



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:35 AM EDT

PDB ID : 2OCE / pdb_00002oce
Title : Crystal structure of Tex family protein PA5201 from Pseudomonas aeruginosa
Authors : Jin, X.; Min, T.; Burley, S.K.; Shapiro, L.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : 2006-12-20
Resolution : 3.10 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

<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

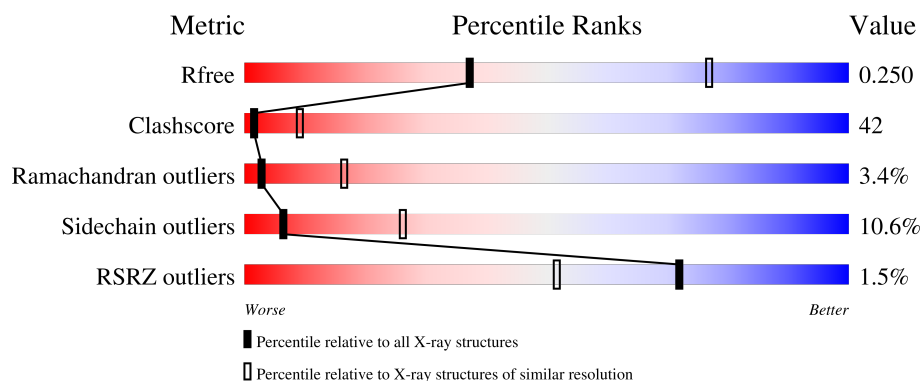
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 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	780	43% 40% 9% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5876 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 Hypothetical protein PA5201.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5610	3532	987	1077	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	cloning artifact	UNP Q9HTY8
A	1	LEU	-	cloning artifact	UNP Q9HTY8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	266	Total	O	0	0
			266	266		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.97Å 113.03Å 144.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.10) 99.7 (50.00-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.64 (at 3.11Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.279 0.224 , 0.250	Depositor DCC
R_{free} test set	943 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5876	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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

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	0.52	0/5699	1.11	38/7711 (0.5%)

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	1	4

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	592	ARG	N-CA-C	19.48	136.99	113.23
1	A	593	SER	N-CA-CB	15.87	137.31	110.49
1	A	561	MET	N-CA-C	14.43	127.05	111.03
1	A	604	LEU	N-CA-CB	12.77	131.42	112.13
1	A	603	ARG	CB-CA-C	12.50	135.30	110.42
1	A	365	LYS	N-CA-C	10.62	123.86	111.11
1	A	586	ASP	N-CA-C	-10.53	96.71	111.24
1	A	592	ARG	CB-CA-C	-10.38	93.92	111.26
1	A	583	ILE	N-CA-C	-8.18	103.21	111.88
1	A	544	SER	N-CA-C	7.91	124.34	111.37
1	A	588	GLU	N-CA-C	-7.71	103.93	112.72
1	A	690	LYS	CB-CA-C	7.64	122.58	109.51
1	A	365	LYS	CB-CA-C	-7.40	98.96	110.81
1	A	572	VAL	N-CA-C	6.70	117.10	108.12
1	A	558	LEU	N-CA-C	-6.41	102.26	110.53
1	A	35	GLY	N-CA-C	6.37	123.81	115.47
1	A	323	ALA	N-CA-C	-6.36	102.09	110.43
1	A	69	GLU	N-CA-C	-6.32	104.47	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	MET	CB-CA-C	-6.24	101.29	110.95
1	A	503	ASN	N-CA-C	6.08	120.56	113.20
1	A	157	ALA	N-CA-C	6.04	117.87	111.28
1	A	604	LEU	N-CA-C	-5.75	103.97	111.74
1	A	569	ALA	N-CA-C	-5.72	104.88	112.94
1	A	213	PHE	CA-C-O	5.72	126.31	119.10
1	A	656	MET	N-CA-C	5.69	117.64	110.24
1	A	488	ASP	N-CA-C	-5.64	105.22	111.36
1	A	97	LEU	N-CA-C	5.54	119.14	112.38
1	A	634	ARG	CA-C-N	5.53	125.47	119.78
1	A	634	ARG	C-N-CA	5.53	125.47	119.78
1	A	702	GLY	N-CA-C	-5.52	108.12	114.69
1	A	480	GLN	N-CA-C	5.41	116.98	111.14
1	A	387	ILE	CB-CA-C	-5.33	105.84	111.23
1	A	690	LYS	N-CA-C	-5.32	101.87	110.32
1	A	649	LEU	N-CA-C	-5.31	106.31	112.89
1	A	504	THR	N-CA-CB	-5.30	101.54	110.49
1	A	456	ASP	CA-C-N	5.28	126.44	119.84
1	A	456	ASP	C-N-CA	5.28	126.44	119.84
1	A	109	LEU	N-CA-C	5.14	121.17	109.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	603	ARG	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	GLU	Peptide
1	A	249	ALA	Peptide
1	A	610	THR	Peptide
1	A	615	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5610	0	5701	477	0
2	A	266	0	0	11	0
All	All	5876	0	5701	477	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 42.

