



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:37 am GMT

PDB ID : 3NZ4
Title : Crystal Structure of a Taxus Phenylalanine Aminomutase
Authors : Feng, L.; Geiger, J.H.
Deposited on : 2010-07-16
Resolution : 2.38 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

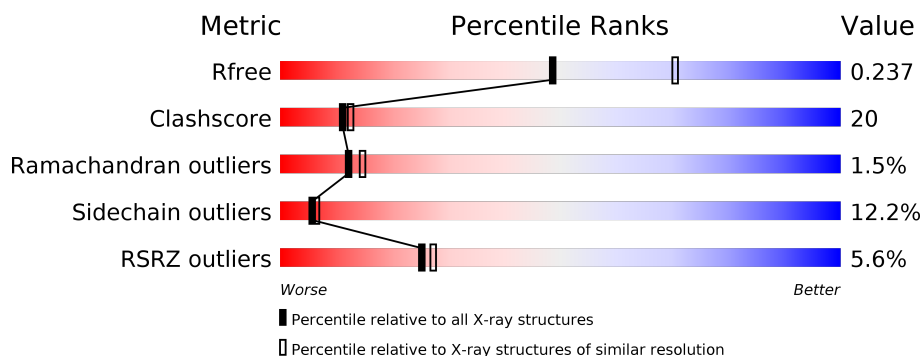
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	100719	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	696	<div> <div>4%</div> <div>60% 27% 6% 6%</div> </div>
1	B	696	<div> <div>6%</div> <div>61% 27% 6% 6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10477 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.

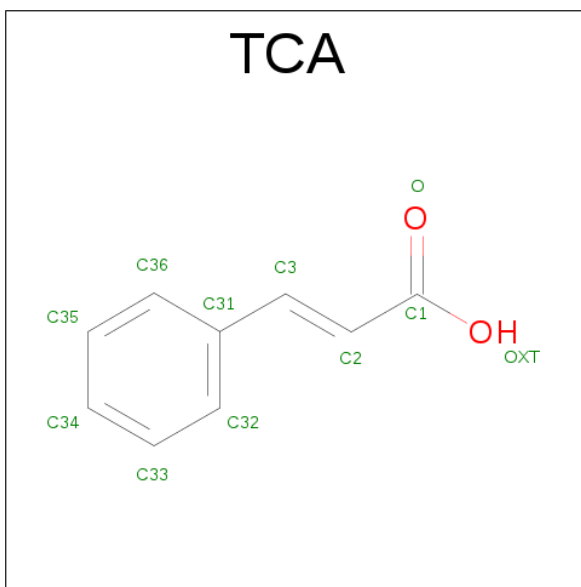
- Molecule 1 is a protein called Phenylalanine ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	2	0
			5086	3219	882	961	24			
1	B	656	Total	C	N	O	S	0	1	0
			5093	3225	882	962	24			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	VAL	ALA	CONFLICT	UNP Q6GZ04
A	196	ILE	VAL	CONFLICT	UNP Q6GZ04
A	473	ASP	GLU	CONFLICT	UNP Q6GZ04
A	556	LYS	GLU	CONFLICT	UNP Q6GZ04
A	634	ASP	GLU	CONFLICT	UNP Q6GZ04
B	128	VAL	ALA	CONFLICT	UNP Q6GZ04
B	196	ILE	VAL	CONFLICT	UNP Q6GZ04
B	473	ASP	GLU	CONFLICT	UNP Q6GZ04
B	556	LYS	GLU	CONFLICT	UNP Q6GZ04
B	634	ASP	GLU	CONFLICT	UNP Q6GZ04

- Molecule 2 is PHENYLETHYLENECARBOXYLIC ACID (three-letter code: TCA) (formula: C₉H₈O₂).



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

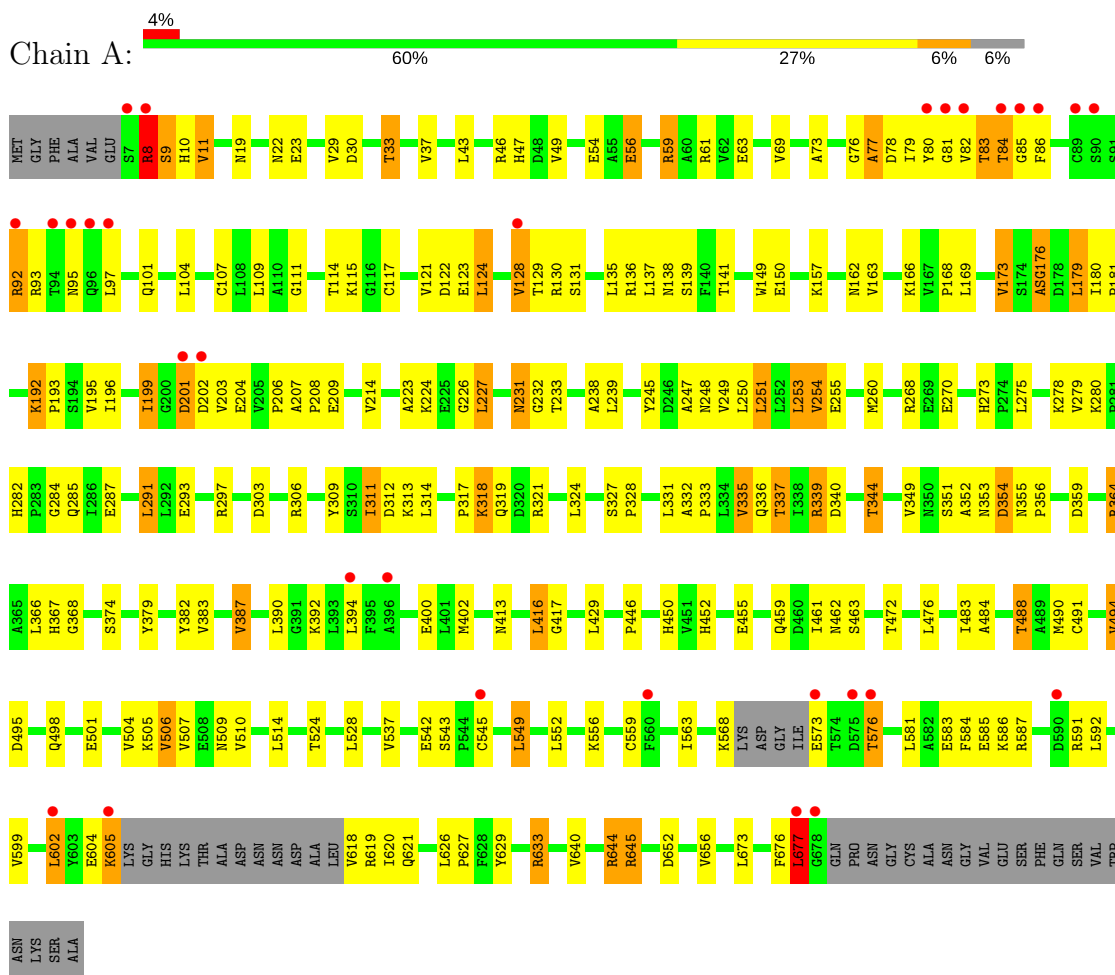
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total	O	0	0
			155	155		
3	B	121	Total	O	0	0
			121	121		

