



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:20 PM GMT

PDB ID : 1T6J
Title : Crystal Structure of Phenylalanine Ammonia Lyase from Rhodosporidium toruloides
Authors : Calabrese, J.C.; Jordan, D.B.
Deposited on : 2004-05-06
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

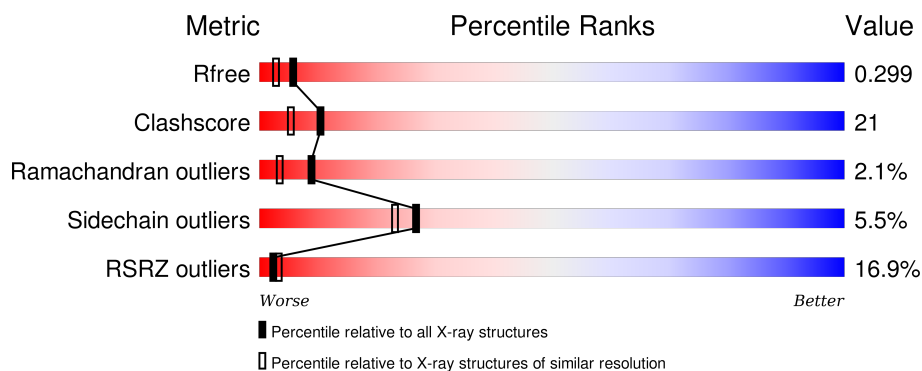
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	714	
1	B	714	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	175	A	211	X	-	-	-
1	175	B	211	X	-	-	-
2	CIN	B	1001	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10300 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 phenylalanine ammonia-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	647	Total	C	N	O	S	Se	0	0	0
			4939	3104	878	940	4	13			
1	B	647	Total	C	N	O	S	Se	0	0	0
			4939	3104	878	940	4	13			

There are 36 discrepancies between the modelled and reference sequences:

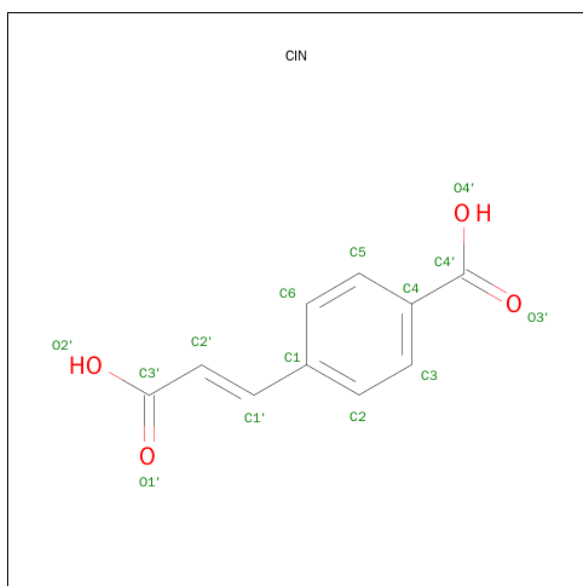
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	51	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	107	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	169	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	211	175	ALA	SEE REMARK 999	UNP P11544
A	211	175	SER	SEE REMARK 999	UNP P11544
A	211	175	GLY	SEE REMARK 999	UNP P11544
A	250	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	278	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	288	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	299	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	304	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	422	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	443	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	448	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	497	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	564	MSE	MET	MODIFIED RESIDUE	UNP P11544
A	714	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	1	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	51	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	107	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	169	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	211	175	ALA	SEE REMARK 999	UNP P11544
B	211	175	SER	SEE REMARK 999	UNP P11544
B	211	175	GLY	SEE REMARK 999	UNP P11544

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Chain	Residue	Modelled	Actual	Comment	Reference
B	250	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	278	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	288	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	299	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	304	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	422	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	443	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	448	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	497	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	564	MSE	MET	MODIFIED RESIDUE	UNP P11544
B	714	MSE	MET	MODIFIED RESIDUE	UNP P11544

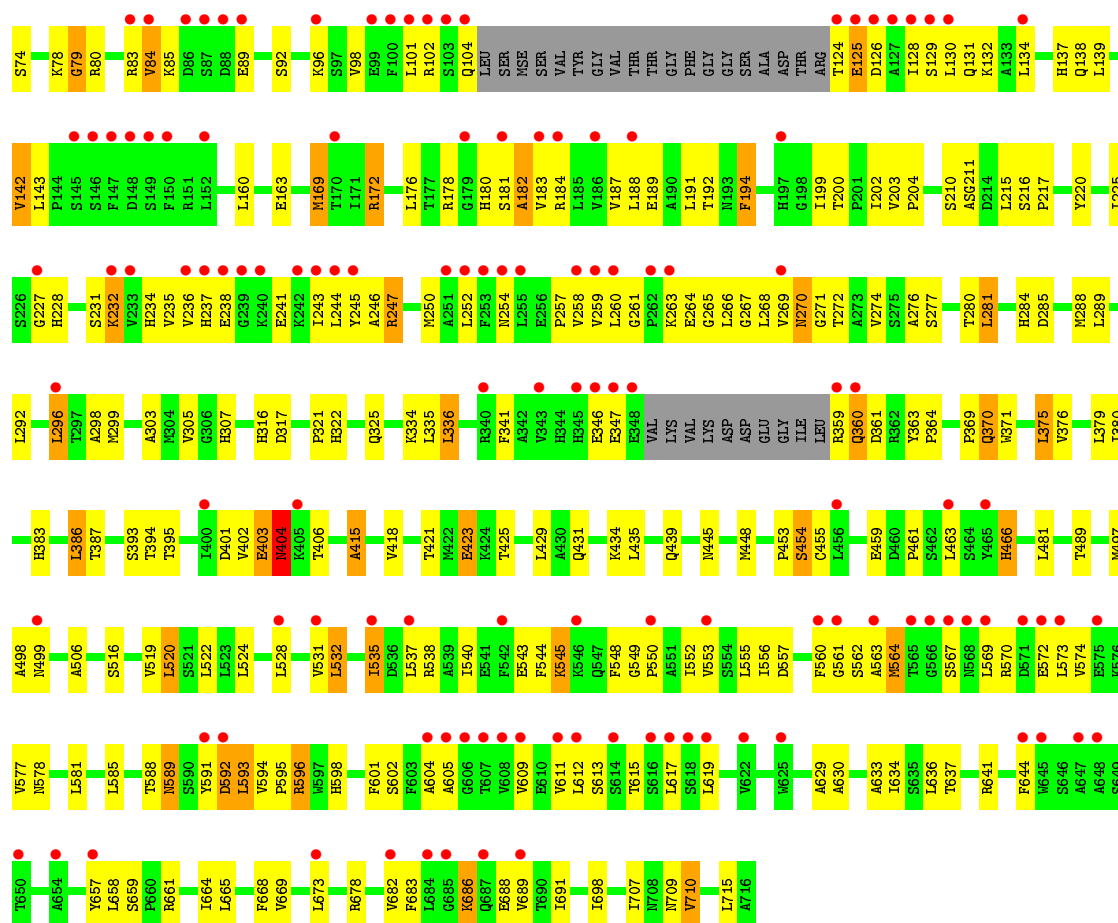
- Molecule 2 is 4-CARBOXYCINNAMIC ACID (three-letter code: CIN) (formula: C₁₀H₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			11	9	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	245	Total	O	0	0
			245	245		
3	B	166	Total	O	0	0
			166	166		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.86Å 107.86Å 204.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.10 24.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.10) 93.6 (24.77-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.298 0.254 , 0.299	Depositor DCC
R_{free} test set	1934 reflections (2.56%)	DCC
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.2	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 75419 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10300	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 175, CIN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/4995	0.64	0/6756
1	B	0.32	0/4995	0.61	0/6756
All	All	0.32	0/9990	0.63	0/13512