All (477) 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:603:ARG:HH22	1:A:620:THR:CG2	1.18	1.56
1:A:198:VAL:HG21	1:A:213:PHE:CZ	1.39	1.55
1:A:198:VAL:HG11	1:A:213:PHE:CD1	1.37	1.54
1:A:198:VAL:HG11	1:A:213:PHE:CG	1.38	1.53
1:A:198:VAL:CG1	1:A:213:PHE:CD1	1.89	1.53
1:A:198:VAL:HG11	1:A:213:PHE:CD2	1.54	1.41
1:A:198:VAL:CG2	1:A:213:PHE:CZ	2.03	1.41
1:A:198:VAL:CG1	1:A:213:PHE:CE1	2.01	1.40
1:A:198:VAL:HG11	1:A:213:PHE:CE1	1.55	1.40
1:A:198:VAL:CB	1:A:213:PHE:CZ	2.14	1.31
1:A:198:VAL:CG1	1:A:213:PHE:CG	2.04	1.30
1:A:198:VAL:HG11	1:A:213:PHE:CE2	1.70	1.27
1:A:198:VAL:HG11	1:A:213:PHE:CZ	1.71	1.25
1:A:198:VAL:CB	1:A:213:PHE:CE1	2.18	1.24
1:A:198:VAL:HG21	1:A:213:PHE:CE2	1.71	1.24
1:A:603:ARG:NH2	1:A:620:THR:CG2	2.04	1.20
1:A:198:VAL:HB	1:A:213:PHE:CE1	1.76	1.18
1:A:615:GLY:O	1:A:616:LEU:HD12	1.40	1.17
1:A:603:ARG:NH2	1:A:620:THR:HG23	1.58	1.17
1:A:212:TYR:OH	1:A:226:ARG:HG3	1.39	1.16
1:A:198:VAL:HG12	1:A:213:PHE:CD1	1.74	1.16
1:A:579:LEU:HD21	1:A:619:VAL:HG22	1.26	1.14
1:A:198:VAL:CG1	1:A:213:PHE:CD2	2.27	1.14
1:A:198:VAL:CG1	1:A:213:PHE:CZ	2.26	1.12
1:A:616:LEU:CB	1:A:617:PRO:HD2	1.80	1.10
1:A:388:ALA:HB2	1:A:454:LEU:HD12	1.33	1.10
1:A:616:LEU:CB	1:A:617:PRO:CD	2.30	1.10
1:A:616:LEU:HB3	1:A:617:PRO:CD	1.80	1.09
1:A:603:ARG:HH22	1:A:620:THR:HG23	0.91	1.05
1:A:653:LYS:HD3	1:A:654:PRO:HD2	1.35	1.05
1:A:616:LEU:HB2	1:A:617:PRO:HD2	1.31	1.05
1:A:12:LEU:HD23	1:A:59:MET:HE2	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ARG:HH22	1:A:620:THR:HG21	1.20	1.02
1:A:619:VAL:HA	1:A:622:ILE:CD1	1.93	0.98
1:A:579:LEU:HD21	1:A:619:VAL:CG2	1.95	0.97
1:A:198:VAL:CG1	1:A:213:PHE:CE2	2.38	0.96
1:A:212:TYR:CE2	1:A:226:ARG:HG2	2.02	0.94
1:A:198:VAL:CG2	1:A:213:PHE:CE2	2.38	0.94
1:A:607:LYS:HE3	1:A:607:LYS:HA	1.49	0.94
1:A:616:LEU:HB3	1:A:617:PRO:HD3	1.50	0.93
1:A:615:GLY:O	1:A:616:LEU:CD1	2.18	0.91
1:A:247:GLU:HG3	1:A:248:GLU:O	1.71	0.91
1:A:249:ALA:HB1	1:A:250:PRO:HD2	1.52	0.90
1:A:198:VAL:HG21	1:A:213:PHE:HZ	1.19	0.89
1:A:579:LEU:HD13	1:A:609:PHE:CG	2.09	0.88
1:A:212:TYR:HE2	1:A:226:ARG:HG2	1.34	0.88
1:A:662:VAL:HG23	1:A:701:ALA:HA	1.56	0.88
1:A:619:VAL:HA	1:A:622:ILE:CG1	2.04	0.88
1:A:203:GLU:HG2	1:A:213:PHE:CZ	2.09	0.87
1:A:601:LEU:HD21	1:A:626:LEU:HD23	1.57	0.87
1:A:653:LYS:HD3	1:A:654:PRO:CD	2.06	0.86
1:A:619:VAL:HA	1:A:622:ILE:HD12	1.56	0.85
1:A:708:LYS:HG2	1:A:710:MET:HE3	1.59	0.85
1:A:612:GLU:O	1:A:613:THR:HG23	1.77	0.84
1:A:249:ALA:HB1	1:A:250:PRO:CD	2.07	0.84
1:A:496:ASN:HD21	1:A:514:SER:H	1.20	0.84
1:A:212:TYR:OH	1:A:226:ARG:CG	2.25	0.84
1:A:223:PRO:HG2	1:A:226:ARG:HB2	1.60	0.83
1:A:653:LYS:H	1:A:656:MET:HE3	1.43	0.83
1:A:619:VAL:HA	1:A:622:ILE:HG13	1.60	0.83
1:A:567:LEU:H	1:A:567:LEU:HD23	1.43	0.82
1:A:682:VAL:HG11	1:A:723:MET:HE3	1.62	0.81
1:A:313:PHE:CE1	1:A:472:GLY:HA3	2.15	0.81
1:A:579:LEU:O	1:A:579:LEU:HD12	1.82	0.80
1:A:203:GLU:HG2	1:A:213:PHE:HZ	1.45	0.80
1:A:286:LYS:HE2	1:A:286:LYS:HA	1.63	0.79
1:A:95:ILE:HD13	1:A:107:LEU:HD23	1.63	0.79
1:A:403:GLY:O	1:A:406:ILE:HD13	1.83	0.79
1:A:388:ALA:CB	1:A:454:LEU:HD12	2.12	0.79
1:A:196:ALA:O	1:A:197:ARG:HD2	1.83	0.79
1:A:530:ALA:C	1:A:531:ASN:HD22	1.92	0.78
1:A:531:ASN:HD22	1:A:531:ASN:N	1.79	0.77