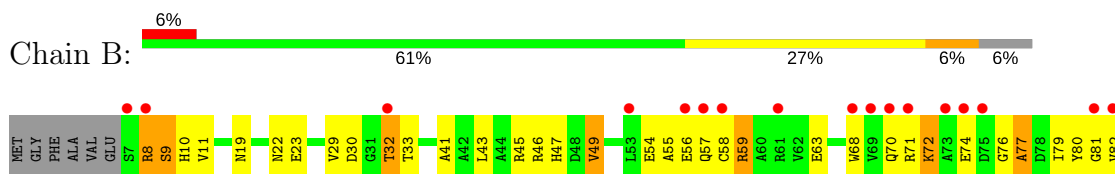
3 Residue-property plots

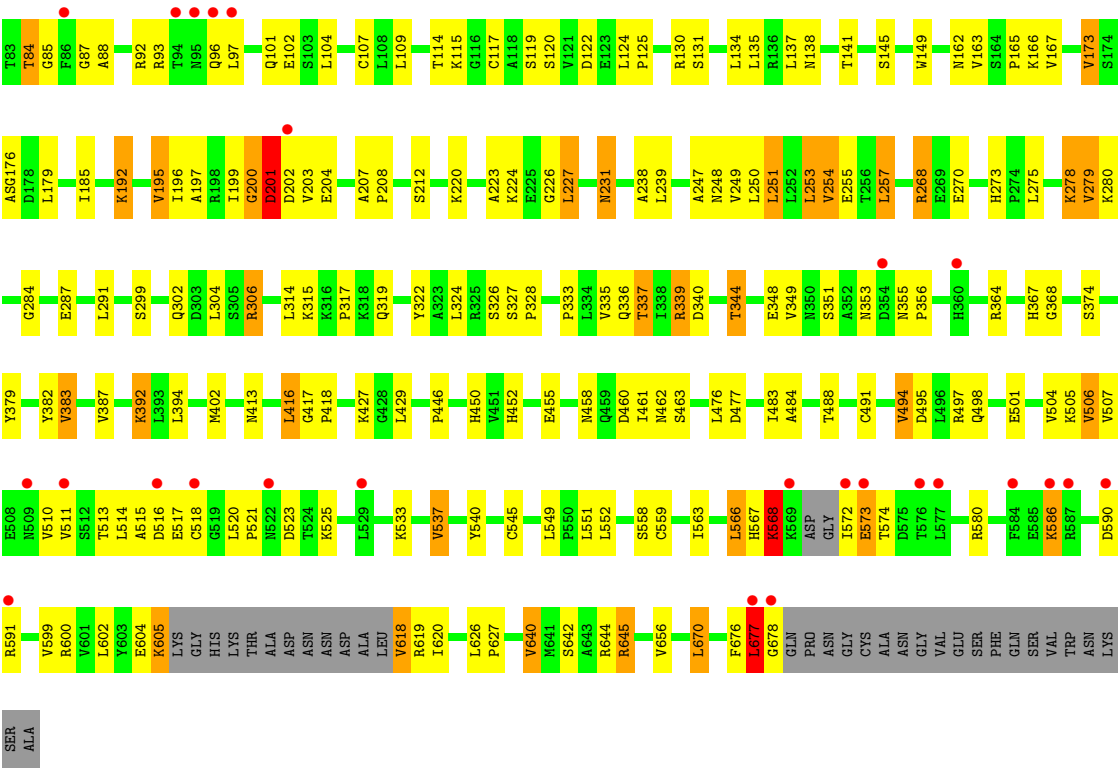
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Phenylalanine ammonia-lyase



• Molecule 1: Phenylalanine ammonia-lyase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.73Å 76.11Å 120.39Å 90.00° 120.43° 90.00°	Depositor
Resolution (Å)	103.81 – 2.38 47.40 – 2.38	Depositor EDS
% Data completeness (in resolution range)	96.8 (103.81-2.38) 96.8 (47.40-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.183 , 0.239 0.183 , 0.237	Depositor DCC
R_{free} test set	5580 reflections (11.24%)	DCC
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10477	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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: MDO, TCA

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	0.50	0/5160	0.64	0/6999
1	B	0.48	0/5166	0.62	0/7006
All	All	0.49	0/10326	0.63	0/14005