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	A	2	1
1	B	2	1
All	All	4	2

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	211	175	C3,C2
1	B	211	175	C3,C2

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	SER	Peptide
1	B	210	SER	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	4939	0	4998	187	0
1	B	4939	0	4998	244	0
2	B	11	0	6	0	0
3	A	245	0	0	6	0
3	B	166	0	0	17	0
All	All	10300	0	10002	427	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 21.

All (427) 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:247:ARG:HB3	1:B:247:ARG:HH11	1.11	1.08
1:A:279:ALA:HA	1:A:422:MSE:HE2	1.42	1.01
1:A:422:MSE:HE3	1:A:510:ALA:HA	1.43	0.99
1:A:593:LEU:HD11	1:A:637:THR:HG21	1.46	0.94
1:A:169:MSE:HE3	1:A:221:ILE:HG23	1.51	0.93
1:A:178:ARG:HE	1:A:394:THR:HG22	1.34	0.91
1:B:247:ARG:HB3	1:B:247:ARG:NH1	1.87	0.89
1:A:422:MSE:HE3	1:A:510:ALA:CA	2.02	0.88
1:A:279:ALA:HA	1:A:422:MSE:CE	2.06	0.85
1:A:383:HIS:O	1:A:387:THR:HG23	1.78	0.83
1:A:549:GLY:O	1:A:552:ILE:HG22	1.79	0.83
1:B:593:LEU:HD11	1:B:637:THR:HG21	1.60	0.83
1:B:383:HIS:O	1:B:387:THR:HG23	1.79	0.83
1:B:176:LEU:HD22	1:B:183:VAL:HG11	1.59	0.82
1:A:369:PRO:HD2	1:A:370:GLN:NE2	1.95	0.81
1:A:87:SER:O	1:A:88:ASP:HB2	1.80	0.80
1:A:605:ALA:O	1:A:608:VAL:HG22	1.85	0.77
1:A:69:LEU:HG	1:A:280:THR:HG23	1.67	0.77
1:B:520:LEU:HD22	1:B:524:LEU:HG	1.68	0.76
1:B:359:ARG:O	1:B:360:GLN:HB2	1.85	0.75
1:B:143:LEU:HD21	1:B:202:ILE:HG22	1.68	0.75
1:A:39:THR:HG22	1:A:41:GLN:HG2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HH22	1:A:86:ASP:HB2	1.52	0.74
1:A:594:VAL:HB	1:A:595:PRO:HD3	1.71	0.72
1:B:463:LEU:HD13	1:B:682:VAL:HG11	1.71	0.72
1:B:288:MSE:HE3	1:B:288:MSE:HA	1.72	0.72
1:B:250:MSE:SE	1:B:257:PRO:HG3	2.40	0.71
1:A:375:LEU:HD21	1:A:431:GLN:HB2	1.70	0.71
1:A:402:VAL:HG23	1:A:403:GLU:H	1.55	0.71
1:B:299:MSE:SE	1:B:665:LEU:HD23	2.41	0.71
1:A:588:THR:HG23	1:A:596:ARG:HE	1.55	0.71
1:B:531:VAL:O	1:B:535:ILE:HG12	1.91	0.70
1:A:263:LYS:HD3	1:A:263:LYS:O	1.92	0.69
1:A:520:LEU:HD22	1:A:524:LEU:HG	1.75	0.69
1:B:556:ILE:HD11	1:B:573:LEU:HD22	1.74	0.69
1:B:169:MSE:HG3	1:B:191:LEU:HD22	1.74	0.69
1:B:69:LEU:HG	1:B:280:THR:HG23	1.75	0.68
1:A:84:VAL:HG12	3:A:908:HOH:O	1.92	0.68
1:A:180:HIS:ND1	1:A:394:THR:HG21	2.08	0.68
1:A:59:THR:HG21	1:A:83:ARG:CD	2.23	0.68
1:B:60:LEU:HD11	1:B:71:ASP:HB3	1.76	0.68
1:A:266:LEU:HD22	1:A:270:ASN:HD21	1.60	0.67
1:B:556:ILE:CD1	1:B:573:LEU:HD22	2.25	0.67
1:A:166:ARG:O	1:A:170:THR:HG23	1.95	0.67
1:A:348:GLU:HB2	1:A:359:ARG:NH2	2.10	0.67
1:A:535:ILE:HD11	1:A:666:TYR:CD1	2.30	0.66
1:A:279:ALA:CA	1:A:422:MSE:HE2	2.23	0.66
1:A:248:GLU:O	1:A:252:LEU:HD13	1.95	0.66
1:B:481:LEU:HD21	1:B:519:VAL:HG23	1.75	0.66
1:B:98:VAL:HG12	1:B:102:ARG:HD2	1.76	0.66
1:A:567:SER:HB2	1:A:569:LEU:HD23	1.75	0.66
1:A:445:ASN:ND2	1:A:448:MSE:HE3	2.11	0.66
1:A:569:LEU:HD12	1:A:612:LEU:HD12	1.78	0.66
1:A:55:PRO:O	1:A:80:ARG:HD2	1.96	0.66
1:A:400:ILE:HG22	1:A:402:VAL:H	1.60	0.65
1:A:552:ILE:O	1:A:556:ILE:HG13	1.96	0.65
1:A:466:HIS:HE1	1:A:533:GLN:HG3	1.62	0.65
1:B:581:LEU:O	1:B:585:LEU:HD13	1.97	0.65
1:B:307:HIS:HD2	1:B:361:ASP:OD1	1.80	0.65
1:B:266:LEU:O	1:B:270:ASN:HB2	1.97	0.65
1:B:137:HIS:CE1	1:B:138:GLN:HG2	2.32	0.64
1:B:707:ILE:O	1:B:710:VAL:HG13	1.97	0.64
1:B:563:ALA:HB1	1:B:617:LEU:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:LEU:O	1:B:439:GLN:HG3	1.97	0.63
1:B:129:SER:HA	1:B:132:LYS:HE2	1.81	0.63
1:B:232:LYS:NZ	1:B:243:ILE:HG22	2.14	0.63
1:A:101:LEU:HD21	1:A:400:ILE:HG12	1.81	0.62
1:B:98:VAL:O	1:B:102:ARG:HG3	1.99	0.62
1:B:138:GLN:OE1	1:B:215:LEU:HD23	1.99	0.62
1:A:316:HIS:CD2	1:A:325:GLN:HE21	2.17	0.62
1:B:633:ALA:O	1:B:637:THR:HG22	1.99	0.62
1:B:598:HIS:O	1:B:602:SER:HB2	1.99	0.62
1:B:386:LEU:HD13	1:B:421:THR:HG21	1.80	0.62
1:A:418:VAL:HG22	1:A:506:ALA:HB1	1.82	0.62
1:A:87:SER:O	1:A:88:ASP:CB	2.47	0.62
1:A:215:LEU:HD12	1:A:269:VAL:O	2.00	0.62
1:B:216:SER:HB3	1:B:217:PRO:HD3	1.82	0.62
1:B:178:ARG:NH1	1:B:393:SER:HA	2.15	0.62
1:B:593:LEU:N	3:B:1046:HOH:O	2.32	0.62
1:B:92:SER:O	1:B:96:LYS:HG3	2.00	0.61
1:B:589:ASN:HD22	1:B:589:ASN:N	1.97	0.61
1:A:593:LEU:CD1	1:A:637:THR:HG21	2.25	0.61
1:B:573:LEU:HD12	1:B:612:LEU:HD11	1.82	0.61
1:B:588:THR:O	1:B:588:THR:HG22	2.00	0.60
1:A:320:ARG:HD3	1:A:325:GLN:HE22	1.66	0.60
1:A:97:SER:O	1:A:101:LEU:HD23	2.02	0.60
1:B:360:GLN:HG2	3:B:1052:HOH:O	2.01	0.60
1:B:160:LEU:HB2	1:B:203:VAL:HG23	1.84	0.60
1:B:347:GLU:HG2	1:B:347:GLU:O	2.02	0.60
1:B:612:LEU:HB3	1:B:615:THR:HG21	1.84	0.59
1:B:453:PRO:HD2	1:B:537:LEU:HD23	1.84	0.59
1:B:228:HIS:HB3	1:B:231:SER:CB	2.32	0.59
1:B:669:VAL:HA	1:B:673:LEU:HD12	1.83	0.59
1:B:96:LYS:HB3	1:B:96:LYS:NZ	2.18	0.59
1:A:585:LEU:HA	1:A:588:THR:HG22	1.83	0.59
1:B:341:PHE:CZ	1:B:657:TYR:HB2	2.38	0.59
1:B:247:ARG:H	1:B:247:ARG:HD2	1.68	0.59
1:B:187:VAL:HG21	1:B:264:GLU:OE1	2.03	0.59
