:CB	2.27	0.55
1:A:420:VAL:O	1:A:420:VAL:CG1	2.54	0.55
1:B:107:PHE:CD1	1:B:107:PHE:N	2.75	0.55
1:A:237:VAL:O	1:A:241:LEU:HB2	2.07	0.55
1:B:28:LEU:HD11	1:B:222:VAL:HG22	1.88	0.55
1:B:105:ARG:NH2	1:B:338:GLN:HG3	2.20	0.55
1:B:30:LEU:O	1:B:34:GLY:HA3	2.07	0.54
1:C:354:GLY:HA2	1:C:355:VAL:O	2.08	0.54
1:A:157:PHE:HD1	1:C:56:MET:HE3	1.73	0.54
1:A:165:ILE:HG21	1:A:184:LEU:HB2	1.87	0.54
1:B:406:LEU:HA	1:B:409:THR:HG22	1.89	0.54
1:B:18:ILE:O	1:B:22:LEU:HB2	2.08	0.53
1:B:20:LEU:HD12	1:B:213:ILE:HG12	1.89	0.53
1:C:239:LEU:HG	1:C:400:VAL:HG23	1.88	0.53
1:C:216:VAL:HG11	1:C:385:MET:HG2	1.91	0.53
1:B:10:TYR:CD1	1:B:11:PRO:HD2	2.43	0.53
1:B:299:TYR:HB2	1:B:303:LEU:HD22	1.91	0.53
1:A:107:PHE:HB3	1:A:230:LYS:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:O	1:A:65:SER:CB	2.49	0.53
1:A:10:TYR:CE2	1:A:11:PRO:HG2	2.44	0.52
1:A:333:LEU:HD12	1:A:337:GLN:HB2	1.91	0.52
1:B:338:GLN:O	1:B:342:VAL:HG23	2.09	0.52
1:B:217:MET:SD	1:B:224:VAL:CG2	2.97	0.52
1:B:333:LEU:HD11	1:B:337:GLN:HG3	1.89	0.52
1:A:333:LEU:CD1	1:A:337:GLN:HB2	2.39	0.52
1:B:354:GLY:CA	1:B:355:VAL:HB	2.40	0.52
1:A:409:THR:HA	1:A:412:VAL:HG12	1.91	0.52
1:B:333:LEU:HD13	1:B:337:GLN:CG	2.26	0.52
1:A:57:LEU:HD13	1:A:198:VAL:HG22	1.90	0.52
1:A:335:VAL:O	1:A:339:LEU:HG	2.10	0.52
1:C:77:ARG:NH1	1:C:170:ASN:OD1	2.43	0.51
1:C:198:VAL:CB	1:C:356:PRO:HG3	2.39	0.51
1:A:54:LEU:C	1:A:56:MET:H	2.15	0.51
1:C:364:CYS:SG	1:C:368:HIS:NE2	2.84	0.51
1:C:194:MET:O	1:C:198:VAL:HG23	2.11	0.51
1:B:306:GLY:O	1:B:310:ASN:HB2	2.10	0.51
1:C:141:ASN:C	1:C:141:ASN:OD1	2.54	0.51
1:C:222:VAL:O	1:C:225:VAL:HG12	2.11	0.51
1:B:25:ILE:HG22	1:B:29:ILE:HD11	1.93	0.50
1:B:155:ILE:CD1	1:B:365:MET:HE2	2.35	0.50
1:A:198:VAL:CG1	1:A:356:PRO:CG	2.89	0.50
1:B:198:VAL:HB	1:B:356:PRO:HG3	1.93	0.50
1:C:117:VAL:HG22	1:C:378:ASN:CG	2.37	0.50
1:C:202:MET:HE2	1:C:276:ARG:NH2	2.27	0.50
1:A:130:LEU:HA	1:A:133:ILE:HG22	1.92	0.50
1:C:409:THR:O	1:C:413:ALA:HB2	2.11	0.50
1:B:13:LEU:O	1:B:14:GLN:C	2.53	0.50
1:B:26:VAL:HG12	1:B:30:LEU:HD12	1.94	0.50
1:A:222:VAL:O	1:A:225:VAL:HG12	2.12	0.49
1:A:370:VAL:HG12	1:A:370:VAL:O	2.12	0.49
1:C:339:LEU:HD12	1:C:340:THR:H	1.77	0.49
1:A:79:GLY:O	1:A:83:VAL:HG23	2.12	0.49