1:A:592:ARG:C	1:A:594:LEU:H	1.91	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:GLU:O	1:A:408:LYS:HE2	1.85	0.77
1:A:500:VAL:HG21	1:A:513:ILE:HD11	1.68	0.76
1:A:579:LEU:HD13	1:A:609:PHE:CD1	2.19	0.76
1:A:481:LEU:O	1:A:485:ARG:HG2	1.86	0.76
1:A:597:ASP:O	1:A:601:LEU:HB3	1.87	0.75
1:A:598:SER:HA	1:A:602:LYS:HB2	1.68	0.75
1:A:465:GLU:HG3	1:A:468:SER:HB2	1.69	0.74
1:A:567:LEU:H	1:A:567:LEU:CD2	2.00	0.74
1:A:302:ARG:HB3	1:A:302:ARG:NH1	2.01	0.74
1:A:631:ARG:HG3	1:A:631:ARG:HH11	1.52	0.74
1:A:88:THR:HG22	1:A:91:LEU:H	1.53	0.74
1:A:591:ILE:O	1:A:591:ILE:HG13	1.86	0.74
1:A:603:ARG:NH2	1:A:620:THR:HG21	1.88	0.72
1:A:223:PRO:HB2	1:A:225:HIS:CE1	2.25	0.71
1:A:579:LEU:CD2	1:A:619:VAL:HG22	2.14	0.71
1:A:263:ARG:O	1:A:263:ARG:HD3	1.91	0.70
1:A:543:VAL:HB	1:A:546:LEU:HB2	1.73	0.70
1:A:545:ARG:HB3	1:A:545:ARG:NH1	2.07	0.70
1:A:212:TYR:CE2	1:A:226:ARG:CG	2.74	0.69
1:A:602:LYS:HA	1:A:602:LYS:NZ	2.07	0.69
1:A:582:ARG:HE	1:A:609:PHE:HZ	1.40	0.69
1:A:606:PRO:C	1:A:608:LYS:H	2.01	0.69
1:A:198:VAL:HB	1:A:213:PHE:CZ	2.05	0.69
1:A:360:TYR:CB	1:A:365:LYS:HD2	2.22	0.69
1:A:590:ASP:O	1:A:591:ILE:HG12	1.92	0.69
1:A:402:ALA:O	1:A:406:ILE:HG23	1.94	0.68
1:A:520:LEU:HD11	1:A:545:ARG:HB2	1.76	0.68
1:A:198:VAL:HG13	1:A:213:PHE:CD2	2.26	0.68
1:A:500:VAL:CG2	1:A:513:ILE:HD11	2.22	0.68
1:A:496:ASN:HD21	1:A:514:SER:N	1.92	0.68
1:A:652:LEU:HA	1:A:656:MET:HE1	1.76	0.68
1:A:579:LEU:HD13	1:A:609:PHE:CB	2.25	0.67
1:A:21:GLN:H	1:A:24:GLN:HE21	1.41	0.67
1:A:586:ASP:HB3	1:A:600:PHE:HZ	1.60	0.67
1:A:623:LEU:HA	1:A:626:LEU:HD21	1.77	0.67
1:A:299:GLY:HA2	1:A:302:ARG:NH1	2.10	0.67
1:A:321:LEU:HD23	1:A:461:LEU:HD12	1.76	0.66
1:A:662:VAL:HG11	1:A:699:VAL:HG21	1.75	0.66
1:A:643:GLN:O	1:A:646:VAL:HG12	1.95	0.66
1:A:60:LEU:C	1:A:60:LEU:HD23	2.21	0.66
1:A:631:ARG:HG3	2:A:836:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ASP:HB3	1:A:600:PHE:CZ	2.31	0.66
1:A:269:GLN:HE21	1:A:269:GLN:HA	1.60	0.65
1:A:496:ASN:ND2	1:A:514:SER:H	1.94	0.65
1:A:332:LEU:HD11	1:A:344:VAL:CG1	2.26	0.65
1:A:627:ASP:HB3	1:A:628:LYS:HD3	1.76	0.65
1:A:256:CYS:O	1:A:260:ILE:HG13	1.96	0.65
1:A:407:LYS:O	1:A:407:LYS:HG3	1.97	0.65
1:A:193:THR:HG22	1:A:218:PRO:HA	1.79	0.65
1:A:198:VAL:HG13	1:A:213:PHE:O	1.96	0.64
1:A:343:LYS:HE2	1:A:343:LYS:H	1.63	0.64
1:A:465:GLU:HG3	1:A:468:SER:CB	2.27	0.64
1:A:396:ARG:HH11	1:A:396:ARG:HB2	1.63	0.64
1:A:269:GLN:HE21	1:A:269:GLN:CA	2.10	0.63
1:A:223:PRO:HG3	1:A:226:ARG:CZ	2.29	0.63
1:A:631:ARG:H	1:A:631:ARG:HD3	1.62	0.63
1:A:531:ASN:N	1:A:531:ASN:ND2	2.47	0.63
1:A:700:LYS:O	1:A:703:ASP:HB2	1.98	0.63
1:A:619:VAL:HG13	1:A:622:ILE:HD12	1.81	0.63
1:A:217:GLU:OE2	1:A:226:ARG:HD2	1.99	0.63
1:A:158:ASP:OD2	1:A:160:LYS:HB3	1.99	0.62
1:A:583:ILE:O	1:A:583:ILE:HG22	1.98	0.62
1:A:65:ARG:NH1	1:A:65:ARG:HB3	2.14	0.62
1:A:540:LEU:O	1:A:546:LEU:HG	1.99	0.62
1:A:286:LYS:HE2	1:A:286:LYS:CA	2.30	0.62
1:A:602:LYS:HA	1:A:602:LYS:HZ1	1.65	0.62
1:A:577:TYR:HB2	1:A:578:PRO:HD3	1.82	0.61
1:A:268:ASN:ND2	1:A:274:ASP:HB3	2.14	0.61
1:A:382:HIS:HA	2:A:875:HOH:O	2.00	0.61
1:A:632:ASP:OD2	1:A:634:ARG:HB2	2.00	0.61
1:A:89:PRO:HD2	1:A:90:GLU:OE1	2.00	0.61
1:A:631:ARG:O	1:A:633:PRO:HD3	2.01	0.61
1:A:212:TYR:CZ	1:A:226:ARG:HG3	2.32	0.60
1:A:607:LYS:HA	1:A:607:LYS:CE	2.28	0.60
1:A:277:LEU:O	1:A:281:VAL:HG23	2.00	0.60