1:B:573:LEU:HD23	1:B:573:LEU:O	2.02	0.59
1:A:601:PHE:HA	1:A:604:ALA:HB3	1.84	0.59
1:A:611:VAL:HG23	1:A:612:LEU:HD13	1.84	0.59
1:A:138:GLN:OE1	1:A:215:LEU:HD23	2.03	0.58
1:B:181:SER:O	1:B:182:ALA:HB3	2.04	0.58
1:B:83:ARG:HG3	1:B:83:ARG:HH11	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:LEU:HD12	1:A:612:LEU:HD13	1.84	0.58
1:B:418:VAL:HG23	1:B:506:ALA:HB1	1.85	0.58
1:B:369:PRO:HD2	1:B:370:GLN:OE1	2.04	0.58
1:A:459:GLU:OE1	1:A:679:ARG:NH1	2.33	0.58
1:B:178:ARG:HH12	1:B:393:SER:HA	1.68	0.58
1:B:228:HIS:HB3	1:B:231:SER:HB2	1.86	0.58
1:B:176:LEU:HD22	1:B:183:VAL:CG1	2.32	0.58
1:A:422:MSE:CE	1:A:510:ALA:HA	2.25	0.58
1:A:633:ALA:O	1:A:637:THR:HG22	2.04	0.57
1:B:481:LEU:CD2	1:B:519:VAL:HG23	2.34	0.57
1:A:367:THR:HA	1:A:370:GLN:NE2	2.20	0.57
1:A:218:LEU:HD13	1:A:274:VAL:HG23	1.85	0.57
1:A:298:ALA:HB1	1:A:336:LEU:HD13	1.86	0.57
1:B:322:HIS:HD2	3:B:1074:HOH:O	1.85	0.57
1:B:637:THR:O	1:B:641:ARG:HG3	2.04	0.57
1:A:368:SER:OG	1:A:369:PRO:HD3	2.05	0.57
1:A:282:ALA:HB3	1:A:422:MSE:HE1	1.87	0.57
1:A:564:MSE:HG3	1:A:567:SER:OG	2.04	0.57
1:A:282:ALA:CB	1:A:422:MSE:HE1	2.34	0.57
1:A:316:HIS:HD2	1:A:325:GLN:HG2	1.69	0.56
1:B:425:THR:O	1:B:429:LEU:HG	2.05	0.56
1:B:553:VAL:O	1:B:556:ILE:HG22	2.04	0.56
1:A:369:PRO:HD2	1:A:370:GLN:HE22	1.65	0.56
1:B:516:SER:HA	1:B:519:VAL:HG22	1.86	0.56
1:A:574:VAL:O	1:A:578:ASN:HB2	2.06	0.56
1:B:305:VAL:HG23	1:B:538:ARG:HD3	1.87	0.56
1:A:400:ILE:HD12	1:A:400:ILE:N	2.19	0.56
1:B:60:LEU:HD22	1:B:62:LEU:HD12	1.87	0.56
1:A:367:THR:C	1:A:370:GLN:HE21	2.07	0.56
1:A:39:THR:CG2	1:A:41:GLN:HG2	2.35	0.56
1:B:630:ALA:O	1:B:634:ILE:HG13	2.06	0.56
1:B:232:LYS:NZ	1:B:232:LYS:HB3	2.20	0.56
1:B:461:PRO:HD2	1:B:592:ASP:HA	1.88	0.55
1:A:612:LEU:O	1:A:615:THR:HG22	2.07	0.55
1:A:445:ASN:HB3	1:A:448:MSE:HB2	1.89	0.55
1:B:316:HIS:CD2	1:B:325:GLN:HE21	2.24	0.55
1:A:176:LEU:HD22	1:A:183:VAL:HG11	1.88	0.55
1:A:422:MSE:HE3	1:A:510:ALA:CB	2.37	0.54
1:B:237:HIS:HD2	1:B:252:LEU:HD21	1.71	0.54
1:B:359:ARG:O	1:B:360:GLN:CB	2.55	0.54
1:B:545:LYS:HD2	1:B:545:LYS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ILE:HG23	1:A:553:VAL:N	2.22	0.54
1:A:316:HIS:HD2	1:A:325:GLN:HE21	1.54	0.54
1:B:55:PRO:O	1:B:80:ARG:HD2	2.07	0.54
1:B:678:ARG:HD2	1:B:691:ILE:CD1	2.38	0.54
1:A:535:ILE:HD11	1:A:666:TYR:CE1	2.42	0.54
1:B:139:LEU:HA	1:B:220:TYR:CE1	2.43	0.54
1:A:41:GLN:O	1:A:42:VAL:HB	2.08	0.54
1:B:217:PRO:HB2	1:B:274:VAL:HG21	1.90	0.53
1:A:169:MSE:HE2	1:A:191:LEU:HD22	1.89	0.53
1:B:180:HIS:CD2	1:B:394:THR:HG21	2.43	0.53
1:B:84:VAL:HG12	3:B:1162:HOH:O	2.08	0.53
1:B:61:GLU:OE2	1:B:85:LYS:HG3	2.08	0.53
1:A:573:LEU:C	1:A:573:LEU:HD23	2.29	0.53
1:B:215:LEU:HD12	1:B:269:VAL:O	2.08	0.53
1:B:445:ASN:HD22	1:B:448:MSE:HG3	1.74	0.53
1:A:305:VAL:O	1:A:305:VAL:HG12	2.08	0.53
1:A:42:VAL:O	1:A:42:VAL:CG1	2.56	0.53
1:B:585:LEU:HD23	3:B:1067:HOH:O	2.06	0.53
1:A:659:SER:O	1:A:663:GLN:HB2	2.07	0.53
1:B:247:ARG:CB	1:B:247:ARG:HH11	2.02	0.53
1:A:563:ALA:HB1	1:A:617:LEU:HD11	1.91	0.53
1:B:375:LEU:CD1	1:B:375:LEU:H	2.21	0.53
1:A:237:HIS:HB3	1:A:242:LYS:HE3	1.90	0.52
1:B:131:GLN:OE1	1:B:261:GLY:O	2.27	0.52
1:A:127:ALA:O	1:A:131:GLN:HG2	2.09	0.52
1:B:192:THR:HG21	3:B:1162:HOH:O	2.10	0.52
1:B:379:LEU:HD23	3:B:1126:HOH:O	2.10	0.52
1:B:543:GLU:HA	1:B:543:GLU:OE1	2.09	0.52
1:A:266:LEU:HD22	1:A:270:ASN:ND2	2.23	0.52
1:A:401:ASP:O	1:A:401:ASP:OD1	2.27	0.52
1:A:402:VAL:HG23	1:A:403:GLU:N	2.24	0.52
1:B:577:VAL:O	1:B:581:LEU:HB2	2.09	0.52
1:B:128:ILE:HD13	1:B:260:LEU:O	2.10	0.52
1:A:573:LEU:HD12	1:A:612:LEU:CD1	2.40	0.52
1:B:459:GLU:HG3	1:B:683:PHE:CG	2.45	0.52
1:B:595:PRO:HG2	3:B:1046:HOH:O	2.10	0.52
1:B:124:THR:HG23	1:B:125:GLU:H	1.75	0.52
1:B:375:LEU:HD12	1:B:375:LEU:N	2.25	0.52
1:A:370:GLN:NE2	1:A:370:GLN:H	2.09	0.51
1:B:611:VAL:HG13	1:B:612:LEU:HD13	1.91	0.51
1:A:615:THR:CG2	1:B:619:LEU:HD12	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:VAL:CG2	1:B:506:ALA:HB1	2.40	0.51
1:B:499:ASN:N	1:B:499:ASN:HD22	2.08	0.51
1:B:284:HIS:HD2	1:B:285:ASP:OD2	1.92	0.51
1:B:172:ARG:HE	1:B:172:ARG:HA	1.76	0.51
1:B:292:LEU:O	1:B:296:LEU:HD13	2.09	0.51
1:A:59:THR:HG21	1:A:83:ARG:HD2	1.92	0.51
1:B:589:ASN:ND2	1:B:589:ASN:N	2.59	0.51
1:B:225:ILE:O	1:B:258:VAL:HG12	2.10	0.51
1:B:553:VAL:C	1:B:556:ILE:HG22	2.30	0.51
1:B:611:VAL:HG13	1:B:612:LEU:H	1.76	0.51
1:B:611:VAL:HG13	1:B:612:LEU:N	2.25	0.51
1:B:277:SER:O	1:B:281:LEU:HD13	2.10	0.51
1:B:601:PHE:HA	1:B:604:ALA:HB3	1.93	0.51
1:A:612:LEU:HB3	1:A:615:THR:HG21	1.92	0.51
1:A:598:HIS:O	1:A:602:SER:HB2	2.11	0.51
1:B:612:LEU:O	1:B:615:THR:HG22	2.11	0.50
1:B:305:VAL:CG2	1:B:538:ARG:HD3	2.41	0.50
1:B:265:GLY:O	1:B:269:VAL:HG22	2.12	0.50
1:A:169:MSE:HE2	1:A:191:LEU:CD2	2.41	0.50
1:A:573:LEU:HD23	1:A:573:LEU:O	2.10	0.50
1:A:588:THR:HG23	1:A:596:ARG:HG3	1.93	0.50
1:B:601:PHE:CZ	1:B:629:ALA:HB1	2.47	0.50