1:C:105:ARG:NH2	1:C:338:GLN:HG3	2.27	0.49
1:B:10:TYR:O	1:B:11:PRO:C	2.55	0.49
1:C:103:MET:HA	1:C:103:MET:HE2	1.95	0.49
1:C:311:MET:HE2	1:C:346:VAL:HG12	1.93	0.49
1:B:105:ARG:NH2	1:B:335:VAL:N	2.56	0.49
1:C:364:CYS:O	1:C:365:MET:C	2.56	0.49
1:A:198:VAL:CG1	1:A:356:PRO:HG3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:VAL:O	1:B:225:VAL:HG12	2.13	0.49
1:C:233:ALA:O	1:C:237:VAL:HG22	2.13	0.48
1:B:343:LEU:O	1:B:347:LEU:HB2	2.13	0.48
1:B:354:GLY:CA	1:B:355:VAL:CB	2.90	0.48
1:C:338:GLN:O	1:C:342:VAL:HG23	2.13	0.48
1:A:59:MET:HB2	1:A:60:PRO:HD3	1.95	0.48
1:C:113:ILE:HG23	1:C:113:ILE:O	2.13	0.48
1:C:237:VAL:O	1:C:241:LEU:HB2	2.13	0.48
1:B:56:MET:HE3	1:C:157:PHE:CD1	2.45	0.48
1:A:306:GLY:O	1:A:310:ASN:HB2	2.14	0.48
1:B:137:ILE:O	1:B:153:PRO:HA	2.14	0.48
1:C:318:GLN:O	1:C:322:THR:HB	2.14	0.48
1:A:188:ASN:ND2	1:B:175:LYS:HE3	2.28	0.48
1:C:10:TYR:OH	1:C:14:GLN:HG2	2.14	0.48
1:C:15:LYS:HB3	1:C:206:PRO:HB3	1.96	0.48
1:B:157:PHE:HA	1:B:160:ILE:HG22	1.96	0.48
1:C:303:LEU:HD11	1:C:409:THR:HG21	1.95	0.48
1:A:57:LEU:O	1:A:61:ILE:CG1	2.56	0.47
1:B:28:LEU:HD21	1:B:222:VAL:HG13	1.95	0.47
1:B:188:ASN:HD21	1:C:175:LYS:HE3	1.79	0.47
1:A:244:LEU:O	1:A:248:PHE:HB2	2.15	0.47
1:A:355:VAL:CG1	1:A:358:ALA:CB	2.69	0.47
1:C:107:PHE:HZ	1:C:237:VAL:HG21	1.80	0.47
1:C:325:ILE:HG12	1:C:386:ILE:HD12	1.97	0.47
1:A:54:LEU:C	1:A:56:MET:N	2.73	0.47
1:B:126:GLN:CB	1:B:127:ALA:HB2	2.44	0.47
1:B:198:VAL:CG1	1:B:356:PRO:CG	2.93	0.47
1:A:242:GLN:O	1:A:246:VAL:HG23	2.14	0.47
1:B:110:GLY:O	1:B:113:ILE:HG22	2.15	0.47
1:C:61:ILE:HG23	1:C:194:MET:HB3	1.95	0.47
1:C:364:CYS:O	1:C:367:LEU:N	2.48	0.47
1:B:107:PHE:HZ	1:B:237:VAL:HG21	1.80	0.47
1:B:349:SER:C	1:B:352:THR:HG23	2.32	0.47
1:B:64:ALA:HB2	1:B:190:LEU:HD23	1.96	0.47
1:B:115:LEU:HD23	1:B:328:ALA:O	2.13	0.47
1:B:337:GLN:O	1:B:341:ILE:HG23	2.14	0.47
1:C:67:VAL:HG11	1:C:187:ILE:HD13	1.98	0.46
1:A:8:ILE:HG23	1:A:15:LYS:NZ	2.30	0.46
1:A:194:MET:O	1:A:198:VAL:HG23	2.15	0.46
1:B:352:THR:O	1:B:352:THR:OG1	2.28	0.46
1:A:141:ASN:ND2	1:C:59:MET:HG3	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:MET:HA	1:A:177:ARG:HG3	1.97	0.46
1:B:263:LYS:HA	1:B:266:LYS:HD2	1.96	0.46