1:A:117:THR:HG21	1:A:172:GLU:OE1	2.02	0.60
1:A:19:ARG:HG2	1:A:19:ARG:HH11	1.66	0.60
1:A:458:LEU:HD21	1:A:495:VAL:HG12	1.83	0.60
1:A:602:LYS:HE3	1:A:603:ARG:HG2	1.83	0.60
1:A:626:LEU:N	1:A:626:LEU:HD22	2.16	0.60
1:A:348:ASP:OD2	1:A:350:THR:N	2.27	0.60
1:A:563:GLY:HA2	2:A:860:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLU:HG3	1:A:63:ARG:HD3	1.83	0.59
1:A:588:GLU:C	1:A:590:ASP:H	2.10	0.59
1:A:94:ASP:HB3	1:A:107:LEU:HD21	1.84	0.59
1:A:391:ASN:C	1:A:391:ASN:HD22	2.10	0.59
1:A:427:TYR:O	1:A:430:SER:HB3	2.02	0.59
1:A:203:GLU:CG	1:A:213:PHE:HZ	2.12	0.59
1:A:594:LEU:O	1:A:595:ILE:HG22	2.02	0.59
1:A:184:LEU:HD22	1:A:256:CYS:SG	2.43	0.59
1:A:348:ASP:OD2	1:A:348:ASP:C	2.45	0.59
1:A:588:GLU:O	1:A:590:ASP:N	2.36	0.59
1:A:603:ARG:O	1:A:623:LEU:HD23	2.02	0.59
1:A:570:SER:OG	1:A:572:VAL:HG23	2.04	0.58
1:A:120:GLN:O	1:A:124:GLU:HG3	2.03	0.58
1:A:254:HIS:HB3	1:A:257:GLU:HG3	1.84	0.58
1:A:65:ARG:HB3	1:A:65:ARG:CZ	2.34	0.58
1:A:195:THR:HG23	1:A:197:ARG:NH1	2.19	0.58
1:A:575:GLU:HG2	1:A:614:PHE:HE2	1.69	0.58
1:A:198:VAL:CG2	1:A:213:PHE:HZ	1.90	0.58
1:A:203:GLU:CG	1:A:213:PHE:CZ	2.85	0.58
1:A:302:ARG:HB3	1:A:302:ARG:CZ	2.34	0.58
1:A:310:ILE:HD11	1:A:478:VAL:CG1	2.33	0.58
1:A:606:PRO:C	1:A:608:LYS:N	2.61	0.58
1:A:299:GLY:HA2	1:A:302:ARG:HH12	1.69	0.57
1:A:615:GLY:O	1:A:616:LEU:CB	2.51	0.57
1:A:212:TYR:CZ	1:A:226:ARG:CG	2.87	0.57
1:A:212:TYR:C	1:A:214:GLU:H	2.12	0.57
1:A:420:SER:O	1:A:453:ARG:NH1	2.37	0.57
1:A:631:ARG:HG3	1:A:631:ARG:NH1	2.16	0.57
1:A:581:GLN:C	1:A:583:ILE:H	2.12	0.57
1:A:100:THR:OG1	1:A:103:ARG:HG2	2.05	0.57
1:A:228:LEU:O	1:A:232:ARG:HB2	2.04	0.57
1:A:249:ALA:CB	1:A:250:PRO:CD	2.78	0.57
1:A:527:HIS:CE1	1:A:543:VAL:HA	2.40	0.57
1:A:619:VAL:CA	1:A:622:ILE:HD12	2.33	0.56
1:A:184:LEU:HD12	1:A:289:LEU:HD13	1.87	0.56
1:A:185:ARG:HD2	2:A:810:HOH:O	2.04	0.56
1:A:615:GLY:O	1:A:616:LEU:HB2	2.03	0.56
1:A:681:LEU:HD23	1:A:682:VAL:N	2.20	0.56
1:A:486:SER:O	1:A:489:ALA:HB3	2.05	0.56
1:A:527:HIS:NE2	1:A:543:VAL:HA	2.20	0.56
1:A:590:ASP:C	1:A:592:ARG:N	2.61	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:LEU:HD23	1:A:682:VAL:H	1.70	0.56
1:A:21:GLN:H	1:A:24:GLN:NE2	2.03	0.56
1:A:4:ILE:O	1:A:8:ILE:HG13	2.06	0.56
1:A:332:LEU:HD11	1:A:344:VAL:HG12	1.88	0.56
1:A:588:GLU:HG3	1:A:600:PHE:CD2	2.40	0.56
1:A:567:LEU:HD23	1:A:567:LEU:N	2.19	0.55
1:A:598:SER:CA	1:A:602:LYS:HB2	2.35	0.55
1:A:626:LEU:HD13	1:A:626:LEU:H	1.71	0.55
1:A:582:ARG:NE	1:A:609:PHE:HZ	2.05	0.55
1:A:684:ILE:HD12	1:A:695:PRO:HD3	1.89	0.55
1:A:360:TYR:HB2	1:A:365:LYS:HD2	1.87	0.55
1:A:641:GLU:OE1	1:A:644:GLU:HB3	2.05	0.55
1:A:656:MET:HB2	1:A:709:VAL:CG1	2.37	0.55
1:A:60:LEU:O	1:A:64:LEU:HB2	2.06	0.55
1:A:360:TYR:CG	1:A:365:LYS:HD2	2.42	0.55
1:A:195:THR:HG23	1:A:197:ARG:HH11	1.71	0.55
1:A:247:GLU:HG3	1:A:248:GLU:C	2.32	0.55
1:A:527:HIS:O	1:A:530:ALA:N	2.38	0.54
1:A:708:LYS:HG2	1:A:710:MET:CE	2.34	0.54
1:A:514:SER:OG	1:A:553:GLN:O	2.25	0.54
1:A:616:LEU:C	1:A:618:THR:H	2.15	0.54
1:A:21:GLN:HB3	1:A:23:GLN:CD	2.32	0.54
1:A:646:VAL:HG13	1:A:646:VAL:O	2.06	0.54
1:A:565:ASN:OD1	1:A:567:LEU:HD21	2.08	0.54
1:A:689:GLU:OE1	1:A:724:ARG:HB2	2.07	0.54
1:A:254:HIS:HD2	1:A:256:CYS:HB2	1.73	0.54
1:A:46:LYS:O	1:A:50:GLY:N	2.37	0.54
1:A:523:ASN:O	1:A:526:ALA:HB3	2.07	0.54