1:A:455:CYS:O	1:A:456:LEU:HB2	2.11	0.50
1:A:588:THR:CG2	1:A:596:ARG:HE	2.24	0.50
1:B:347:GLU:OE1	1:B:347:GLU:N	2.45	0.50
1:A:570:ARG:HG3	1:A:570:ARG:HH11	1.75	0.50
1:A:339:SER:O	1:A:344:HIS:HE1	1.95	0.50
1:B:235:VAL:HG22	1:B:236:VAL:N	2.26	0.50
1:B:678:ARG:HD2	1:B:691:ILE:HD11	1.93	0.49
1:B:163:GLU:OE2	1:B:281:LEU:HD23	2.12	0.49
1:B:296:LEU:CD2	1:B:524:LEU:HD22	2.42	0.49
1:B:588:THR:HG23	1:B:591:TYR:CD1	2.48	0.49
1:B:258:VAL:HG22	1:B:259:VAL:N	2.28	0.49
1:A:42:VAL:O	1:A:42:VAL:HG13	2.11	0.49
1:A:620:ALA:HB2	1:B:613:SER:O	2.13	0.49
1:B:183:VAL:HG23	1:B:264:GLU:HG3	1.94	0.49
1:A:359:ARG:O	1:A:360:GLN:HG3	2.12	0.49
1:A:277:SER:O	1:A:281:LEU:HD22	2.11	0.49
1:B:172:ARG:NH1	1:B:268:LEU:HA	2.27	0.49
1:B:346:GLU:OE1	1:B:359:ARG:HD2	2.12	0.49
1:B:415:ALA:HB1	1:B:418:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ARG:H	1:B:247:ARG:CD	2.26	0.49
1:B:401:ASP:CG	1:B:404:ASN:HB2	2.33	0.49
1:B:560:PHE:O	1:B:562:SER:N	2.44	0.49
1:B:260:LEU:HD22	1:B:264:GLU:O	2.11	0.49
1:B:375:LEU:CD1	1:B:375:LEU:N	2.76	0.49
1:B:204:PRO:HG2	3:B:1014:HOH:O	2.13	0.49
1:A:637:THR:O	1:A:641:ARG:HG3	2.13	0.48
1:B:124:THR:HG23	1:B:125:GLU:N	2.28	0.48
1:B:589:ASN:H	1:B:589:ASN:ND2	2.10	0.48
1:A:214:ASP:O	1:A:218:LEU:HB2	2.13	0.48
1:A:59:THR:HG21	1:A:83:ARG:HD3	1.95	0.48
1:A:209:ILE:HD11	1:A:500:GLN:OE1	2.13	0.48
1:A:124:THR:O	1:A:125:GLU:HG3	2.13	0.48
1:A:370:GLN:CD	1:A:370:GLN:H	2.16	0.48
1:B:564:MSE:SE	1:B:567:SER:OG	2.82	0.48
1:A:375:LEU:HD23	1:A:432:ILE:HG13	1.96	0.48
1:A:443:MSE:SE	1:A:531:VAL:HG12	2.63	0.48
1:A:262:PRO:C	1:A:264:GLU:H	2.17	0.48
1:A:686:LYS:HE2	3:A:733:HOH:O	2.13	0.48
1:B:194:PHE:CE2	1:B:199:ILE:HG22	2.49	0.48
1:A:569:LEU:N	1:A:569:LEU:HD22	2.29	0.48
1:A:560:PHE:HE1	1:A:625:TRP:CG	2.32	0.48
1:B:570:ARG:O	1:B:574:VAL:HG23	2.13	0.48
1:B:129:SER:HA	1:B:132:LYS:CE	2.43	0.48
1:B:232:LYS:HZ2	1:B:243:ILE:HG22	1.78	0.48
1:B:203:VAL:HG12	1:B:220:TYR:HB3	1.95	0.47
1:B:596:ARG:HB3	3:B:1046:HOH:O	2.13	0.47
1:A:401:ASP:O	1:A:403:GLU:N	2.48	0.47
1:B:556:ILE:HG23	1:B:557:ASP:N	2.30	0.47
1:A:266:LEU:O	1:A:270:ASN:HB2	2.14	0.47
1:A:346:GLU:HB3	1:A:359:ARG:NH2	2.29	0.47
1:B:305:VAL:O	1:B:305:VAL:HG12	2.15	0.47
1:B:172:ARG:HH11	1:B:268:LEU:HA	1.78	0.47
1:A:124:THR:HG23	1:A:124:THR:O	2.15	0.47
1:A:435:LEU:O	1:A:439:GLN:HG3	2.15	0.47
1:B:528:LEU:HD23	1:B:698:ILE:CG2	2.45	0.47
1:A:601:PHE:HA	1:A:604:ALA:CB	2.45	0.47
1:B:601:PHE:CE2	1:B:629:ALA:HB1	2.49	0.47
1:A:367:THR:O	1:A:370:GLN:HG2	2.15	0.47
1:B:41:GLN:O	1:B:42:VAL:HB	2.15	0.47
1:B:334:LYS:HE2	1:B:661:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:TRP:O	1:B:375:LEU:HD13	2.15	0.46
1:B:363:TYR:CD1	1:B:363:TYR:N	2.83	0.46
1:A:247:ARG:HA	1:A:250:MSE:HE3	1.96	0.46
1:A:548:PHE:HD1	1:A:636:LEU:HD12	1.80	0.46
1:A:619:LEU:HD12	1:B:615:THR:CG2	2.46	0.46
1:A:444:LEU:HD13	1:A:471:ASP:HB2	1.96	0.46
1:A:552:ILE:CG2	1:A:553:VAL:N	2.79	0.46
1:A:135:LEU:O	1:A:139:LEU:HD22	2.16	0.46
1:B:709:ASN:HB3	3:B:1166:HOH:O	2.15	0.46
1:A:41:GLN:O	1:A:42:VAL:CB	2.62	0.46
1:B:686:LYS:HB2	1:B:686:LYS:NZ	2.30	0.46
1:B:707:ILE:HA	1:B:710:VAL:CG1	2.46	0.46
1:B:60:LEU:HD22	1:B:62:LEU:CD1	2.46	0.46
1:B:402:VAL:C	1:B:404:ASN:H	2.19	0.46
1:A:181:SER:O	1:A:182:ALA:HB3	2.15	0.46
1:B:375:LEU:HD21	1:B:431:GLN:HB2	1.98	0.46
1:B:499:ASN:N	1:B:499:ASN:ND2	2.64	0.46
1:B:188:LEU:HD12	1:B:188:LEU:N	2.31	0.46
1:B:605:ALA:O	1:B:609:VAL:HG23	2.16	0.46
1:B:232:LYS:HE2	1:B:245:TYR:CE1	2.51	0.45
1:B:125:GLU:OE1	1:B:125:GLU:HA	2.16	0.45
1:A:307:HIS:N	1:A:307:HIS:CD2	2.84	0.45
1:A:262:PRO:O	1:A:264:GLU:N	2.49	0.45
1:A:589:ASN:N	1:A:589:ASN:OD1	2.43	0.45
1:A:288:MSE:HE3	1:A:708:ASN:ND2	2.32	0.45
1:B:528:LEU:O	1:B:531:VAL:HG12	2.15	0.45
1:B:272:THR:HG22	1:B:276:ALA:HB2	1.97	0.45
1:B:549:GLY:N	1:B:550:PRO:HD2	2.31	0.45
1:A:603:PHE:HD2	1:A:603:PHE:O	1.99	0.45
1:A:696:SER:O	1:A:700:GLU:HG3	2.17	0.45
1:B:68:ASN:OD1	1:B:71:ASP:OD1	2.35	0.45
1:A:606:GLY:HA3	1:B:602:SER:O	2.17	0.45
1:A:232:LYS:HE2	1:A:245:TYR:CZ	2.52	0.45
1:B:298:ALA:HB1	1:B:336:LEU:HD13	1.99	0.45
1:A:535:ILE:HG13	1:A:536:ASP:N	2.31	0.45
1:B:569:LEU:HD12	1:B:569:LEU:N	2.32	0.45
1:A:234:HIS:HD2	3:A:953:HOH:O	1.98	0.45
1:B:528:LEU:HD23	1:B:698:ILE:HG23	1.99	0.45
1:A:316:HIS:CD2	1:A:325:GLN:HG2	2.51	0.45
1:B:363:TYR:HD1	1:B:363:TYR:N	2.15	0.45
1:B:184:ARG:HH11	1:B:184:ARG:HG3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:TRP:CE2	1:A:679:ARG:HG2	2.52	0.45
1:A:225:ILE:HG13	1:A:226:SER:N	2.32	0.45
1:B:497:MSE:O	1:B:498:ALA:HB3	2.15	0.45
1:B:69:LEU:O	1:B:73:VAL:HG23	2.17	0.45
1:B:259:VAL:O	1:B:259:VAL:HG23	2.16	0.45
1:A:669:VAL:HG12	1:A:675:VAL:HG13	1.98	0.45
1:B:78:LYS:O	1:B:79:GLY:C	2.55	0.45
1:A:623:ASN:O	1:A:627:VAL:HG23	2.17	0.45
1:B:271:GLY:HA3	3:B:1139:HOH:O	2.17	0.44
1:A:415:ALA:HB1	1:A:418:VAL:HG13	1.99	0.44
1:A:427:LEU:O	1:A:431:GLN:HG2	2.16	0.44
