Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:49 AM GMT

PDB ID : 2OCE
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

1 Overall quality at a glance (i)

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.
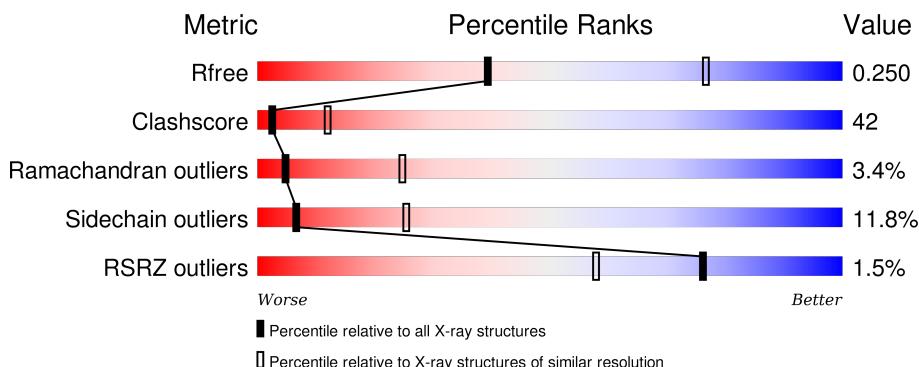
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 <=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	
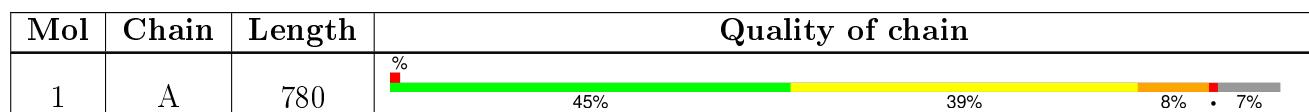
2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	729	5610	3532	987	1077	14	0	0	0

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
			Total	O		
2	A	266	266	266	0	0

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 errors 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: Hypothetical protein PA5201
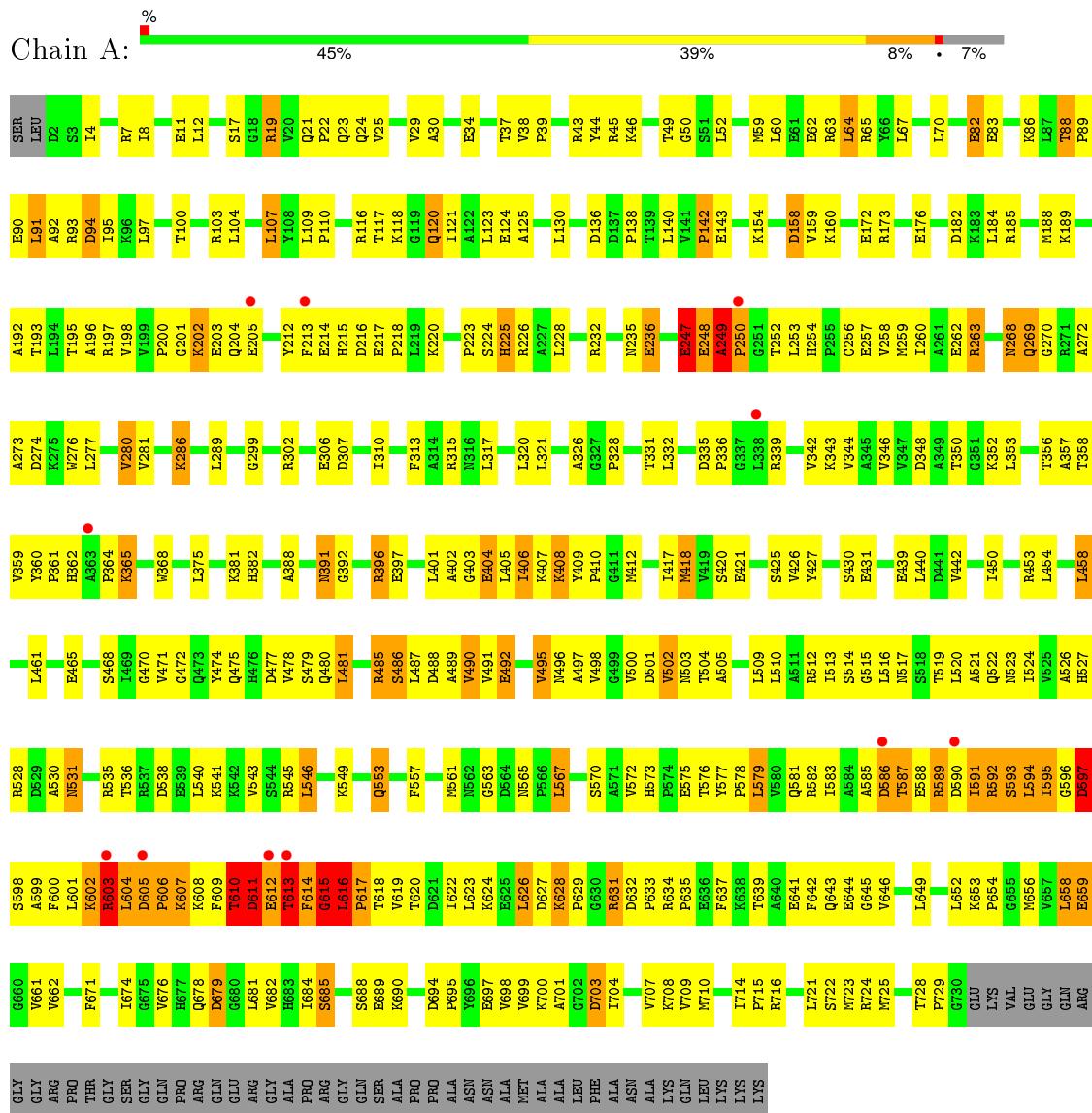
4   Data and refinement statistics (i)