1:A:142:PRO:HG2	1:A:143:GLU:OE2	2.08	0.54
1:A:588:GLU:C	1:A:590:ASP:N	2.64	0.54
1:A:592:ARG:C	1:A:594:LEU:N	2.61	0.54
1:A:722:SER:OG	1:A:724:ARG:HG2	2.08	0.54
1:A:252:THR:HG22	1:A:253:LEU:N	2.22	0.54
1:A:620:THR:HG22	1:A:620:THR:O	2.07	0.54
1:A:140:LEU:O	1:A:272:ALA:HB3	2.08	0.53
1:A:197:ARG:HH12	1:A:216:ASP:CG	2.16	0.53
1:A:212:TYR:C	1:A:214:GLU:N	2.62	0.53
1:A:618:THR:O	1:A:622:ILE:HG13	2.08	0.53
1:A:515:GLY:O	1:A:516:LEU:HD23	2.08	0.53
1:A:592:ARG:HG2	1:A:592:ARG:HH11	1.74	0.53
1:A:215:HIS:CD2	1:A:216:ASP:H	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:HIS:O	1:A:528:ARG:C	2.52	0.53
1:A:618:THR:O	1:A:622:ILE:HD11	2.09	0.53
1:A:90:GLU:CD	1:A:90:GLU:H	2.17	0.53
1:A:610:THR:C	1:A:611:ASP:O	2.51	0.53
1:A:616:LEU:C	1:A:618:THR:N	2.67	0.53
1:A:109:LEU:HB2	1:A:110:PRO:HD3	1.90	0.53
1:A:336:PRO:HA	1:A:342:VAL:HG23	1.90	0.53
1:A:17:SER:HB2	2:A:843:HOH:O	2.08	0.53
1:A:728:THR:HB	1:A:729:PRO:HD2	1.90	0.53
1:A:332:LEU:HD13	1:A:346:VAL:HG22	1.90	0.53
1:A:618:THR:O	1:A:622:ILE:CG1	2.57	0.53
1:A:502:VAL:HG21	1:A:540:LEU:HD21	1.90	0.52
1:A:653:LYS:H	1:A:656:MET:CE	2.16	0.52
1:A:417:ILE:CD1	1:A:637:PHE:HZ	2.21	0.52
1:A:595:ILE:HG13	1:A:595:ILE:O	2.10	0.52
1:A:674:ILE:HG22	1:A:674:ILE:O	2.10	0.52
1:A:474:TYR:HB3	1:A:477:ASP:OD2	2.10	0.52
1:A:628:LYS:HD3	1:A:628:LYS:N	2.25	0.52
1:A:688:SER:OG	1:A:689:GLU:N	2.43	0.52
1:A:25:VAL:O	1:A:29:VAL:HG23	2.10	0.51
1:A:249:ALA:CB	1:A:250:PRO:HD2	2.35	0.51
1:A:490:VAL:CG2	1:A:491:VAL:N	2.72	0.51
1:A:676:VAL:HG12	1:A:676:VAL:O	2.09	0.51
1:A:619:VAL:CA	1:A:622:ILE:HG13	2.35	0.51
1:A:707:VAL:HG12	1:A:723:MET:HG3	1.91	0.51
1:A:604:LEU:O	1:A:605:ASP:O	2.29	0.51
1:A:212:TYR:HE2	1:A:226:ARG:CG	2.13	0.51
1:A:391:ASN:C	1:A:391:ASN:ND2	2.68	0.51
1:A:652:LEU:HD21	1:A:658:LEU:HD21	1.91	0.51
1:A:202:LYS:NZ	1:A:205:GLU:HG2	2.26	0.51
1:A:430:SER:OG	1:A:431:GLU:N	2.43	0.51
1:A:643:GLN:C	1:A:645:GLY:N	2.69	0.51
1:A:223:PRO:HB2	1:A:225:HIS:NE2	2.27	0.50
1:A:662:VAL:HG11	1:A:699:VAL:CG2	2.40	0.50
1:A:306:GLU:O	1:A:307:ASP:C	2.54	0.50
1:A:258:VAL:O	1:A:262:GLU:HG3	2.12	0.50
1:A:120:GLN:HA	1:A:123:LEU:HD12	1.94	0.50
1:A:37:THR:OG1	1:A:514:SER:HB2	2.11	0.50
1:A:403:GLY:HA2	1:A:406:ILE:HD12	1.93	0.50
1:A:409:TYR:N	1:A:410:PRO:HD3	2.26	0.50
1:A:616:LEU:O	1:A:620:THR:N	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:VAL:O	1:A:623:LEU:HD13	2.12	0.50
1:A:173:ARG:NH1	2:A:862:HOH:O	2.43	0.49
1:A:653:LYS:CD	1:A:654:PRO:HD2	2.25	0.49
1:A:88:THR:HG23	1:A:90:GLU:OE1	2.12	0.49
1:A:497:ALA:O	1:A:633:PRO:HG2	2.12	0.49
1:A:224:SER:O	1:A:228:LEU:HD12	2.13	0.49
1:A:517:ASN:OD1	1:A:519:THR:HB	2.12	0.49
1:A:223:PRO:HG3	1:A:226:ARG:NH2	2.27	0.49
1:A:335:ASP:O	1:A:342:VAL:HG23	2.11	0.49
1:A:403:GLY:O	1:A:404:GLU:C	2.54	0.49
1:A:492:GLU:O	1:A:496:ASN:OD1	2.30	0.49
1:A:652:LEU:HD23	1:A:656:MET:SD	2.52	0.49
1:A:641:GLU:CG	1:A:641:GLU:O	2.59	0.49
1:A:662:VAL:CG2	1:A:700:LYS:O	2.61	0.49
1:A:248:GLU:O	1:A:248:GLU:OE2	2.30	0.49
1:A:694:ASP:OD2	1:A:697:GLU:HG2	2.13	0.49
1:A:362:HIS:CD2	1:A:397:GLU:HB2	2.48	0.48
1:A:408:LYS:HB3	1:A:409:TYR:CD1	2.47	0.48
1:A:49:THR:HG21	1:A:52:LEU:HB2	1.95	0.48
1:A:521:ALA:O	1:A:522:GLN:C	2.56	0.48
1:A:173:ARG:O	1:A:176:GLU:HG2	2.14	0.48
1:A:189:LYS:O	1:A:189:LYS:HG2	2.12	0.48