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	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	MDO	Mainchain,Peptide
1	B	176	MDO	Mainchain,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	5086	0	5146	224	0
1	B	5093	0	5164	211	1
2	A	11	0	7	1	0
2	B	11	0	7	2	0
3	A	155	0	0	7	0
3	B	121	0	0	8	0
All	All	10477	0	10324	410	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (410) 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:76:GLY:CA	1:A:77:ALA:HB2	1.79	1.13
1:A:402:MET:HE3	1:A:413:ASN:HA	1.13	1.12
1:A:76:GLY:HA2	1:A:77:ALA:HB2	1.12	1.10
1:B:572:ILE:HG13	1:B:573:GLU:H	1.03	1.10
1:B:506:VAL:HG11	1:B:599:VAL:HG21	1.26	1.08
1:A:101:GLN:HE21	1:A:226:GLY:N	1.55	1.04
1:B:114:THR:HG21	1:B:117:CYS:HB2	1.40	1.01
1:B:284:GLY:H	1:B:336:GLN:HE21	1.10	0.96
1:A:76:GLY:HA2	1:A:77:ALA:CB	1.94	0.96
1:B:605:LYS:HE3	1:B:605:LYS:HA	1.50	0.93
1:A:114:THR:HB	1:A:122:ASP:HB2	1.50	0.93
1:A:355:ASN:HD21	1:A:368:GLY:H	1.15	0.93
1:A:402:MET:CE	1:A:413:ASN:HA	1.97	0.92
1:A:417:GLY:HA3	3:A:745:HOH:O	1.69	0.92
1:A:76:GLY:CA	1:A:77:ALA:CB	2.49	0.91
1:A:82:VAL:HG13	1:A:224:LYS:HB2	1.52	0.90
1:B:572:ILE:HG13	1:B:573:GLU:N	1.83	0.90
1:B:417:GLY:HA3	3:B:742:HOH:O	1.72	0.90
1:A:284:GLY:H	1:A:336:GLN:HE21	1.17	0.89
1:A:101:GLN:NE2	1:A:226:GLY:H	1.70	0.89
1:A:101:GLN:NE2	1:A:226:GLY:N	2.21	0.87
1:A:101:GLN:HE21	1:A:226:GLY:H	0.92	0.87
1:A:124:LEU:HG	1:A:128:VAL:HG11	1.55	0.86
1:A:201:ASP:O	1:A:203:VAL:HG13	1.76	0.86
1:A:352:ALA:HB3	1:B:279:VAL:CG1	2.06	0.85
1:A:83:THR:O	1:A:83:THR:HG22	1.77	0.84
1:B:71[A]:ARG:O	1:B:72:LYS:CB	2.25	0.84
1:B:71[B]:ARG:O	1:B:72:LYS:HB2	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLN:HE21	1:B:226:GLY:H	1.26	0.83
1:A:488:THR:HG22	1:A:656:VAL:HG21	1.61	0.83
1:A:506:VAL:HG11	1:A:599:VAL:HG21	1.60	0.82
1:B:114:THR:CG2	1:B:117:CYS:HB2	2.08	0.82
1:A:166:LYS:HE2	3:A:796:HOH:O	1.78	0.82
1:A:104:LEU:HD11	2:A:699:TCA:H33	1.60	0.81
1:B:572:ILE:O	1:B:573:GLU:HB2	1.79	0.81
1:A:157:LYS:HE3	1:A:214:VAL:O	1.81	0.81
1:B:355:ASN:HD21	1:B:368:GLY:H	1.29	0.80
1:A:93:ARG:NH1	1:B:314:LEU:HA	1.97	0.79
1:B:572:ILE:CG1	1:B:573:GLU:H	1.91	0.78
1:B:131:SER:HB3	1:B:238:ALA:HB1	1.64	0.78
1:A:355:ASN:ND2	1:A:368:GLY:H	1.80	0.78
1:B:55:ALA:O	1:B:59:ARG:HB2	1.84	0.78
1:A:78:ASP:O	1:A:79:ILE:HG13	1.83	0.78
1:A:319:GLN:HE21	1:B:367:HIS:HB3	1.49	0.78
1:A:260:MET:HG2	1:A:490:MET:HG2	1.64	0.77
1:B:677:LEU:HG	1:B:678:GLY:H	1.49	0.77
1:A:114:THR:HG22	1:A:115:LYS:N	1.99	0.77
1:B:56:GLU:HG2	3:B:778:HOH:O	1.84	0.77
1:B:604:GLU:OE2	1:B:644:ARG:HD2	1.83	0.77
1:B:402:MET:HE3	1:B:413:ASN:HA	1.66	0.77
1:B:355:ASN:ND2	1:B:368:GLY:H	1.83	0.76
1:A:273:HIS:CD2	1:A:275:LEU:H	2.04	0.76
1:B:506:VAL:CG1	1:B:599:VAL:HG21	2.12	0.76
1:A:114:THR:HG22	1:A:115:LYS:H	1.50	0.76
1:A:382:TYR:OH	1:B:337:THR:HG21	1.86	0.75
1:B:302:GLN:O	1:B:306:ARG:HG3	1.85	0.75
1:A:461:ILE:CD1	1:B:392:LYS:HG3	2.17	0.75
1:A:82:VAL:HG12	1:A:223:ALA:HB1	1.70	0.74
1:B:101:GLN:HE21	1:B:226:GLY:N	1.85	0.74
1:B:165:PRO:HG3	1:B:185:ILE:HD13	1.68	0.74
1:A:166:LYS:HD3	1:A:196:ILE:CG2	2.18	0.74
1:B:498:GLN:NE2	1:B:620:ILE:H	1.85	0.74
1:B:273:HIS:HD2	1:B:275:LEU:H	1.33	0.73
1:B:488:THR:HG22	1:B:656:VAL:HG21	1.71	0.73
1:A:559:CYS:O	1:A:563:ILE:HG23	1.89	0.73
1:B:498:GLN:HE22	1:B:620:ILE:HG22	1.53	0.73
1:B:402:MET:CE	1:B:413:ASN:HA	2.18	0.72
1:B:201:ASP:HB3	1:B:203:VAL:HG13	1.71	0.72
1:A:545:CYS:O	1:A:552:LEU:HD12	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LYS:O	1:B:315:LYS:HG2	1.88	0.72
1:A:248:ASN:HD21	1:A:339:ARG:HE	1.36	0.72
1:A:352:ALA:HB3	1:B:279:VAL:HG13	1.71	0.72
1:A:273:HIS:HD2	1:A:275:LEU:H	1.36	0.71
1:B:516:ASP:OD2	1:B:525:LYS:NZ	2.22	0.71
1:B:71[A]:ARG:O	1:B:72:LYS:HB3	1.90	0.71
1:A:82:VAL:O	1:A:83:THR:OG1	2.08	0.71
1:B:200:GLY:O	1:B:202:ASP:N	2.21	0.71
1:A:201:ASP:O	1:A:203:VAL:N	2.20	0.70
1:B:567:HIS:O	1:B:568:LYS:HB3	1.90	0.70
1:A:676:PHE:O	1:A:677:LEU:O	2.09	0.69
1:A:82:VAL:CG1	1:A:224:LYS:HB2	2.23	0.69
1:A:232:GLY:HA2	1:A:353:ASN:HD22	1.58	0.69
1:A:484:ALA:O	1:A:488:THR:HG23	1.92	0.69
1:A:83:THR:O	1:A:83:THR:CG2	2.42	0.68
1:A:233:THR:H	1:A:353:ASN:ND2	1.92	0.68
1:A:270:GLU:OE1	1:B:367:HIS:HD2	1.77	0.68
1:A:461:ILE:HD11	1:B:392:LYS:HG3	1.74	0.68
1:A:293:GLU:OE1	1:A:297:ARG:NH1	2.26	0.68
1:A:337:THR:HG21	1:B:382:TYR:OH	1.93	0.67
1:B:173:VAL:HG13	1:B:462:ASN:HB2	1.75	0.67
1:B:80:TYR:H	1:B:367:HIS:HE1	1.43	0.67
1:B:545:CYS:O	1:B:552:LEU:HD12	1.95	0.67
1:B:104:LEU:HD11	2:B:699:TCA:H33	1.77	0.66
1:A:383:VAL:HG23	1:A:472:THR:HG21	1.75	0.66
1:B:101:GLN:NE2	1:B:226:GLY:H	1.93	0.66