1:B:203:VAL:HG12	1:B:220:TYR:CB	2.48	0.44
1:B:445:ASN:ND2	1:B:448:MSE:HG3	2.32	0.44
1:B:236:VAL:HA	1:B:241:GLU:HA	1.99	0.44
1:B:341:PHE:HE2	1:B:658:LEU:HG	1.81	0.44
1:B:189:GLU:HA	1:B:192:THR:OG1	2.17	0.44
1:A:160:LEU:HB2	1:A:203:VAL:HG22	1.99	0.44
1:A:549:GLY:N	1:A:550:PRO:HD2	2.32	0.44
1:B:589:ASN:H	1:B:589:ASN:HD22	1.65	0.44
1:B:228:HIS:HB3	1:B:231:SER:HB3	1.99	0.44
1:A:459:GLU:HG3	1:A:683:PHE:CG	2.53	0.44
1:A:90:ILE:O	1:A:94:ILE:HG13	2.17	0.44
1:B:664:ILE:HG22	1:B:710:VAL:HG23	2.00	0.44
1:A:536:ASP:O	1:A:540:ILE:HG13	2.18	0.43
1:B:519:VAL:HA	1:B:522:LEU:HD12	2.00	0.43
1:B:535:ILE:HG12	1:B:535:ILE:H	1.55	0.43
1:B:142:VAL:HG13	3:B:1118:HOH:O	2.17	0.43
1:B:181:SER:HA	3:B:1109:HOH:O	2.18	0.43
1:A:208:THR:OG1	1:A:214:ASP:HA	2.18	0.43
1:B:89:GLU:H	1:B:89:GLU:CD	2.22	0.43
1:B:244:LEU:HD12	1:B:244:LEU:N	2.33	0.43
1:B:130:LEU:O	1:B:134:LEU:HD13	2.18	0.43
1:B:335:LEU:HD11	1:B:715:LEU:HD21	2.00	0.43
1:B:187:VAL:HG22	1:B:258:VAL:HG21	2.00	0.43
1:B:184:ARG:NH1	1:B:184:ARG:HG3	2.33	0.43
1:A:460:ASP:HA	1:A:461:PRO:HD3	1.92	0.43
1:A:645:TRP:CD2	1:A:679:ARG:HG2	2.54	0.43
1:B:303:ALA:O	1:B:538:ARG:HD2	2.18	0.43
1:A:60:LEU:HB2	1:A:80:ARG:NE	2.34	0.42
1:A:48:VAL:O	1:A:52:LEU:HG	2.19	0.42
1:B:591:TYR:HB2	1:B:596:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ASP:OD1	1:B:570:ARG:NH1	2.51	0.42
1:A:567:SER:CB	1:A:569:LEU:HD23	2.45	0.42
1:B:386:LEU:HD12	1:B:386:LEU:HA	1.88	0.42
1:B:364:PRO:HB2	3:B:1058:HOH:O	2.19	0.42
1:A:363:TYR:CD1	1:A:363:TYR:N	2.86	0.42
1:B:202:ILE:HD11	1:B:234:HIS:HB2	2.01	0.42
1:A:528:LEU:HD21	1:A:669:VAL:HG21	2.02	0.42
1:B:101:LEU:O	1:B:104:GLN:N	2.48	0.42
1:B:540:ILE:HD11	1:B:644:PHE:CD2	2.55	0.42
1:B:688:GLU:O	1:B:689:VAL:C	2.57	0.42
1:B:423:GLU:OE2	1:B:489:THR:HG23	2.19	0.42
1:A:601:PHE:CZ	1:A:629:ALA:HB1	2.55	0.42
1:B:376:VAL:O	1:B:380:ILE:HG13	2.20	0.42
1:A:313:PRO:HG3	1:A:333:ARG:CZ	2.49	0.42
1:B:69:LEU:CD1	1:B:387:THR:HA	2.49	0.42
1:B:572:GLU:OE2	1:B:611:VAL:HG23	2.20	0.42
1:B:236:VAL:HG22	1:B:241:GLU:HB3	2.01	0.42
1:B:669:VAL:O	1:B:673:LEU:HB2	2.18	0.42
1:A:267:GLY:O	1:A:396:ASP:OD2	2.38	0.42
1:B:387:THR:HG22	3:B:1152:HOH:O	2.20	0.42
1:A:139:LEU:HA	1:A:220:TYR:CE1	2.55	0.42
1:B:336:LEU:HD12	1:B:336:LEU:HA	1.91	0.42
1:B:555:LEU:HD12	1:B:555:LEU:N	2.35	0.42
1:B:272:THR:CG2	1:B:272:THR:O	2.68	0.42
1:B:96:LYS:HB3	1:B:96:LYS:HZ3	1.83	0.41
1:B:548:PHE:O	1:B:552:ILE:HG13	2.20	0.41
1:A:346:GLU:HB3	1:A:359:ARG:CZ	2.50	0.41
1:B:102:ARG:HH12	1:B:184:ARG:NH2	2.18	0.41
1:B:270:ASN:HD22	1:B:270:ASN:HA	1.60	0.41
1:B:434:LYS:HG3	3:B:1081:HOH:O	2.19	0.41
1:A:422:MSE:CE	1:A:510:ALA:HB1	2.51	0.41
1:B:316:HIS:HD2	1:B:325:GLN:HE21	1.67	0.41
1:A:190:ALA:HA	3:A:926:HOH:O	2.18	0.41
1:B:548:PHE:CZ	1:B:633:ALA:HB2	2.55	0.41
1:B:264:GLU:HG2	1:B:264:GLU:O	2.20	0.41
1:A:45:VAL:HG23	3:A:789:HOH:O	2.19	0.41
1:B:573:LEU:HD23	1:B:577:VAL:CG2	2.51	0.41
1:A:188:LEU:HD12	1:A:188:LEU:N	2.35	0.41
1:A:434:LYS:O	1:A:438:THR:HG23	2.20	0.41
1:A:127:ALA:HB1	1:A:262:PRO:HG3	2.02	0.41
1:B:74:SER:O	1:B:78:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:PHE:C	1:B:544:PHE:CD1	2.94	0.41
1:A:228:HIS:HB3	1:A:231:SER:HB2	2.02	0.41
1:B:360:GLN:HG2	1:B:360:GLN:O	2.20	0.41
1:A:124:THR:C	1:A:125:GLU:HG3	2.41	0.41
1:A:424:LYS:HB3	1:A:424:LYS:NZ	2.36	0.41
1:A:532:LEU:HD12	1:A:532:LEU:HA	1.92	0.41
1:B:535:ILE:HD12	1:B:658:LEU:HD21	2.02	0.41
1:A:176:LEU:HD22	1:A:183:VAL:CG1	2.50	0.41
1:B:532:LEU:HA	1:B:532:LEU:HD12	1.82	0.41
1:A:422:MSE:CE	1:A:510:ALA:CB	2.98	0.41
1:B:594:VAL:N	1:B:595:PRO:HD2	2.36	0.41
1:B:678:ARG:CD	1:B:691:ILE:HD11	2.50	0.41
1:A:570:ARG:NH1	1:A:570:ARG:HG3	2.35	0.41
1:B:564:MSE:HG3	1:B:569:LEU:HD22	2.02	0.41
1:A:661:ARG:HD3	1:A:714:MSE:O	2.21	0.41
1:A:491:HIS:HE1	3:A:776:HOH:O	2.03	0.41
1:B:178:ARG:HD3	1:B:394:THR:HG23	2.03	0.40
1:B:271:GLY:HA2	1:B:395:THR:O	2.21	0.40
1:B:69:LEU:HD13	1:B:387:THR:HG22	2.04	0.40
1:B:138:GLN:HE21	1:B:216:SER:HA	1.85	0.40
1:B:668:PHE:O	1:B:673:LEU:HG	2.22	0.40
1:B:455:CYS:O	1:B:466:HIS:HB3	2.20	0.40
1:A:69:LEU:HD22	1:A:387:THR:HG22	2.03	0.40
1:A:608:VAL:CG2	1:A:609:VAL:N	2.84	0.40
1:B:232:LYS:HZ2	1:B:232:LYS:HB3	1.85	0.40
1:B:83:ARG:HG3	1:B:83:ARG:NH1	2.35	0.40
1:B:84:VAL:O	1:B:85:LYS:C	2.59	0.40
1:B:172:ARG:NH1	1:B:267:GLY:O	2.49	0.40
1:A:426:ARG:NE	1:A:484:LEU:O	2.50	0.40
1:A:146:SER:OG	1:A:147:PHE:N	2.54	0.40
1:A:128:ILE:HG23	1:A:129:SER:N	2.35	0.40
1:A:54:ALA:HA	1:A:55:PRO:HD3	1.89	0.40
1:B:180:HIS:HD2	1:B:394:THR:HG21	1.85	0.40
1:A:52:LEU:HD12	1:A:712:LEU:HD22	2.04	0.40
1:A:541:GLU:O	1:A:545:LYS:HG3	2.22	0.40
1:B:316:HIS:HD2	1:B:325:GLN:HG2	1.85	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	640/714 (90%)	587 (92%)	44 (7%)	9 (1%)	14	7
1	B	640/714 (90%)	571 (89%)	51 (8%)	18 (3%)	6	2
All	All	1280/1428 (90%)	1158 (90%)	95 (7%)	27 (2%)	9	3