1:A:570:SER:C	1:A:572:VAL:H	2.20	0.48
1:A:594:LEU:C	1:A:596:GLY:N	2.71	0.48
1:A:408:LYS:HB3	1:A:409:TYR:CE1	2.48	0.48
1:A:520:LEU:O	1:A:524:ILE:HG12	2.14	0.48
1:A:708:LYS:CG	1:A:710:MET:HE3	2.39	0.48
1:A:223:PRO:HG3	1:A:226:ARG:NE	2.28	0.48
1:A:490:VAL:HG22	1:A:491:VAL:N	2.29	0.48
1:A:674:ILE:HD11	1:A:721:LEU:HD21	1.96	0.48
1:A:658:LEU:HD12	1:A:658:LEU:H	1.78	0.48
1:A:82:GLU:HG3	1:A:83:GLU:N	2.28	0.47
1:A:136:ASP:HB2	2:A:800:HOH:O	2.14	0.47
1:A:425:SER:O	1:A:426:VAL:C	2.56	0.47
1:A:585:ALA:O	1:A:586:ASP:C	2.57	0.47
1:A:159:VAL:HG13	1:A:160:LYS:N	2.30	0.47
1:A:184:LEU:CD1	1:A:289:LEU:HD13	2.44	0.47
1:A:368:TRP:CE2	1:A:401:LEU:HD23	2.49	0.47
1:A:253:LEU:HD21	1:A:258:VAL:HG22	1.95	0.47
1:A:471:VAL:HG22	1:A:475:GLN:HE22	1.80	0.47
1:A:643:GLN:C	1:A:645:GLY:H	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:LYS:HE3	1:A:710:MET:CE	2.45	0.47
1:A:187:PHE:CD1	1:A:259:MET:HE1	2.49	0.47
1:A:268:ASN:C	1:A:268:ASN:HD22	2.23	0.47
1:A:276:TRP:O	1:A:280:VAL:HG12	2.15	0.47
1:A:359:VAL:HG23	1:A:361:PRO:HD3	1.96	0.47
1:A:381:LYS:HD2	2:A:1045:HOH:O	2.15	0.47
1:A:408:LYS:HD2	2:A:967:HOH:O	2.14	0.47
1:A:500:VAL:HG22	1:A:509:LEU:HD21	1.96	0.47
1:A:579:LEU:HD12	1:A:579:LEU:C	2.38	0.47
1:A:641:GLU:O	1:A:641:GLU:CD	2.58	0.47
1:A:215:HIS:CD2	1:A:216:ASP:N	2.83	0.47
1:A:545:ARG:HB3	1:A:545:ARG:HH11	1.79	0.47
1:A:138:PRO:HA	1:A:273:ALA:HB3	1.96	0.46
1:A:520:LEU:HA	1:A:523:ASN:HB2	1.96	0.46
1:A:409:TYR:CD2	1:A:412:MET:HE2	2.50	0.46
1:A:590:ASP:C	1:A:592:ARG:H	2.23	0.46
1:A:49:THR:HG22	1:A:52:LEU:HG	1.97	0.46
1:A:656:MET:HB2	1:A:709:VAL:HG11	1.96	0.46
1:A:317:LEU:HD22	1:A:487:LEU:HG	1.98	0.46
1:A:339:ARG:HA	1:A:364:PRO:HD2	1.98	0.46
1:A:417:ILE:HG22	1:A:418:MET:N	2.30	0.46
1:A:500:VAL:HG11	1:A:510:LEU:HD13	1.98	0.46
1:A:125:ALA:HA	1:A:154:LYS:HD3	1.97	0.46
1:A:501:ASP:O	1:A:503:ASN:N	2.49	0.46
1:A:254:HIS:CD2	1:A:256:CYS:HB2	2.50	0.46
1:A:689:GLU:OE2	1:A:689:GLU:HA	2.15	0.46
1:A:116:ARG:HH11	1:A:116:ARG:HG2	1.81	0.45
1:A:21:GLN:HB2	1:A:24:GLN:HG3	1.98	0.45
1:A:588:GLU:OE1	1:A:588:GLU:HA	2.17	0.45
1:A:601:LEU:HD11	1:A:626:LEU:CD2	2.46	0.45
1:A:642:PHE:CG	1:A:643:GLN:N	2.84	0.45
1:A:716:ARG:HG3	1:A:716:ARG:HH11	1.81	0.45
1:A:103:ARG:HE	1:A:182:ASP:CG	2.25	0.45
1:A:627:ASP:CB	1:A:628:LYS:HD3	2.43	0.45
1:A:310:ILE:CG1	1:A:478:VAL:HG11	2.47	0.45
1:A:632:ASP:C	1:A:634:ARG:H	2.24	0.45
1:A:201:GLY:C	1:A:203:GLU:H	2.25	0.45
1:A:576:THR:O	1:A:577:TYR:C	2.57	0.45
1:A:215:HIS:C	1:A:216:ASP:OD1	2.59	0.45
1:A:408:LYS:C	1:A:410:PRO:HD3	2.41	0.45
1:A:587:THR:O	1:A:587:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HB3	1:A:44:TYR:CD1	2.51	0.45
1:A:188:MET:O	1:A:192:ALA:HB3	2.17	0.45
1:A:362:HIS:NE2	1:A:397:GLU:HB2	2.32	0.45
1:A:604:LEU:O	1:A:605:ASP:C	2.58	0.45
1:A:570:SER:C	1:A:572:VAL:N	2.74	0.45
1:A:620:THR:O	1:A:624:LYS:HE2	2.17	0.45
1:A:501:ASP:C	1:A:503:ASN:N	2.75	0.44
1:A:605:ASP:O	1:A:606:PRO:O	2.36	0.44
1:A:339:ARG:HA	1:A:364:PRO:CD	2.46	0.44
1:A:596:GLY:O	1:A:597:ASP:O	2.35	0.44
1:A:603:ARG:CZ	1:A:620:THR:HG23	2.36	0.44
1:A:595:ILE:C	1:A:597:ASP:H	2.25	0.44
1:A:612:GLU:O	1:A:613:THR:CG2	2.59	0.44
1:A:421:GLU:HG2	1:A:450:ILE:HD11	1.98	0.44
1:A:465:GLU:HG3	1:A:468:SER:OG	2.18	0.44
1:A:470:GLY:HA2	1:A:475:GLN:OE1	2.17	0.44