1:A:82:VAL:O	1:A:83:THR:CB	2.42	0.66
1:B:273:HIS:CD2	1:B:275:LEU:H	2.13	0.66
1:B:501:GLU:O	1:B:504:VAL:HG12	1.96	0.66
1:A:166:LYS:HD3	1:A:196:ILE:HG23	1.76	0.66
1:A:303:ASP:OD1	1:A:306:ARG:NH1	2.29	0.66
1:B:131:SER:CB	1:B:238:ALA:HB1	2.25	0.66
1:A:253:LEU:HD13	1:A:483:ILE:HG21	1.76	0.66
1:B:284:GLY:H	1:B:336:GLN:NE2	1.90	0.66
1:B:340:ASP:O	1:B:344:THR:HG23	1.96	0.66
1:B:114:THR:HG21	1:B:117:CYS:CB	2.22	0.66
1:A:450:HIS:O	1:A:452:HIS:HD2	1.79	0.65
1:A:321:ARG:HG2	1:B:458:ASN:HA	1.77	0.65
1:B:559:CYS:O	1:B:563:ILE:HG23	1.96	0.65
1:B:501:GLU:OE1	1:B:619:ARG:HD2	1.95	0.65
1:B:124:LEU:HD12	1:B:125:PRO:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:VAL:HG13	1:A:82:VAL:HG11	1.77	0.65
1:B:101:GLN:NE2	1:B:226:GLY:N	2.45	0.65
1:B:333:PRO:O	1:B:337:THR:CG2	2.45	0.65
1:B:71[B]:ARG:O	1:B:72:LYS:CB	2.46	0.64
1:A:10:HIS:HE1	1:A:255:GLU:OE1	1.79	0.64
1:B:101:GLN:HE22	1:B:227:LEU:H	1.45	0.64
1:A:250:LEU:O	1:A:254:VAL:HG13	1.97	0.64
1:A:73:ALA:HB1	1:A:97:LEU:HD13	1.78	0.64
1:A:232:GLY:CA	1:A:353:ASN:HD22	2.11	0.64
1:B:306:ARG:HH11	1:B:306:ARG:HB3	1.63	0.63
1:B:572:ILE:O	1:B:573:GLU:CB	2.45	0.63
1:A:163:VAL:HG22	1:A:199:ILE:HG23	1.79	0.63
1:B:166:LYS:HB2	1:B:196:ILE:HG23	1.80	0.63
1:B:224:LYS:HG3	1:B:224:LYS:O	1.98	0.63
1:B:76:GLY:O	1:B:77:ALA:O	2.17	0.63
1:B:81:GLY:HA2	1:B:227:LEU:HD12	1.79	0.63
1:B:163:VAL:HG22	1:B:199:ILE:HD13	1.81	0.63
1:A:81:GLY:HA2	1:A:227:LEU:HD12	1.81	0.63
1:A:311:ILE:O	1:A:312:ASP:HB2	1.98	0.63
1:B:253:LEU:HD13	1:B:483:ILE:HG21	1.81	0.62
1:A:510:VAL:O	1:A:514:LEU:HB2	1.99	0.62
1:B:43:LEU:O	1:B:130:ARG:NH2	2.31	0.62
1:B:192:LYS:O	1:B:195:VAL:HG13	1.99	0.62
1:A:111:GLY:HA3	1:A:168:PRO:HG2	1.80	0.61
1:B:202:ASP:O	1:B:204:GLU:HG2	1.99	0.61
1:B:510:VAL:O	1:B:514:LEU:HB2	1.99	0.61
1:A:124:LEU:HD13	1:A:169:LEU:HD12	1.82	0.61
1:A:340:ASP:O	1:A:344:THR:HG23	2.01	0.61
1:A:268:ARG:NH2	1:A:317:PRO:O	2.33	0.60
1:A:367:HIS:HB3	1:B:319:GLN:HE21	1.66	0.60
1:B:71[A]:ARG:O	1:B:72:LYS:HB2	2.01	0.60
1:B:46:ARG:O	1:B:49:VAL:HG13	2.01	0.60
1:B:379:TYR:O	1:B:383:VAL:HG12	2.02	0.60
1:A:260:MET:CG	1:A:490:MET:HG2	2.31	0.60
1:A:501:GLU:OE1	1:A:619:ARG:HD2	2.02	0.60
1:B:10:HIS:HD2	1:B:287:GLU:OE1	1.85	0.60
1:B:268:ARG:NH2	1:B:317:PRO:O	2.29	0.60
1:A:604:GLU:O	1:A:605:LYS:C	2.39	0.59
1:A:248:ASN:ND2	1:A:339:ARG:HE	2.00	0.59
1:B:43:LEU:HD22	1:B:134:LEU:HD22	1.84	0.59
1:B:165:PRO:CG	1:B:185:ILE:HD13	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:TYR:H	1:A:367:HIS:HE1	1.50	0.59
1:A:461:ILE:HD12	1:B:392:LYS:HG3	1.84	0.59
1:B:333:PRO:O	1:B:337:THR:HG23	2.01	0.59
1:B:450:HIS:O	1:B:452:HIS:HD2	1.86	0.59
1:A:30:ASP:OD1	1:A:33:THR:HG22	2.03	0.58
1:B:79:ILE:HB	1:B:82:VAL:HG22	1.85	0.58
1:A:114:THR:CG2	1:A:115:LYS:H	2.16	0.58
1:A:402:MET:HE3	1:A:413:ASN:CA	2.09	0.58
1:B:600:ARG:NH2	3:B:776:HOH:O	2.28	0.58
1:A:284:GLY:H	1:A:336:GLN:NE2	1.94	0.58
1:B:192:LYS:HG3	3:B:757:HOH:O	2.04	0.58
1:B:416:LEU:HD13	1:B:417:GLY:N	2.18	0.58
1:A:114:THR:HB	1:A:122:ASP:CB	2.30	0.58
1:A:10:HIS:HD2	1:A:287:GLU:OE1	1.86	0.58
1:A:101:GLN:HE21	1:A:226:GLY:CA	2.17	0.57
1:A:318:LYS:HG3	1:A:318:LYS:O	2.04	0.57
1:A:355:ASN:ND2	1:A:356:PRO:HA	2.19	0.57
1:A:645:ARG:NH1	1:A:652:ASP:OD2	2.37	0.57
1:B:47:HIS:HD2	1:B:162:ASN:OD1	1.86	0.57
1:A:173:VAL:HG13	1:A:462:ASN:HB2	1.84	0.57
1:A:101:GLN:NE2	1:A:226:GLY:CA	2.67	0.57
1:A:556:LYS:HE2	1:A:585:GLU:OE2	2.04	0.57
1:B:19:ASN:HB3	1:B:23:GLU:OE2	2.05	0.57
1:A:114:THR:CG2	1:A:115:LYS:N	2.68	0.57
1:A:383:VAL:O	1:A:387:VAL:HG13	2.05	0.56
1:B:484:ALA:O	1:B:488:THR:HG23	2.04	0.56
1:A:291:LEU:HD21	1:A:673:LEU:HD22	1.86	0.56
1:A:92:ARG:HA	1:A:92:ARG:CZ	2.36	0.56
1:A:273:HIS:HD2	1:A:275:LEU:N	2.04	0.56
1:B:223:ALA:O	1:B:224:LYS:HB3	2.05	0.56
1:B:506:VAL:O	1:B:510:VAL:HG23	2.05	0.56
1:B:284:GLY:N	1:B:336:GLN:HE21	1.92	0.56
1:B:495:ASP:CB	1:B:640:VAL:HG13	2.36	0.56
1:A:29:VAL:HG13	1:A:138:ASN:HD22	1.71	0.55
1:A:344:THR:HB	3:B:744:HOH:O	2.05	0.55
1:B:166:LYS:HE3	1:B:196:ILE:HG21	1.88	0.55
1:A:383:VAL:CG2	1:A:472:THR:HG21	2.36	0.55
1:A:59:ARG:HG2	1:A:149:TRP:CD2	2.42	0.55
1:A:364:ARG:HD3	1:A:366:LEU:HD21	1.88	0.55
1:A:56:GLU:HA	1:A:56:GLU:OE2	2.05	0.55
1:A:131:SER:HB3	1:A:238:ALA:HB1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:HIS:O	1:B:567:HIS:CG	2.59	0.55
1:B:114:THR:HG22	1:B:115:LYS:N	2.22	0.54
1:B:79:ILE:HB	1:B:82:VAL:CG2	2.37	0.54
1:A:86:PHE:CE1	1:A:104:LEU:HB2	2.43	0.54
1:B:540:TYR:CE1	1:B:551:LEU:HD22	2.42	0.54
1:B:498:GLN:HE21	1:B:620:ILE:H	1.54	0.54
1:B:248:ASN:HD21	1:B:339:ARG:HE	1.55	0.54
1:A:166:LYS:HD3	1:A:196:ILE:HG21	1.87	0.54