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	B	238	GLU
1	B	360	GLN
1	B	454	SER
1	A	88	ASP
1	A	238	GLU
1	A	263	LYS
1	A	402	VAL
1	A	466	HIS
1	B	246	ALA
1	B	263	LYS
1	B	466	HIS
1	B	592	ASP
1	A	125	GLU
1	A	454	SER
1	B	182	ALA
1	B	227	GLY
1	B	42	VAL
1	B	403	GLU
1	B	404	ASN
1	B	415	ALA
1	B	561	GLY
1	B	593	LEU
1	B	126	ASP
1	B	321	PRO

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Mol	Chain	Res	Type
1	B	79	GLY
1	A	321	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	538/573 (94%)	516 (96%)	22 (4%)	37	36
1	B	538/573 (94%)	501 (93%)	37 (7%)	19	15
All	All	1076/1146 (94%)	1017 (94%)	59 (6%)	27	23

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	72	VAL
1	A	139	LEU
1	A	172	ARG
1	A	183	VAL
1	A	203	VAL
1	A	281	LEU
1	A	288	MSE
1	A	289	LEU
1	A	317	ASP
1	A	336	LEU
1	A	370	GLN
1	A	394	THR
1	A	465	TYR
1	A	520	LEU
1	A	532	LEU
1	A	533	GLN
1	A	578	ASN
1	A	603	PHE
1	A	659	SER
1	A	675	VAL