1:B:339:LEU:CD1	1:B:343:LEU:CG	2.93	0.46
1:C:270:LEU:O	1:C:274:VAL:HG23	2.15	0.46
1:C:105:ARG:NH2	1:C:335:VAL:HA	2.30	0.46
1:B:85:ILE:O	1:B:88:TYR:HB3	2.16	0.46
1:B:107:PHE:CZ	1:B:237:VAL:HG21	2.50	0.46
1:C:181:GLU:O	1:C:185:ASP:HB2	2.15	0.46
1:B:205:ALA:N	1:B:206:PRO:HD2	2.30	0.46
1:B:212:LEU:O	1:B:216:VAL:HG23	2.16	0.46
1:B:370:VAL:O	1:B:370:VAL:CG1	2.59	0.46
1:C:243:ILE:HA	1:C:247:TYR:CD2	2.49	0.46
1:C:117:VAL:HG23	1:C:377:PRO:HB2	1.97	0.46
1:A:11:PRO:HB2	1:A:14:GLN:NE2	2.30	0.46
1:A:299:TYR:O	1:A:303:LEU:HB2	2.15	0.46
1:A:409:THR:O	1:A:413:ALA:HB2	2.16	0.46
1:A:10:TYR:OH	1:A:14:GLN:HG2	2.15	0.46
1:B:198:VAL:CG1	1:B:356:PRO:HG2	2.43	0.46
1:C:117:VAL:HG23	1:C:118:GLY:N	2.30	0.46
1:C:273:PHE:HB2	1:C:399:MET:HG3	1.98	0.46
1:A:336:GLY:O	1:A:339:LEU:HD12	2.15	0.45
1:C:329:LEU:HD23	1:C:372:LEU:HD21	1.98	0.45
1:A:198:VAL:CB	1:A:356:PRO:HG3	2.46	0.45
1:B:305:LEU:HD23	1:B:309:ILE:HD11	1.97	0.45
1:B:198:VAL:HG11	1:B:356:PRO:CG	2.45	0.45
1:C:51:VAL:HG22	1:C:387:LEU:HD23	1.97	0.45
1:A:276:ARG:HD2	1:A:394:ASP:HB3	1.99	0.45
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.76	0.45
1:B:54:LEU:C	1:B:56:MET:H	2.24	0.45
1:B:205:ALA:O	1:B:209:VAL:HB	2.16	0.45
1:A:17:LEU:HD22	1:A:392:ILE:CD1	2.47	0.45
1:A:105:ARG:NH2	1:A:335:VAL:HA	2.32	0.45
1:B:391:ALA:O	1:B:395:MET:HG3	2.17	0.45
1:A:193:ALA:O	1:A:197:ILE:HG13	2.16	0.45
1:A:251:LEU:HD22	1:A:256:ILE:HG21	1.99	0.45
1:C:107:PHE:O	1:C:109:PRO:HD3	2.17	0.45
1:B:134:LEU:O	1:B:137:ILE:HG12	2.17	0.45
1:B:181:GLU:O	1:B:185:ASP:HB2	2.17	0.45
1:B:339:LEU:CD1	1:B:339:LEU:C	2.90	0.45
1:C:311:MET:HB3	1:C:346:VAL:HG13	1.97	0.45
1:C:59:MET:HB2	1:C:60:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:VAL:O	1:C:213:ILE:HG13	2.17	0.45
1:A:278:SER:HB3	1:A:307:ALA:HA	1.98	0.44
1:A:339:LEU:HG	1:A:339:LEU:H	1.60	0.44
1:B:55:CYS:O	1:B:58:VAL:HG12	2.17	0.44
1:B:352:THR:O	1:B:355:VAL:CG1	2.63	0.44
1:A:310:ASN:HD21	1:A:401:ASN:HA	1.82	0.44
1:C:213:ILE:HG13	1:C:213:ILE:H	1.64	0.44
1:C:325:ILE:HD13	1:C:382:ALA:HB1	1.98	0.44
1:B:224:VAL:HG12	1:B:385:MET:HE1	2.00	0.44
1:C:107:PHE:CZ	1:C:237:VAL:HG21	2.53	0.44
1:A:213:ILE:H	1:A:213:ILE:HG13	1.65	0.44
1:B:98:THR:O	1:B:102:ILE:HB	2.18	0.44