1:A:44:TYR:CE2	1:A:573:HIS:HB2	2.52	0.44
1:A:439:GLU:HG2	1:A:440:LEU:N	2.32	0.44
1:A:120:GLN:N	1:A:120:GLN:OE1	2.50	0.44
1:A:567:LEU:HG	1:A:577:TYR:CE1	2.53	0.44
1:A:575:GLU:HG2	1:A:614:PHE:CE2	2.51	0.44
1:A:38:VAL:N	1:A:39:PRO:HD2	2.32	0.44
1:A:627:ASP:OD1	1:A:628:LYS:HD2	2.18	0.44
1:A:667:ASN:OD1	1:A:667:ASN:C	2.61	0.44
1:A:579:LEU:HD13	1:A:609:PHE:HB3	1.99	0.44
1:A:335:ASP:C	1:A:342:VAL:HG23	2.43	0.43
1:A:498:VAL:O	1:A:498:VAL:HG12	2.18	0.43
1:A:626:LEU:HD22	1:A:626:LEU:H	1.82	0.43
1:A:254:HIS:CD2	1:A:256:CYS:H	2.36	0.43
1:A:118:LYS:HA	1:A:121:ILE:HD12	1.99	0.43
1:A:320:LEU:HD12	1:A:320:LEU:HA	1.86	0.43
1:A:662:VAL:HG21	1:A:700:LYS:O	2.18	0.43
1:A:594:LEU:O	1:A:595:ILE:CG2	2.67	0.43
1:A:313:PHE:CE2	1:A:475:GLN:HA	2.54	0.43
1:A:232:ARG:O	1:A:236:GLU:HB2	2.19	0.43
1:A:579:LEU:CD1	1:A:609:PHE:CB	2.94	0.43
1:A:594:LEU:C	1:A:596:GLY:H	2.25	0.43
1:A:684:ILE:HG23	1:A:685:SER:N	2.34	0.43
1:A:67:LEU:O	1:A:70:LEU:HB3	2.19	0.43
1:A:254:HIS:HB3	1:A:257:GLU:CG	2.49	0.43
1:A:317:LEU:CD2	1:A:487:LEU:HG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:VAL:O	1:A:622:ILE:HB	2.19	0.43
1:A:659:GLU:OE1	1:A:704:ILE:HD11	2.19	0.43
1:A:585:ALA:O	1:A:586:ASP:HB2	2.18	0.43
1:A:618:THR:O	1:A:622:ILE:CD1	2.67	0.43
1:A:93:ARG:O	1:A:97:LEU:HG	2.19	0.42
1:A:302:ARG:O	1:A:306:GLU:HG3	2.19	0.42
1:A:310:ILE:HD11	1:A:478:VAL:HG11	2.00	0.42
1:A:500:VAL:HG13	1:A:505:ALA:HB2	2.01	0.42
1:A:642:PHE:CD1	1:A:643:GLN:N	2.87	0.42
1:A:388:ALA:HB2	1:A:454:LEU:CD1	2.25	0.42
1:A:44:TYR:O	1:A:45:ARG:NE	2.53	0.42
1:A:313:PHE:CD1	1:A:472:GLY:HA3	2.55	0.42
1:A:646:VAL:O	1:A:646:VAL:CG1	2.67	0.42
1:A:599:ALA:O	1:A:600:PHE:HB3	2.19	0.42
1:A:626:LEU:O	1:A:629:PRO:HD3	2.19	0.42
1:A:671:PHE:HB3	1:A:679:ASP:OD2	2.19	0.42
1:A:89:PRO:O	1:A:92:ALA:HB3	2.19	0.42
1:A:503:ASN:HA	1:A:528:ARG:HD2	2.02	0.42
1:A:142:PRO:O	1:A:143:GLU:C	2.61	0.42
1:A:545:ARG:HH11	1:A:545:ARG:CB	2.33	0.42
1:A:43:ARG:HB3	1:A:44:TYR:CE1	2.54	0.42
1:A:332:LEU:HD21	1:A:375:LEU:HD22	2.02	0.42
1:A:401:LEU:HD13	1:A:401:LEU:C	2.45	0.42
1:A:535:ARG:O	1:A:536:THR:HG23	2.20	0.42
1:A:634:ARG:HA	1:A:635:PRO:HD3	1.87	0.42
1:A:682:VAL:HG22	1:A:721:LEU:HB2	2.00	0.42
1:A:392:GLY:N	1:A:421:GLU:OE2	2.50	0.42
1:A:407:LYS:O	1:A:408:LYS:HD3	2.19	0.42
1:A:353:LEU:HD11	1:A:356:THR:HG22	2.02	0.42
1:A:596:GLY:O	1:A:597:ASP:C	2.62	0.42
1:A:344:VAL:N	1:A:357:ALA:O	2.48	0.42
1:A:487:LEU:O	1:A:491:VAL:HG23	2.19	0.42
1:A:360:TYR:CD1	1:A:360:TYR:N	2.88	0.41
1:A:417:ILE:HD13	1:A:637:PHE:HZ	1.85	0.41
1:A:348:ASP:OD1	1:A:352:LYS:HB3	2.20	0.41
1:A:541:LYS:HG2	2:A:873:HOH:O	2.20	0.41
1:A:653:LYS:N	1:A:656:MET:HE3	2.23	0.41
1:A:90:GLU:OE1	1:A:90:GLU:N	2.43	0.41
1:A:202:LYS:HZ1	1:A:205:GLU:HG2	1.85	0.41
1:A:478:VAL:CG1	1:A:479:SER:N	2.83	0.41
1:A:577:TYR:N	1:A:578:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:SER:O	1:A:596:GLY:N	2.54	0.41
1:A:594:LEU:HD12	1:A:595:ILE:H	1.85	0.41
1:A:714:ILE:N	1:A:715:PRO:CD	2.84	0.41
1:A:91:LEU:O	1:A:95:ILE:HG12	2.18	0.41
1:A:70:LEU:HD12	1:A:104:LEU:HD22	2.02	0.41
1:A:220:LYS:O	1:A:220:LYS:HG2	2.20	0.41
1:A:704:ILE:C	1:A:705:VAL:HG13	2.46	0.41
1:A:259:MET:HA	1:A:262:GLU:OE2	2.20	0.41
1:A:601:LEU:HD11	1:A:626:LEU:HD23	2.03	0.41
1:A:615:GLY:O	1:A:616:LEU:CG	2.68	0.41