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 29.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.10) 99.8 (29.99-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.18	Depositor
$<I/\sigma(I)>$ [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 (5.12%)	DCC
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<\|L\|> = 0.48, <L^2> = 0.31$	Xtriage
Outliers	0 of 18408 reflections	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<\|L\|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.40	0/5699	0.73	9/7711 (0.1%)

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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	593	SER	N-CA-CB	17.87	137.31	110.50
1	A	603	ARG	CB-CA-C	12.45	135.30	110.40
1	A	604	LEU	N-CA-CB	10.51	131.42	110.40
1	A	592	ARG	N-CA-C	9.63	136.99	111.00
1	A	592	ARG	CB-CA-C	-8.24	93.92	110.40
1	A	690	LYS	CB-CA-C	6.09	122.58	110.40
1	A	561	MET	N-CA-C	5.94	127.05	111.00
1	A	365	LYS	CB-CA-C	-5.72	98.96	110.40
1	A	586	ASP	N-CA-C	-5.29	96.71	111.00

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	470	0
2	A	266	0	0	11	0
All	All	5876	0	5701	470	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 (470) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:653:LYS:H	1:A:656:MET:HE3	1.30	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:212:TYR:HH	1:A:226:ARG:HG3	1.34	0.90
1:A:198:VAL:HG21	1:A:213:PHE:HZ	1.19	0.89
1:A:708:LYS:HG2	1:A:710:MET:HE3	1.56	0.88
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	1:A:286:LYS:HE2	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:531:ASN:N	1:A:531:ASN:HD22	1.79	0.77
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:567:LEU:H	1:A:567:LEU:CD2	2.00	0.74
1:A:465:GLU:HG3	1:A:468:SER:HB2	1.69	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:591:ILE:HG13	1:A:591:ILE:O	1.86	0.74
1:A:88:THR:HG22	1:A:91:LEU:H	1.53	0.74
1:A:592:ARG:C	1:A:594:LEU:H	1.91	0.72
1:A:603:ARG:NH2	1:A:620:THR:HG21	1.88	0.72
1:A:530:ALA:C	1:A:531:ASN:HD22	1.92	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:NZ	1:A:602:LYS:HA	2.07	0.69
1:A:582:ARG:HE	1:A:609:PHE:HZ	1.40	0.69
1:A:198:VAL:HB	1:A:213:PHE:CZ	2.05	0.69
1:A:590:ASP:O	1:A:591:ILE:HG12	1.92	0.69
1:A:360:TYR:CB	1:A:365:LYS:HD2	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ASN:HD21	1:A:514:SER:N	1.92	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:631:ARG:HG3	2:A:836:HOH:O	1.96	0.66
1:A:586:ASP:HB3	1:A:600:PHE:CZ	2.31	0.66
1:A:496:ASN:ND2	1:A:514:SER:H	1.94	0.65
1:A:269:GLN:HE21	1:A:269:GLN:HA	1.60	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:HG3	1:A:407:LYS:O	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:465:GLU:HG3	1:A:468:SER:CB	2.27	0.64
1:A:343:LYS:HE2	1:A:343:LYS:H	1.63	0.64
1:A:396:ARG:HH11	1:A:396:ARG:HB2	1.63	0.64
1:A:606:PRO:C	1:A:608:LYS:H	2.01	0.64
1:A:269:GLN:CA	1:A:269:GLN:HE21	2.10	0.63
1:A:223:PRO:HG3	1:A:226:ARG:CZ	2.29	0.63
1:A:631:ARG:HD3	1:A:631:ARG:H	1.62	0.63
1:A:700:LYS:O	1:A:703:ASP:HB2	1.98	0.63
1:A:531:ASN:ND2	1:A:531:ASN:N	2.47	0.63
1:A:619:VAL:HG13	1:A:622:ILE:HD12	1.81	0.63