1:A:46:ARG:O	1:A:49:VAL:HG12	2.08	0.54
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.89	0.54
1:A:101:GLN:HE22	1:A:227:LEU:H	1.56	0.54
1:A:333:PRO:O	1:A:337:THR:CG2	2.55	0.54
1:A:114:THR:HG21	1:A:117:CYS:HB2	1.90	0.54
1:A:128:VAL:HG12	1:A:129:THR:N	2.23	0.54
1:A:573:GLU:OE1	1:A:576:THR:HG21	2.08	0.54
1:B:101:GLN:HE21	1:B:226:GLY:CA	2.21	0.54
1:B:29:VAL:HG13	1:B:138:ASN:HD22	1.73	0.53
1:B:416:LEU:O	1:B:417:GLY:C	2.47	0.53
1:A:491:CYS:HA	1:A:494:VAL:HG13	1.89	0.53
1:B:383:VAL:O	1:B:387:VAL:HG13	2.07	0.53
1:B:495:ASP:HB3	1:B:640:VAL:HG13	1.89	0.53
1:B:355:ASN:ND2	1:B:356:PRO:HA	2.24	0.53
1:A:400:GLU:OE2	1:B:460:ASP:OD2	2.26	0.53
1:A:124:LEU:HG	1:A:128:VAL:CG1	2.32	0.52
1:A:270:GLU:OE1	1:B:367:HIS:CD2	2.61	0.52
1:A:80:TYR:HD1	1:A:84:THR:HG21	1.74	0.52
1:A:446:PRO:HD3	1:B:446:PRO:HD3	1.91	0.52
1:B:88:ALA:HB2	1:B:458:ASN:HB2	1.90	0.52
1:B:114:THR:CG2	1:B:115:LYS:N	2.73	0.52
1:B:201:ASP:C	1:B:203:VAL:H	2.13	0.52
1:B:333:PRO:O	1:B:337:THR:HG22	2.10	0.52
1:B:30:ASP:OD1	1:B:33:THR:HG23	2.10	0.52
1:A:284:GLY:N	1:A:336:GLN:HE21	1.97	0.52
1:A:353:ASN:O	1:A:354:ASP:HB2	2.09	0.52
1:A:76:GLY:HA3	1:A:77:ALA:HB2	1.84	0.52
1:B:416:LEU:HD22	1:B:416:LEU:C	2.29	0.52
1:A:417:GLY:HA2	1:A:644:ARG:HH22	1.74	0.52
1:A:43:LEU:HD12	3:A:845:HOH:O	2.10	0.51
1:A:333:PRO:O	1:A:337:THR:HG22	2.10	0.51
1:B:339:ARG:HG2	3:B:753:HOH:O	2.11	0.51
1:B:82:VAL:HG13	1:B:224:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71[B]:ARG:NH1	1:B:74:GLU:OE1	2.44	0.51
1:B:513:THR:O	1:B:517:GLU:HG3	2.11	0.51
1:B:537:VAL:HA	1:B:540:TYR:CE2	2.45	0.51
1:A:136:ARG:NH1	1:A:231:ASN:O	2.35	0.51
1:A:352:ALA:HB3	1:B:279:VAL:HG11	1.89	0.51
1:A:121:VAL:O	1:A:122:ASP:CG	2.49	0.51
1:A:37:VAL:HG13	1:A:245:TYR:HB2	1.92	0.51
1:B:201:ASP:O	1:B:202:ASP:HB3	2.11	0.51
1:A:335:VAL:O	1:A:339:ARG:HB2	2.11	0.51
1:A:59:ARG:O	1:A:63:GLU:HG3	2.11	0.50
1:B:87:GLY:HA3	1:B:455:GLU:OE2	2.11	0.50
1:B:626:LEU:HB3	1:B:627:PRO:HD3	1.93	0.50
1:A:122:ASP:OD2	1:A:122:ASP:C	2.50	0.50
1:B:568:LYS:O	1:B:568:LYS:HG2	2.10	0.50
1:A:285:GLN:HB2	1:A:332:ALA:HB2	1.94	0.49
1:B:278:LYS:HD2	1:B:278:LYS:C	2.32	0.49
1:A:677:LEU:C	1:A:677:LEU:HD23	2.32	0.49
1:A:629:TYR:O	1:A:633:ARG:HB2	2.12	0.49
1:A:11:VAL:HG11	1:A:676:PHE:HE2	1.77	0.49
1:A:507:VAL:HG22	1:A:592:LEU:HD11	1.95	0.49
1:B:247:ALA:O	1:B:251:LEU:HB2	2.12	0.49
1:B:248:ASN:ND2	1:B:339:ARG:HE	2.10	0.49
1:A:192:LYS:HG3	3:A:738:HOH:O	2.12	0.49
1:A:166:LYS:HD2	1:A:204:GLU:OE2	2.13	0.49
1:A:93:ARG:HH11	1:B:314:LEU:HD23	1.76	0.49
1:A:314:LEU:HD23	1:B:93:ARG:HH11	1.78	0.48
1:A:327:SER:OG	1:A:328:PRO:HD3	2.13	0.48
1:B:567:HIS:HB2	1:B:574:THR:OG1	2.13	0.48
1:B:207:ALA:HB3	1:B:208:PRO:HD3	1.95	0.48
1:B:344:THR:HG22	3:B:711:HOH:O	2.13	0.48
1:B:495:ASP:HB3	1:B:640:VAL:CG1	2.43	0.48
1:A:383:VAL:HG23	1:A:472:THR:CG2	2.42	0.48
1:A:80:TYR:CD1	1:A:84:THR:HG21	2.48	0.48
1:A:128:VAL:CG1	1:A:129:THR:N	2.75	0.48
1:B:642:SER:OG	1:B:644:ARG:HG2	2.13	0.48
1:A:282:HIS:HB3	1:A:336:GLN:HE22	1.78	0.48
1:B:618:VAL:O	1:B:618:VAL:CG2	2.62	0.48
1:A:354:ASP:HB2	3:A:748:HOH:O	2.13	0.48
1:B:677:LEU:CG	1:B:678:GLY:H	2.20	0.48
1:B:192:LYS:O	1:B:195:VAL:CG1	2.61	0.47
1:B:379:TYR:O	1:B:383:VAL:CG1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:SER:HA	1:A:463:SER:HB2	1.96	0.47
1:A:450:HIS:O	1:A:452:HIS:CD2	2.65	0.47
1:B:85:GLY:N	1:B:92:ARG:O	2.47	0.47
1:A:80:TYR:CD1	1:A:84:THR:CG2	2.98	0.47
1:B:101:GLN:NE2	1:B:226:GLY:CA	2.77	0.47
1:B:572:ILE:CG1	1:B:573:GLU:N	2.62	0.47
1:B:231:ASN:HD22	1:B:231:ASN:HA	1.53	0.47
1:A:254:VAL:HG21	1:A:390:LEU:HD22	1.97	0.47
1:A:47:HIS:HD2	1:A:162:ASN:OD1	1.97	0.47
1:A:498:GLN:NE2	1:A:620:ILE:H	2.13	0.47
1:B:59:ARG:HG2	1:B:149:TRP:CE2	2.50	0.47
1:B:55:ALA:HB1	1:B:59:ARG:HG3	1.96	0.47
1:B:605:LYS:HA	1:B:605:LYS:CE	2.23	0.47
1:B:41:ALA:O	1:B:45:ARG:HB2	2.15	0.47
1:A:130:ARG:NH2	3:A:845:HOH:O	2.47	0.46
1:A:223:ALA:O	1:A:224:LYS:HB3	2.15	0.46
1:A:131:SER:CB	1:A:238:ALA:HB1	2.45	0.46
1:A:461:ILE:HG22	1:B:322:TYR:HB3	1.97	0.46
1:B:192:LYS:HB3	1:B:195:VAL:HG12	1.97	0.46
1:B:450:HIS:O	1:B:452:HIS:CD2	2.68	0.46
1:A:207:ALA:N	1:A:208:PRO:CD	2.79	0.46
1:B:59:ARG:NH1	1:B:63:GLU:OE2	2.48	0.46
1:B:676:PHE:O	1:B:677:LEU:C	2.54	0.46
1:B:10:HIS:HE1	1:B:255:GLU:OE1	1.99	0.46
1:B:80:TYR:H	1:B:367:HIS:CE1	2.29	0.46
1:A:618:VAL:HG23	1:A:621:GLN:OE1	2.16	0.46
1:A:626:LEU:HB3	1:A:627:PRO:HD3	1.96	0.46
1:B:227:LEU:O	1:B:231:ASN:HB2	2.15	0.46
1:B:84:THR:HG22	1:B:85:GLY:O	2.15	0.46
1:A:506:VAL:CG1	1:A:599:VAL:HG21	2.39	0.46
1:B:322:TYR:O	1:B:326:SER:HB3	2.16	0.46
1:A:247:ALA:O	1:A:251:LEU:HB2	2.16	0.45