1:B:202:MET:HE2	1:B:276:ARG:HH22	1.82	0.44
1:C:311:MET:HE2	1:C:346:VAL:CG1	2.48	0.44
1:A:57:LEU:HB3	1:A:194:MET:HE2	1.99	0.44
1:B:67:VAL:HG11	1:B:187:ILE:HD13	2.00	0.44
1:C:193:ALA:O	1:C:197:ILE:HG13	2.17	0.44
1:C:195:TYR:CE1	1:C:355:VAL:HG22	2.53	0.44
1:C:51:VAL:HG22	1:C:387:LEU:CD2	2.47	0.44
1:C:173:ASN:HB3	1:C:176:VAL:HB	2.00	0.44
1:C:325:ILE:HG21	1:C:367:LEU:HD21	1.99	0.44
1:A:93:SER:OG	1:A:311:MET:HB2	2.18	0.43
1:B:10:TYR:CE2	1:B:14:GLN:HB3	2.48	0.43
1:A:325:ILE:HA	1:A:325:ILE:HD13	1.74	0.43
1:A:15:LYS:NZ	1:A:203:GLN:OE1	2.51	0.43
1:A:241:LEU:HD23	1:A:245:LEU:HD23	2.00	0.43
1:A:303:LEU:HD11	1:A:409:THR:HG21	2.00	0.43
1:B:10:TYR:CD2	1:B:11:PRO:HG2	2.53	0.43
1:C:155:ILE:O	1:C:159:ILE:HD12	2.18	0.43
1:C:205:ALA:N	1:C:206:PRO:HD2	2.33	0.43
1:A:57:LEU:HB3	1:A:194:MET:HE3	2.00	0.43
1:A:263:LYS:HA	1:A:266:LYS:HD2	2.01	0.43
1:B:54:LEU:C	1:B:56:MET:N	2.76	0.43
1:A:248:PHE:HZ	1:A:262:ILE:HG13	1.84	0.43
1:B:63:PHE:O	1:B:67:VAL:HG23	2.18	0.43
1:B:243:ILE:HA	1:B:247:TYR:CD2	2.53	0.43
1:C:250:LEU:HA	1:C:253:ILE:HG22	2.01	0.43
1:A:202:MET:HE2	1:A:276:ARG:NH2	2.34	0.43
1:B:190:LEU:O	1:B:194:MET:HG2	2.19	0.43
1:A:74:SER:HB3	1:A:166:THR:HG21	2.01	0.43
1:B:104:ALA:O	1:B:107:PHE:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:THR:HG23	1:B:341:ILE:HD11	2.00	0.43
1:C:107:PHE:HB3	1:C:230:LYS:HD3	2.00	0.43
1:C:117:VAL:HG21	1:C:377:PRO:C	2.44	0.43
1:C:310:ASN:ND2	1:C:401:ASN:HA	2.33	0.43
1:C:155:ILE:HD11	1:C:365:MET:HE3	2.01	0.43
1:A:98:THR:O	1:A:102:ILE:HB	2.19	0.42
1:A:310:ASN:HD22	1:A:401:ASN:CG	2.27	0.42
1:B:16:ILE:HG21	1:B:391:ALA:HB2	2.01	0.42
1:C:127:ALA:HA	1:C:128:PRO:HD3	1.71	0.42
1:A:55:CYS:O	1:A:58:VAL:HG12	2.18	0.42
1:A:178:LYS:HD3	1:C:185:ASP:OD1	2.19	0.42
1:B:339:LEU:C	1:B:339:LEU:HD12	2.45	0.42
1:C:10:TYR:CE2	1:C:14:GLN:CB	3.00	0.42
1:C:130:LEU:HA	1:C:133:ILE:HG22	2.00	0.42
1:A:166:THR:HA	1:A:169:MET:HE2	2.00	0.42
1:A:141:ASN:HA	1:A:142:PRO:HD3	1.84	0.42
1:B:352:THR:O	1:B:353:ALA:C	2.62	0.42
1:B:80:ARG:HG3	1:B:81:VAL:H	1.85	0.42
1:B:329:LEU:HD12	1:B:329:LEU:HA	1.88	0.42
1:B:77:ARG:NH1	1:B:170:ASN:OD1	2.53	0.42
1:B:242:GLN:O	1:B:246:VAL:HG23	2.19	0.42