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Mol	Chain	Res	Type
1	A	679	ARG
1	B	50	LYS
1	B	84	VAL
1	B	125	GLU
1	B	142	VAL
1	B	169	MSE
1	B	172	ARG
1	B	194	PHE
1	B	200	THR
1	B	232	LYS
1	B	247	ARG
1	B	254	ASN
1	B	270	ASN
1	B	281	LEU
1	B	289	LEU
1	B	296	LEU
1	B	317	ASP
1	B	336	LEU
1	B	370	GLN
1	B	375	LEU
1	B	386	LEU
1	B	403	GLU
1	B	404	ASN
1	B	406	THR
1	B	423	GLU
1	B	454	SER
1	B	520	LEU
1	B	532	LEU
1	B	535	ILE
1	B	545	LYS
1	B	564	MSE
1	B	578	ASN
1	B	589	ASN
1	B	596	ARG
1	B	636	LEU
1	B	659	SER
1	B	686	LYS
1	B	710	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	138	GLN
1	A	234	HIS
1	A	237	HIS
1	A	316	HIS
1	A	344	HIS
1	A	370	GLN
1	A	383	HIS
1	A	408	HIS
1	A	412	ASN
1	A	483	HIS
1	A	491	HIS
1	A	533	GLN
1	A	694	ASN
1	B	44	GLN
1	B	137	HIS
1	B	138	GLN
1	B	158	ASN
1	B	180	HIS
1	B	193	ASN
1	B	254	ASN
1	B	270	ASN
1	B	284	HIS
1	B	294	GLN
1	B	307	HIS
1	B	316	HIS
1	B	322	HIS
1	B	331	ASN
1	B	383	HIS
1	B	392	GLN
1	B	404	ASN
1	B	436	ASN
1	B	445	ASN
1	B	491	HIS
1	B	499	ASN
1	B	559	HIS
1	B	578	ASN
1	B	589	ASN
1	B	663	GLN
1	B	694	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	175	A	211	1	11,14,15	1.35	2 (18%)	6,19,21	3.72	2 (33%)
1	175	B	211	1	11,14,15	1.27	1 (9%)	6,19,21	3.80	2 (33%)

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	175	A	211	1	2/2/5/7	0/3/25/26	0/1/1/1
1	175	B	211	1	2/2/5/7	0/3/25/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	175	C3-C5	-2.76	1.47	1.52
1	B	211	175	C3-C5	-2.67	1.48	1.52
1	A	211	175	O6-C5	2.25	1.26	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	175	O6-C5-N0	-2.42	123.03	125.75
1	A	211	175	C-CA-N0	2.28	119.49	113.58
1	A	211	175	C0-C2-N2	8.18	129.22	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	175	C0-C2-N2	8.53	129.92	112.68

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	211	175	C3
1	A	211	175	C2
1	B	211	175	C3
1	B	211	175	C2

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	CIN	B	1001	-	8,11,14	1.56	2 (25%)	9,13,18	0.38	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	CIN	B	1001	-	-	0/3/5/9	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	CIN	C6-C1	2.19	1.43	1.39
2	B	1001	CIN	C2-C1	2.32	1.43	1.39