1:B:200:GLY:C	1:B:202:ASP:H	2.15	0.45
1:B:306:ARG:NH1	1:B:306:ARG:HB3	2.29	0.45
1:B:586:LYS:HB3	1:B:586:LYS:HE3	1.84	0.45
1:B:677:LEU:HG	1:B:678:GLY:N	2.26	0.45
1:A:93:ARG:HG3	1:B:314:LEU:HD22	1.97	0.45
1:A:93:ARG:HH11	1:B:314:LEU:CD2	2.30	0.45
1:A:416:LEU:C	1:A:416:LEU:CD2	2.85	0.45
1:B:10:HIS:CD2	1:B:287:GLU:OE1	2.68	0.45
1:A:150:GLU:CD	1:A:150:GLU:H	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLU:HG3	1:A:543:SER:N	2.32	0.45
1:A:84:THR:HG23	1:A:85:GLY:O	2.17	0.45
1:A:86:PHE:CD1	1:A:104:LEU:HD13	2.52	0.45
1:A:573:GLU:OE1	1:A:576:THR:CG2	2.65	0.45
1:B:515:ALA:HA	1:B:520:LEU:HD22	1.99	0.45
1:B:68:TRP:O	1:B:71[A]:ARG:O	2.35	0.45
1:A:180:ILE:HB	1:A:181:PRO:HD3	1.99	0.44
1:A:618:VAL:HG22	1:A:618:VAL:O	2.17	0.44
1:B:166:LYS:CE	1:B:196:ILE:HG21	2.47	0.44
1:B:491:CYS:HA	1:B:494:VAL:HG13	1.98	0.44
1:A:416:LEU:HD22	1:A:416:LEU:C	2.38	0.44
1:A:495:ASP:CB	1:A:640:VAL:HG12	2.47	0.44
1:A:640:VAL:HG23	1:A:640:VAL:O	2.17	0.44
1:B:82:VAL:CG1	1:B:224:LYS:HB2	2.47	0.44
1:A:331:LEU:O	1:A:335:VAL:HG13	2.18	0.44
1:A:8:ARG:O	1:A:9:SER:HB2	2.18	0.44
1:A:355:ASN:HD21	1:A:368:GLY:N	1.98	0.44
1:A:80:TYR:O	1:A:84:THR:HG22	2.18	0.44
1:B:327:SER:OG	1:B:328:PRO:HD3	2.18	0.44
1:A:501:GLU:O	1:A:504:VAL:HG12	2.18	0.44
1:A:176:MDO:CB2	1:A:179:LEU:HD21	2.48	0.43
1:A:313:LYS:HG3	1:A:314:LEU:N	2.33	0.43
1:A:8:ARG:O	1:A:9:SER:CB	2.65	0.43
1:B:250:LEU:O	1:B:254:VAL:HG13	2.17	0.43
1:B:645:ARG:HG3	1:B:645:ARG:O	2.18	0.43
1:A:206:PRO:HG2	1:A:209:GLU:OE2	2.18	0.43
1:B:114:THR:HB	1:B:122:ASP:CB	2.48	0.43
1:A:135:LEU:HD22	1:A:349:VAL:HG13	1.99	0.43
1:A:233:THR:H	1:A:353:ASN:HD22	1.66	0.43
1:A:78:ASP:C	1:A:79:ILE:HG13	2.38	0.43
1:B:117:CYS:HB3	1:B:120:SER:O	2.19	0.43
1:A:280:LYS:HE3	1:B:348:GLU:OE1	2.18	0.43
1:B:518:CYS:O	1:B:580:ARG:HD3	2.19	0.43
1:A:581:LEU:O	1:A:584:PHE:HB3	2.18	0.43
1:B:335:VAL:O	1:B:339:ARG:HB2	2.18	0.43
1:A:79:ILE:HB	1:A:82:VAL:HG23	2.01	0.43
1:A:80:TYR:HB3	1:A:367:HIS:CE1	2.54	0.42
1:A:367:HIS:HD2	1:B:270:GLU:OE1	2.02	0.42
1:A:10:HIS:CD2	1:A:287:GLU:OE1	2.69	0.42
1:A:192:LYS:HA	1:A:193:PRO:HD3	1.89	0.42
1:A:505:LYS:HB3	1:A:505:LYS:HE2	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:MET:HE3	1:A:413:ASN:HD22	1.85	0.42
1:A:80:TYR:CB	1:A:367:HIS:CE1	3.02	0.42
1:B:417:GLY:HA2	1:B:418:PRO:HD3	1.91	0.42
1:B:670:LEU:N	1:B:670:LEU:HD23	2.35	0.42
1:A:19:ASN:HB3	1:A:23:GLU:OE2	2.20	0.42
1:B:8:ARG:O	1:B:9:SER:CB	2.68	0.42
1:B:68:TRP:CZ2	1:B:72:LYS:HE3	2.55	0.42
1:A:92:ARG:NE	1:A:92:ARG:HA	2.35	0.42
1:B:32:THR:HG21	1:B:57:GLN:OE1	2.19	0.42
1:B:604:GLU:O	1:B:605:LYS:C	2.57	0.42
1:A:364:ARG:HG2	1:A:364:ARG:HH11	1.84	0.42
1:A:379:TYR:O	1:A:383:VAL:HG13	2.19	0.41
1:A:583:GLU:O	1:A:587:ARG:HG2	2.20	0.41
1:B:114:THR:HB	1:B:122:ASP:HB2	2.02	0.41
1:B:251:LEU:HD11	1:B:335:VAL:HB	2.02	0.41
1:B:507:VAL:O	1:B:511:VAL:HG23	2.19	0.41
1:A:10:HIS:HB2	1:A:339:ARG:HD3	2.00	0.41
1:A:351:SER:HB2	1:B:280:LYS:HA	2.02	0.41
1:B:374:SER:HA	1:B:463:SER:HB2	2.02	0.41
1:A:459:GLN:NE2	3:A:811:HOH:O	2.37	0.41
1:B:201:ASP:O	1:B:202:ASP:CB	2.66	0.41
1:A:29:VAL:HG12	1:A:141:THR:HG21	2.01	0.41
1:A:260:MET:HG2	1:A:490:MET:CG	2.42	0.41
1:A:30:ASP:OD1	1:A:33:THR:CG2	2.67	0.41
1:A:402:MET:CE	1:A:413:ASN:HD22	2.33	0.41
1:A:359:ASP:HB3	1:A:364:ARG:HD2	2.02	0.41
1:A:524:THR:O	1:A:528:LEU:HG	2.20	0.41
1:B:173:VAL:HG13	1:B:173:VAL:O	2.20	0.41
1:B:173:VAL:CG1	1:B:462:ASN:HB2	2.48	0.41
1:A:333:PRO:O	1:A:337:THR:HG23	2.21	0.41
1:A:490:MET:O	1:A:494:VAL:HG12	2.20	0.41
1:A:583:GLU:OE2	1:A:587:ARG:NE	2.48	0.41
1:B:196:ILE:HG13	1:B:197:ALA:N	2.36	0.41
1:A:231:ASN:HA	1:A:231:ASN:HD22	1.54	0.41
1:B:427:LYS:N	3:B:714:HOH:O	2.53	0.41
1:B:520:LEU:HA	1:B:521:PRO:HD3	1.90	0.41
1:A:549:LEU:HD12	1:A:549:LEU:HA	1.80	0.41
1:A:602:LEU:HD22	1:A:602:LEU:HA	1.98	0.41
1:A:280:LYS:HA	1:B:351:SER:HB2	2.03	0.41
1:B:677:LEU:CG	1:B:678:GLY:N	2.83	0.41
1:A:309:TYR:O	1:A:313:LYS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:LEU:HD22	1:B:257:LEU:HD22	2.03	0.40
1:B:135:LEU:HD22	1:B:349:VAL:HG13	2.03	0.40
1:A:114:THR:CG2	1:A:117:CYS:HB2	2.51	0.40
1:A:251:LEU:HD11	1:A:335:VAL:HB	2.04	0.40
1:A:273:HIS:CD2	1:A:275:LEU:HB3	2.56	0.40
1:A:8:ARG:CG	1:A:9:SER:H	2.34	0.40
1:B:220:LYS:HD3	1:B:220:LYS:HA	1.86	0.40
1:B:80:TYR:OH	2:B:699:TCA:C3	2.69	0.40
1:B:82:VAL:HG12	1:B:223:ALA:HB1	2.04	0.40
1:B:327:SER:N	1:B:328:PRO:CD	2.85	0.40
1:A:498:GLN:HE22	1:A:620:ILE:HG22	1.87	0.40
1:B:567:HIS:O	1:B:568:LYS:CB	2.67	0.40
1:B:498:GLN:HE22	1:B:620:ILE:H	1.67	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:SER:OG	1:B:477:ASP:OD2[2_556]	2.15	0.05