1:B:322:THR:CG2	1:B:341:ILE:HD11	2.49	0.42
1:A:75:PRO:HA	1:A:76:ALA:HA	1.73	0.42
1:A:137:ILE:O	1:A:153:PRO:HA	2.19	0.42
1:C:356:PRO:HG2	1:C:357:GLY:H	1.85	0.42
1:B:29:ILE:HG12	1:B:29:ILE:H	1.70	0.42
1:A:10:TYR:CD2	1:A:10:TYR:C	2.98	0.42
1:A:168:LEU:HD11	1:C:193:ALA:HA	2.01	0.42
1:A:181:GLU:O	1:A:185:ASP:HB2	2.20	0.42
1:B:310:ASN:ND2	1:B:401:ASN:OD1	2.53	0.42
1:B:10:TYR:CD2	1:B:10:TYR:C	2.98	0.41
1:B:311:MET:HE2	1:B:346:VAL:CG1	2.50	0.41
1:C:197:ILE:O	1:C:201:VAL:HG23	2.20	0.41
1:C:324:PHE:HD2	1:C:386:ILE:HD11	1.85	0.41
1:A:303:LEU:HD12	1:A:303:LEU:HA	1.82	0.41
1:B:209:VAL:O	1:B:213:ILE:HG13	2.19	0.41
1:A:157:PHE:CD1	1:C:56:MET:HE3	2.55	0.41
1:C:152:LEU:HD12	1:C:152:LEU:HA	1.85	0.41
1:C:335:VAL:O	1:C:339:LEU:HG	2.20	0.41
1:A:126:GLN:HB2	1:A:127:ALA:HB2	2.01	0.41
1:B:241:LEU:HD23	1:B:245:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:MET:HE2	1:B:294:ILE:HD11	2.01	0.41
1:C:106:LEU:HD22	1:C:106:LEU:HA	1.88	0.41
1:B:35:TYR:HB2	1:B:38:ALA:HB3	2.02	0.41
1:C:113:ILE:O	1:C:113:ILE:CG2	2.68	0.41
1:C:155:ILE:CD1	1:C:365:MET:HE2	2.46	0.41
1:A:129:PRO:O	1:A:130:LEU:C	2.64	0.41
1:A:236:TYR:O	1:A:240:THR:HG23	2.20	0.41
1:A:259:ILE:H	1:A:259:ILE:HG13	1.75	0.41
1:B:57:LEU:HB3	1:B:194:MET:CE	2.51	0.41
1:A:28:LEU:HD21	1:A:222:VAL:HG13	2.02	0.41
1:A:61:ILE:HG23	1:A:194:MET:HB3	2.03	0.41
1:B:325:ILE:HA	1:B:325:ILE:HD13	1.85	0.41
1:B:337:GLN:H	1:B:337:GLN:HG2	1.54	0.41
1:C:259:ILE:H	1:C:259:ILE:HG13	1.74	0.41
1:A:54:LEU:CD2	1:A:387:LEU:HD11	2.47	0.41
1:A:134:LEU:O	1:A:137:ILE:HG12	2.20	0.41
1:A:205:ALA:O	1:A:209:VAL:HB	2.20	0.41
1:B:103:MET:SD	1:B:237:VAL:HG23	2.60	0.41
1:B:173:ASN:HB3	1:B:176:VAL:HB	2.02	0.41
1:C:61:ILE:HG12	1:C:61:ILE:H	1.78	0.41
1:A:73:ILE:O	1:A:73:ILE:HG22	2.20	0.41
1:A:88:TYR:O	1:A:92:THR:HG23	2.21	0.41
1:A:212:LEU:HD11	1:A:387:LEU:HD23	2.02	0.41
1:C:105:ARG:HH22	1:C:335:VAL:N	2.19	0.40
1:A:11:PRO:HB2	1:A:14:GLN:HB2	2.03	0.40
1:A:17:LEU:CD2	1:A:392:ILE:HD13	2.51	0.40
1:A:25:ILE:O	1:A:29:ILE:HG12	2.21	0.40
1:A:352:THR:O	1:A:355:VAL:HG11	2.21	0.40
1:C:35:TYR:O	1:C:36:ALA:C	2.64	0.40
1:C:73:ILE:HD12	1:C:350:ILE:HD12	2.02	0.40
1:C:137:ILE:O	1:C:153:PRO:HA	2.21	0.40