1:A:641:GLU:O	1:A:641:GLU:HG2	2.20	0.41
1:A:698:VAL:HG12	1:A:699:VAL:N	2.36	0.41
1:A:7:ARG:NH1	2:A:829:HOH:O	2.50	0.41
1:A:45:ARG:HA	1:A:45:ARG:HD3	1.82	0.41
1:A:331:THR:HG22	1:A:332:LEU:N	2.35	0.41
1:A:375:LEU:O	1:A:376:ALA:C	2.64	0.41
1:A:589:ARG:H	1:A:589:ARG:HG3	1.68	0.41
1:A:19:ARG:HG2	1:A:19:ARG:NH1	2.34	0.41
1:A:465:GLU:O	1:A:466:PRO:C	2.63	0.41
1:A:466:PRO:C	1:A:468:SER:H	2.29	0.41
1:A:496:ASN:HB3	1:A:557:PHE:CD2	2.55	0.41
1:A:299:GLY:CA	1:A:302:ARG:HH12	2.32	0.40
1:A:520:LEU:CD1	1:A:545:ARG:HB2	2.49	0.40
1:A:614:PHE:CD1	1:A:614:PHE:N	2.89	0.40
1:A:678:GLN:HA	1:A:678:GLN:HE21	1.87	0.40
1:A:103:ARG:NH1	1:A:103:ARG:HG3	2.35	0.40
1:A:326:ALA:HB2	1:A:637:PHE:CE1	2.55	0.40
1:A:388:ALA:CA	1:A:454:LEU:HD12	2.51	0.40
1:A:581:GLN:C	1:A:583:ILE:N	2.78	0.40
1:A:30:ALA:O	1:A:34:GLU:HB2	2.20	0.40
1:A:521:ALA:O	1:A:524:ILE:N	2.53	0.40
1:A:708:LYS:HE3	1:A:710:MET:HE3	2.03	0.40
1:A:252:THR:HG22	1:A:253:LEU:H	1.87	0.40
1:A:336:PRO:HA	1:A:342:VAL:CG2	2.51	0.40
1:A:550:THR:O	1:A:551:PHE:C	2.61	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	727/780 (93%)	593 (82%)	109 (15%)	25 (3%)	3 16

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	PRO
1	A	249	ALA
1	A	597	ASP
1	A	605	ASP
1	A	606	PRO
1	A	611	ASP
1	A	613	THR
1	A	616	LEU
1	A	589	ARG
1	A	250	PRO
1	A	270	GLY
1	A	603	ARG
1	A	685	SER
1	A	405	LEU
1	A	587	THR
1	A	610	THR
1	A	594	LEU
1	A	617	PRO
1	A	200	PRO
1	A	485	ARG
1	A	502	VAL
1	A	595	ILE
1	A	328	PRO
1	A	591	ILE
1	A	615	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	594/630 (94%)	531 (89%)	63 (11%)	6 26

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	22	PRO
1	A	62	GLU
1	A	63	ARG
1	A	64	LEU
1	A	82	GLU
1	A	86	LYS
1	A	88	THR
1	A	91	LEU
1	A	107	LEU
1	A	112	LYS
1	A	120	GLN
1	A	130	LEU
1	A	158	ASP
1	A	202	LYS
1	A	204	GLN
1	A	225	HIS
1	A	236	GLU
1	A	245	VAL
1	A	247	GLU
1	A	248	GLU
1	A	269	GLN
1	A	280	VAL
1	A	286	LYS
1	A	315	ARG
1	A	320	LEU
1	A	358	THR
1	A	391	ASN
1	A	396	ARG
1	A	404	GLU

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Mol	Chain	Res	Type
1	A	406	ILE
1	A	418	MET
1	A	442	VAL
1	A	458	LEU
1	A	480	GLN
1	A	481	LEU
1	A	488	ASP
1	A	490	VAL
1	A	492	GLU
1	A	495	VAL
1	A	504	THR
1	A	531	ASN
1	A	546	LEU
1	A	549	LYS
1	A	553	GLN
1	A	567	LEU
1	A	579	LEU
1	A	602	LYS
1	A	607	LYS
1	A	611	ASP
1	A	612	GLU
1	A	613	THR
1	A	614	PHE
1	A	616	LEU
1	A	626	LEU
1	A	631	ARG
1	A	639	THR
1	A	649	LEU
1	A	658	LEU
1	A	659	GLU
1	A	661	VAL
1	A	679	ASP
1	A	723	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	24	GLN
1	A	254	HIS
1	A	268	ASN
1	A	269	GLN

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Mol	Chain	Res	Type
1	A	362	HIS
1	A	391	ASN
1	A	473	GLN
1	A	480	GLN
1	A	496	ASN
1	A	522	GLN
1	A	523	ASN
1	A	531	ASN
1	A	562	ASN
1	A	678	GLN
1	A	717	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](#)

There are no ligands in this entry.

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	729/780 (93%)	-0.08	11 (1%)	72 52	10, 29, 69, 70	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	PHE	6.6
1	A	591	ILE	3.5
1	A	249	ALA	3.5
1	A	617	PRO	2.9
1	A	205	GLU	2.8
1	A	620	THR	2.2
1	A	584	ALA	2.1
1	A	593	SER	2.1
1	A	603	ARG	2.1
1	A	610	THR	2.1
1	A	592	ARG	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.