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	649/696 (93%)	618 (95%)	23 (4%)	8 (1%)	15	20
1	B	650/696 (93%)	602 (93%)	37 (6%)	11 (2%)	11	12
All	All	1299/1392 (93%)	1220 (94%)	60 (5%)	19 (2%)	12	15

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	77	ALA
1	A	83	THR
1	A	677	LEU
1	B	9	SER
1	B	72	LYS
1	B	77	ALA
1	B	201	ASP
1	B	568	LYS
1	B	573	GLU
1	A	201	ASP
1	A	202	ASP
1	B	566	LEU
1	B	677	LEU
1	A	354	ASP
1	B	70	GLN
1	B	8	ARG
1	A	8	ARG
1	B	200	GLY

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	556/586 (95%)	492 (88%)	64 (12%)	6	8
1	B	557/586 (95%)	486 (87%)	71 (13%)	5	6
All	All	1113/1172 (95%)	978 (88%)	135 (12%)	6	6

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	11	VAL
1	A	22	ASN
1	A	33	THR
1	A	54	GLU

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Mol	Chain	Res	Type
1	A	56	GLU
1	A	59	ARG
1	A	61	ARG
1	A	84	THR
1	A	92	ARG
1	A	95	ASN
1	A	107	CYS
1	A	109	LEU
1	A	123	GLU
1	A	124	LEU
1	A	128	VAL
1	A	137	LEU
1	A	139	SER
1	A	173	VAL
1	A	179	LEU
1	A	192	LYS
1	A	195	VAL
1	A	199	ILE
1	A	227	LEU
1	A	231	ASN
1	A	239	LEU
1	A	249	VAL
1	A	251	LEU
1	A	253	LEU
1	A	254	VAL
1	A	278	LYS
1	A	279	VAL
1	A	291	LEU
1	A	311	ILE
1	A	318	LYS
1	A	324	LEU
1	A	335	VAL
1	A	337	THR
1	A	339	ARG
1	A	344	THR
1	A	364	ARG
1	A	387	VAL
1	A	392	LYS
1	A	394	LEU
1	A	416	LEU
1	A	429	LEU
1	A	455	GLU

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Mol	Chain	Res	Type
1	A	476	LEU
1	A	488	THR
1	A	494	VAL
1	A	506	VAL
1	A	509	ASN
1	A	537	VAL
1	A	549	LEU
1	A	568	LYS
1	A	576	THR
1	A	586	LYS
1	A	591	ARG
1	A	602	LEU
1	A	605	LYS
1	A	633	ARG
1	A	644	ARG
1	A	645	ARG
1	A	677	LEU
1	B	11	VAL
1	B	22	ASN
1	B	32	THR
1	B	49	VAL
1	B	54	GLU
1	B	58	CYS
1	B	59	ARG
1	B	84	THR
1	B	96	GLN
1	B	97	LEU
1	B	102	GLU
1	B	107	CYS
1	B	109	LEU
1	B	137	LEU
1	B	145	SER
1	B	167	VAL
1	B	173	VAL
1	B	179	LEU
1	B	192	LYS
1	B	195	VAL
1	B	201	ASP
1	B	212	SER
1	B	227	LEU
1	B	231	ASN
1	B	239	LEU