1:B:10:TYR:CG	1:B:11:PRO:CD	2.96	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	412/422 (98%)	369 (90%)	39 (10%)	4 (1%)	12	40
1	B	406/422 (96%)	376 (93%)	25 (6%)	5 (1%)	10	36
1	C	411/422 (97%)	382 (93%)	25 (6%)	4 (1%)	12	40
All	All	1229/1266 (97%)	1127 (92%)	89 (7%)	13 (1%)	11	38

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	356	PRO
1	C	127	ALA
1	B	255	GLY
1	A	11	PRO
1	B	149	GLY
1	A	255	GLY
1	A	355	VAL
1	A	356	PRO
1	B	355	VAL
1	C	355	VAL
1	C	356	PRO
1	B	11	PRO
1	C	11	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	322/330 (98%)	260 (81%)	62 (19%)	1	6
1	B	317/330 (96%)	257 (81%)	60 (19%)	1	6
1	C	320/330 (97%)	253 (79%)	67 (21%)	1	5
All	All	959/990 (97%)	770 (80%)	189 (20%)	1	6

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	9	GLU
1	A	10	TYR
1	A	13	LEU
1	A	14	GLN
1	A	28	LEU
1	A	41	THR
1	A	54	LEU
1	A	55	CYS
1	A	57	LEU
1	A	61	ILE
1	A	62	VAL
1	A	65	SER
1	A	81	VAL
1	A	84	LYS
1	A	85	ILE
1	A	90	LEU
1	A	102	ILE
1	A	106	LEU
1	A	107	PHE
1	A	125	HIS
1	A	148	ASN
1	A	150	GLN
1	A	152	LEU
1	A	155	ILE
1	A	159	ILE
1	A	174	GLU
1	A	203	GLN
1	A	209	VAL
1	A	213	ILE
1	A	225	VAL
1	A	232	THR
1	A	239	LEU
1	A	241	LEU
1	A	246	VAL
1	A	252	LYS
1	A	259	ILE
1	A	266	LYS
1	A	270	LEU
1	A	279	SER
1	A	303	LEU
1	A	305	LEU

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Mol	Chain	Res	Type
1	A	312	ASP
1	A	325	ILE
1	A	329	LEU
1	A	333	LEU
1	A	337	GLN
1	A	338	GLN
1	A	339	LEU
1	A	341	ILE
1	A	347	LEU
1	A	352	THR
1	A	355	VAL
1	A	366	VAL
1	A	372	LEU
1	A	374	LEU
1	A	394	ASP
1	A	397	ARG
1	A	398	THR
1	A	400	VAL
1	A	411	ILE
1	A	414	LYS
1	B	10	TYR
1	B	12	VAL
1	B	13	LEU
1	B	14	GLN
1	B	22	LEU
1	B	28	LEU
1	B	29	ILE
1	B	41	THR
1	B	54	LEU
1	B	55	CYS
1	B	57	LEU
1	B	61	ILE
1	B	65	SER
1	B	81	VAL
1	B	85	ILE
1	B	90	LEU
1	B	91	LEU
1	B	102	ILE
1	B	106	LEU
1	B	107	PHE
1	B	120	GLN
1	B	131	VAL

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Mol	Chain	Res	Type
1	B	148	ASN
1	B	150	GLN
1	B	155	ILE
1	B	174	GLU
1	B	203	GLN
1	B	209	VAL
1	B	213	ILE
1	B	219	GLU
1	B	222	VAL
1	B	230	LYS
1	B	232	THR
1	B	239	LEU
1	B	241	LEU
1	B	245	LEU
1	B	246	VAL
1	B	259	ILE
1	B	266	LYS
1	B	303	LEU
1	B	305	LEU
1	B	312	ASP
1	B	325	ILE
1	B	329	LEU
1	B	333	LEU
1	B	337	GLN