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	633/714 (88%)	0.83	84 (13%)  	23, 42, 88, 103	0
1	B	633/714 (88%)	1.09	130 (20%)  	23, 48, 87, 101	0
All	All	1266/1428 (88%)	0.96	214 (16%)  	23, 45, 88, 103	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	ALA	10.0
1	A	124	THR	9.0
1	A	611	VAL	6.5
1	B	239	GLY	6.5
1	A	569	LEU	6.5
1	A	127	ALA	6.4
1	B	254	ASN	6.4
1	B	347	GLU	6.2
1	B	56	THR	6.1
1	B	238	GLU	6.0
1	B	360	GLN	5.8
1	B	134	LEU	5.8
1	B	614	SER	5.7
1	A	40	THR	5.7
1	B	348	GLU	5.6
1	B	237	HIS	5.6
1	A	239	GLY	5.4
1	A	347	GLU	5.3
1	A	561	GLY	5.2
1	B	130	LEU	5.1
1	A	39	THR	5.1
1	B	684	LEU	5.1
1	B	251	ALA	5.0
1	B	359	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	227	GLY	5.0
1	B	553	VAL	5.0
1	A	359	ARG	4.9
1	A	606	GLY	4.8
1	B	40	THR	4.7
1	B	648	ALA	4.7
1	B	463	LEU	4.6
1	A	565	THR	4.6
1	B	260	LEU	4.6
1	B	101	LEU	4.5
1	B	129	SER	4.4
1	B	346	GLU	4.4
1	B	565	THR	4.4
1	B	262	PRO	4.4
1	B	57	ASP	4.3
1	B	563	ALA	4.3
1	A	126	ASP	4.3
1	A	348	GLU	4.3
1	B	608	VAL	4.3
1	B	560	PHE	4.2
1	A	566	GLY	4.2
1	B	236	VAL	4.1
1	B	647	ALA	4.1
1	B	240	LYS	4.0
1	A	101	LEU	4.0
1	A	238	GLU	3.9
1	A	630	ALA	3.9
1	A	41	GLN	3.9
1	A	346	GLU	3.9
1	A	563	ALA	3.8
1	B	605	ALA	3.8
1	A	571	ASP	3.8
1	A	609	VAL	3.8
1	A	617	LEU	3.8
1	B	616	SER	3.8
1	B	148	ASP	3.8
1	B	39	THR	3.8
1	A	619	LEU	3.8
1	A	568	ASN	3.7
1	A	634	ILE	3.7
1	B	345	HIS	3.7
1	A	240	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	128	ILE	3.6
1	A	605	ALA	3.6
1	B	606	GLY	3.6
1	B	124	THR	3.5
1	B	104	GLN	3.5
1	B	685	GLY	3.4
1	B	89	GLU	3.4
1	B	689	VAL	3.4
1	B	465	TYR	3.4
1	B	612	LEU	3.4
1	B	245	TYR	3.4
1	A	553	VAL	3.4
1	B	88	ASP	3.4
1	A	125	GLU	3.4
1	B	242	LYS	3.4
1	A	562	SER	3.4
1	A	552	ILE	3.4
1	B	41	GLN	3.3
1	B	145	SER	3.3
1	B	609	VAL	3.3
1	B	152	LEU	3.3
1	A	403	GLU	3.3
1	B	126	ASP	3.2
1	A	550	PRO	3.2
1	B	561	GLY	3.2
1	B	86	ASP	3.1
1	B	102	ARG	3.1
1	B	625	TRP	3.1
1	A	683	PHE	3.1
1	B	604	ALA	3.1
1	B	58	SER	3.1
1	A	531	VAL	3.1
1	B	400	ILE	3.1
1	B	617	LEU	3.0
1	B	197	HIS	3.0
1	B	568	ASN	3.0
1	B	149	SER	3.0
1	B	255	LEU	3.0
1	A	360	GLN	3.0
1	B	244	LEU	3.0
1	A	256	GLU	3.0
1	B	84	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	463	LEU	2.9
1	B	100	PHE	2.9
1	B	125	GLU	2.9
1	B	233	VAL	2.9
1	B	611	VAL	2.9
1	A	549	GLY	2.9
1	B	622	VAL	2.9
1	B	682	VAL	2.9
1	A	618	SER	2.9
1	A	296	LEU	2.8
1	A	567	SER	2.8
1	A	625	TRP	2.8
1	B	232	LYS	2.8
1	B	243	ILE	2.8
1	B	673	LEU	2.8
1	A	102	ARG	2.8
1	A	614	SER	2.8
1	B	650	THR	2.8
1	B	340	ARG	2.7
1	A	128	ILE	2.7
1	B	252	LEU	2.7
1	A	560	PHE	2.7
1	B	253	PHE	2.7
1	A	574	VAL	2.7
1	B	170	THR	2.7
1	A	616	SER	2.6
1	B	537	LEU	2.6
1	B	179	GLY	2.6
1	A	620	ALA	2.6
1	A	170	THR	2.6
1	A	254	ASN	2.6
1	A	534	ALA	2.5
1	B	569	LEU	2.5
1	B	575	GLU	2.5
1	A	530	CYS	2.5
1	B	654	ALA	2.5
1	B	99	GLU	2.5
1	B	150	PHE	2.5
1	B	83	ARG	2.5
1	B	567	SER	2.4
1	B	96	LYS	2.4
1	B	186	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	646	SER	2.4
1	A	622	VAL	2.4
1	B	259	VAL	2.4
1	B	184	ARG	2.4
1	B	146	SER	2.4
1	B	456	LEU	2.4
1	B	618	SER	2.4
1	B	263	LYS	2.4
1	A	608	VAL	2.3
1	B	343	VAL	2.3
1	A	556	ILE	2.3
1	A	632	SER	2.3
1	B	592	ASP	2.3
1	B	405	LYS	2.3
1	B	550	PRO	2.3
1	A	647	ALA	2.3
1	A	57	ASP	2.3
1	A	402	VAL	2.3
1	B	573	LEU	2.3
1	B	531	VAL	2.3
1	A	183	VAL	2.2
1	A	555	LEU	2.2
1	A	684	LEU	2.2
1	B	499	ASN	2.2
1	A	262	PRO	2.2
1	B	591	TYR	2.2
1	B	687	GLN	2.2
1	B	528	LEU	2.2
1	B	103	SER	2.2
1	B	619	LEU	2.2
1	A	293	SER	2.2
1	B	87	SER	2.2
1	A	221	ILE	2.2
1	B	188	LEU	2.1
1	A	499	ASN	2.1
1	B	183	VAL	2.1
1	A	134	LEU	2.1
1	A	573	LEU	2.1
1	B	542	PHE	2.1
1	B	644	PHE	2.1
1	A	577	VAL	2.1
1	B	258	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	345	HIS	2.1
1	A	638	ARG	2.1
1	A	639	GLN	2.1
1	A	223	ALA	2.1
1	B	571	ASP	2.1
1	B	181	SER	2.1
1	B	572	GLU	2.1
1	A	237	HIS	2.1
1	A	607	THR	2.1
1	A	621	ALA	2.1
1	B	546	LYS	2.1
1	A	454	SER	2.1
1	A	245	TYR	2.1
1	B	535	ILE	2.0
1	A	268	LEU	2.0
1	B	296	LEU	2.0
1	B	607	THR	2.0
1	B	566	GLY	2.0
1	B	645	TRP	2.0
1	B	147	PHE	2.0
1	B	269	VAL	2.0
1	B	657	TYR	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	175	A	211	14/15	0.89	0.15	-	36,40,44,44	0
1	175	B	211	14/15	0.90	0.14	-	37,43,44,45	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CIN	B	1001	11/14	0.61	0.35	7.62	83,84,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.