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Mol	Chain	Res	Type
1	B	249	VAL
1	B	251	LEU
1	B	253	LEU
1	B	254	VAL
1	B	257	LEU
1	B	268	ARG
1	B	278	LYS
1	B	279	VAL
1	B	291	LEU
1	B	299	SER
1	B	304	LEU
1	B	306	ARG
1	B	324	LEU
1	B	337	THR
1	B	339	ARG
1	B	344	THR
1	B	353	ASN
1	B	364	ARG
1	B	383	VAL
1	B	392	LYS
1	B	394	LEU
1	B	416	LEU
1	B	429	LEU
1	B	461	ILE
1	B	476	LEU
1	B	494	VAL
1	B	497	ARG
1	B	505	LYS
1	B	506	VAL
1	B	523	ASP
1	B	533	LYS
1	B	537	VAL
1	B	549	LEU
1	B	558	SER
1	B	566	LEU
1	B	568	LYS
1	B	586	LYS
1	B	590	ASP
1	B	591	ARG
1	B	602	LEU
1	B	605	LYS
1	B	618	VAL

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Mol	Chain	Res	Type
1	B	640	VAL
1	B	645	ARG
1	B	670	LEU
1	B	677	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	19	ASN
1	A	47	HIS
1	A	101	GLN
1	A	138	ASN
1	A	231	ASN
1	A	248	ASN
1	A	273	HIS
1	A	319	GLN
1	A	336	GLN
1	A	353	ASN
1	A	355	ASN
1	A	367	HIS
1	A	413	ASN
1	A	452	HIS
1	A	459	GLN
1	A	486	HIS
1	A	498	GLN
1	A	594	ASN
1	B	10	HIS
1	B	19	ASN
1	B	47	HIS
1	B	96	GLN
1	B	101	GLN
1	B	138	ASN
1	B	231	ASN
1	B	248	ASN
1	B	273	HIS
1	B	319	GLN
1	B	336	GLN
1	B	355	ASN
1	B	367	HIS
1	B	413	ASN
1	B	452	HIS

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Mol	Chain	Res	Type
1	B	459	GLN
1	B	498	GLN
1	B	557	GLN
1	B	594	ASN
1	B	621	GLN

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	MDO	A	176	1	12,13,14	3.60	4 (33%)	12,18,20	7.34	4 (33%)
1	MDO	B	176	1	12,13,14	3.55	3 (25%)	12,18,20	7.57	6 (50%)

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	MDO	A	176	1	-	0/4/23/24	0/1/1/1
1	MDO	B	176	1	-	0/4/23/24	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	MDO	C2-N3	-3.74	1.30	1.39
1	A	176	MDO	C2-N3	-3.14	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	MDO	CA-C1	-2.16	1.48	1.51
1	A	176	MDO	C1-N2	3.61	1.37	1.32
1	B	176	MDO	C1-N2	4.14	1.38	1.32
1	B	176	MDO	O2-C2	10.49	1.45	1.23
1	A	176	MDO	O2-C2	11.01	1.47	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	MDO	C2-CA2-N2	-10.74	101.08	108.93
1	A	176	MDO	C2-CA2-N2	-10.03	101.59	108.93
1	A	176	MDO	O2-C2-CA2	-9.95	125.61	130.97
1	B	176	MDO	O2-C2-CA2	-7.40	126.98	130.97
1	B	176	MDO	O2-C2-N3	-2.16	119.91	124.49
1	B	176	MDO	CA3-N3-C1	2.04	129.59	127.20
1	A	176	MDO	CA2-N2-C1	4.05	109.45	105.41
1	B	176	MDO	CA2-N2-C1	4.29	109.68	105.41
1	A	176	MDO	CA2-C2-N3	20.41	112.41	103.30
1	B	176	MDO	CA2-C2-N3	21.97	113.11	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	176	MDO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TCA	A	699	-	8,11,11	0.37	0	9,13,13	1.46	2 (22%)
2	TCA	B	699	-	8,11,11	0.42	0	9,13,13	1.11	1 (11%)

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	TCA	A	699	-	-	0/3/5/5	0/1/1/1
2	TCA	B	699	-	-	0/3/5/5	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	699	TCA	C31-C3-C2	-3.27	113.01	125.88
2	A	699	TCA	C36-C31-C32	2.03	120.68	117.63
2	B	699	TCA	C36-C31-C32	2.33	121.12	117.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	699	TCA	1	0
2	B	699	TCA	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	653/696 (93%)	0.13	30 (4%) 33 35	28, 43, 68, 93	2 (0%)
1	B	655/696 (94%)	0.31	43 (6%) 19 20	28, 46, 74, 93	2 (0%)
All	All	1308/1392 (93%)	0.22	73 (5%) 25 27	28, 44, 73, 93	4 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	SER	7.4
1	B	678	GLY	6.2
1	A	7	SER	5.9
1	A	678	GLY	5.7
1	B	572	ILE	5.6
1	B	8	ARG	5.2
1	B	57	GLN	4.8
1	B	73	ALA	4.6
1	A	86	PHE	4.4
1	A	94	THR	4.4
1	A	85	GLY	4.3
1	B	56	GLU	4.1
1	B	202	ASP	3.8
1	A	590	ASP	3.7
1	A	95	ASN	3.6
1	B	61	ARG	3.6
1	B	518	CYS	3.6
1	B	53	LEU	3.5
1	B	569	LYS	3.5
1	B	82	VAL	3.5
1	B	584	PHE	3.4
1	A	202	ASP	3.3
1	A	90	SER	3.2
1	A	82	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	591	ARG	3.2
1	A	80	TYR	3.2
1	A	677	LEU	3.1
1	B	68	TRP	3.1
1	B	511	VAL	3.0
1	B	509	ASN	3.0
1	A	8	ARG	3.0
1	B	516	ASP	3.0
1	B	58	CYS	2.9
1	A	96	GLN	2.9
1	A	97	LEU	2.9
1	B	32	THR	2.8
1	B	590	ASP	2.8
1	A	573	GLU	2.8
1	B	587	ARG	2.8
1	A	92	ARG	2.8
1	B	576	THR	2.8
1	B	522	ASN	2.7
1	A	575	ASP	2.7
1	B	71[A]	ARG	2.7
1	A	201	ASP	2.6
1	B	81	GLY	2.6
1	B	97	LEU	2.6
1	B	69	VAL	2.6
1	B	74	GLU	2.5
1	A	602	LEU	2.5
1	A	545	CYS	2.5
1	A	394	LEU	2.5
1	A	89	CYS	2.5
1	B	529	LEU	2.4
1	B	70	GLN	2.4
1	B	577	LEU	2.4
1	B	86	PHE	2.4
1	B	586	LYS	2.4
1	B	354	ASP	2.3
1	A	128	VAL	2.3
1	B	95	ASN	2.3
1	B	677	LEU	2.3
1	A	560	PHE	2.3
1	A	396	ALA	2.3
1	A	84	THR	2.2
1	B	360	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	75	ASP	2.2
1	B	96	GLN	2.1
1	A	605	LYS	2.1
1	B	573	GLU	2.1
1	B	94	THR	2.1
1	A	576	THR	2.0
1	A	81	GLY	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	MDO	B	176	13/14	0.96	0.16	-	33,35,36,37	0
1	MDO	A	176	13/14	0.98	0.12	-	34,36,37,37	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(Å ²)	Q<0.9
2	TCA	B	699	11/11	0.93	0.17	0.20	60,61,62,62	0
2	TCA	A	699	11/11	0.93	0.14	-0.23	46,49,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.