1	B	338	GLN
1	B	339	LEU
1	B	341	ILE
1	B	344	THR
1	B	347	LEU
1	B	352	THR
1	B	355	VAL
1	B	374	LEU
1	B	377	PRO
1	B	394	ASP
1	B	397	ARG
1	B	411	ILE
1	B	414	LYS
1	B	416	GLU
1	C	8	ILE
1	C	9	GLU
1	C	10	TYR
1	C	13	LEU

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Mol	Chain	Res	Type
1	C	14	GLN
1	C	22	LEU
1	C	28	LEU
1	C	29	ILE
1	C	41	THR
1	C	43	VAL
1	C	54	LEU
1	C	57	LEU
1	C	61	ILE
1	C	65	SER
1	C	84	LYS
1	C	85	ILE
1	C	90	LEU
1	C	91	LEU
1	C	102	ILE
1	C	106	LEU
1	C	107	PHE
1	C	126	GLN
1	C	140	THR
1	C	148	ASN
1	C	150	GLN
1	C	152	LEU
1	C	159	ILE
1	C	174	GLU
1	C	181	GLU
1	C	203	GLN
1	C	209	VAL
1	C	213	ILE
1	C	219	GLU
1	C	222	VAL
1	C	230	LYS
1	C	232	THR
1	C	241	LEU
1	C	246	VAL
1	C	252	LYS
1	C	259	ILE
1	C	266	LYS
1	C	270	LEU
1	C	285	THR
1	C	287	ARG
1	C	303	LEU
1	C	305	LEU

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Mol	Chain	Res	Type
1	C	312	ASP
1	C	325	ILE
1	C	329	LEU
1	C	333	LEU
1	C	335	VAL
1	C	337	GLN
1	C	338	GLN
1	C	339	LEU
1	C	341	ILE
1	C	344	THR
1	C	347	LEU
1	C	350	ILE
1	C	352	THR
1	C	366	VAL
1	C	374	LEU
1	C	394	ASP
1	C	397	ARG
1	C	398	THR
1	C	400	VAL
1	C	411	ILE
1	C	414	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	108	ASN
1	A	132	HIS
1	A	310	ASN
1	A	368	HIS
1	B	108	ASN
1	B	132	HIS
1	B	150	GLN
1	B	173	ASN
1	B	310	ASN
1	B	318	GLN
1	B	368	HIS
1	C	14	GLN
1	C	108	ASN
1	C	150	GLN
1	C	264	HIS
1	C	310	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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	414/422 (98%)	-0.51	4 (0%)	79 62	65, 105, 140, 182	0
1	B	408/422 (96%)	-0.39	2 (0%)	87 76	63, 101, 147, 196	0
1	C	413/422 (97%)	-0.42	1 (0%)	91 85	64, 111, 154, 196	0
All	All	1235/1266 (97%)	-0.44	7 (0%)	85 73	63, 105, 148, 196	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	GLN	2.9
1	A	7	TYR	2.9
1	B	312	ASP	2.8
1	A	167	TYR	2.3
1	A	278	SER	2.3
1	C	76	ALA	2.0
1	A	8	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](#)

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
2	HG	A	501	1/1	0.99	0.07	140,140,140,140	1
2	HG	B	501	1/1	0.99	0.05	137,137,137,137	1
2	HG	C	501	1/1	0.99	0.06	128,128,128,128	1

6.5 Other polymers [i](#)

There are no such residues in this entry.