1:A:12:LEU:HD23	1:A:59:MET:CE	2.29	0.63
1:A:217:GLU:OE2	1:A:226:ARG:HD2	1.99	0.63
1:A:583:ILE:HG22	1:A:583:ILE:O	1.98	0.62
1:A:158:ASP:OD2	1:A:160:LYS:HB3	1.99	0.62
1:A:65:ARG:HB3	1:A:65:ARG:NH1	2.14	0.62
1:A:540:LEU:O	1:A:546:LEU:HG	1.99	0.62
1:A:286:LYS:CA	1:A:286:LYS:HE2	2.30	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:60:LEU:C	1:A:60:LEU:HD23	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PRO:HD2	1:A:90:GLU:OE1	2.00	0.61
1:A:12:LEU:HA	1:A:59:MET:HE1	1.82	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:602:LYS:HE3	1:A:603:ARG:HG2	1.83	0.60
1:A:458:LEU:HD21	1:A:495:VAL:HG12	1.83	0.60
1:A:19:ARG:HG2	1:A:19:ARG:HH11	1.66	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
1:A:11:GLU:HG3	1:A:63:ARG:HD3	1.83	0.59
1:A:94:ASP:HB3	1:A:107:LEU:HD21	1.84	0.59
1:A:427:TYR:O	1:A:430:SER:HB3	2.02	0.59
1:A:594:LEU:O	1:A:595:ILE:HG22	2.02	0.59
1:A:203:GLU:CG	1:A:213:PHE:HZ	2.12	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:184:LEU:HD22	1:A:256:CYS:SG	2.43	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:615:GLY:O	1:A:616:LEU:HB2	2.03	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:615:GLY:O	1:A:616:LEU:CB	2.51	0.57
1:A:299:GLY:HA2	1:A:302:ARG:HH12	1.69	0.57
1:A:212:TYR:CZ	1:A:226:ARG:CG	2.87	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: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:228:LEU:O	1:A:232:ARG:HB2	2.04	0.57
1:A:100:THR:OG1	1:A:103:ARG:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:681:LEU:HD23	1:A:682:VAL:N	2.20	0.56
1:A:527:HIS:NE2	1:A:543:VAL:HA	2.20	0.56
1:A:486:SER:O	1:A:489:ALA:HB3	2.05	0.56
1:A:11:GLU:HB3	1:A:59:MET:HE3	1.86	0.56
1:A:681:LEU:HD23	1:A:682:VAL:H	1.70	0.56
1:A:646:VAL:HG13	1:A:646:VAL:O	2.06	0.56
1:A:21:GLN:H	1:A:24:GLN:NE2	2.03	0.56
1:A:588:GLU:HG3	1:A:600:PHE:CD2	2.40	0.56
1:A:332:LEU:HD11	1:A:344:VAL:HG12	1.88	0.56
1:A:4:ILE:O	1:A:8:ILE:HG13	2.06	0.56
1:A:598:SER:CA	1:A:602:LYS:HB2	2.35	0.55
1:A:626:LEU:H	1:A:626:LEU:HD13	1.71	0.55
1:A:567:LEU:N	1:A:567:LEU:HD23	2.19	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:653:LYS:N	1:A:656:MET:HE3	2.10	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:391:ASN:HD22	1:A:391:ASN:C	2.10	0.55
1:A:708:LYS:HG2	1:A:710:MET:CE	2.34	0.54
1:A:527:HIS:O	1:A:530:ALA:N	2.38	0.54
1:A:565:ASN:OD1	1:A:567:LEU:HD21	2.08	0.54
1:A:348:ASP:C	1:A:348:ASP:OD2	2.45	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:523:ASN:O	1:A:526:ALA:HB3	2.07	0.54
1:A:46:LYS:O	1:A:50:GLY:N	2.37	0.54
1:A:142:PRO:HG2	1:A:143:GLU:OE2	2.08	0.54
1:A:12:LEU:HD23	1:A:59:MET:HE2	1.90	0.54
1:A:722:SER:OG	1:A:724:ARG:HG2	2.08	0.54
1:A:588:GLU:C	1:A:590:ASP:H	2.10	0.54
1:A:620:THR:HG22	1:A:620:THR:O	2.07	0.54
1:A:252:THR:HG22	1:A:253:LEU:N	2.22	0.54
1:A:140:LEU:O	1:A:272:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:THR:O	1:A:622:ILE:HG13	2.08	0.53
1:A:592:ARG:HH11	1:A:592:ARG:HG2	1.74	0.53
1:A:515:GLY:O	1:A:516:LEU:HD23	2.08	0.53
1:A:618:THR:O	1:A:622:ILE:HD11	2.09	0.53
1:A:215:HIS:CD2	1:A:216:ASP:H	2.26	0.53
1:A:592:ARG:C	1:A:594:LEU:N	2.61	0.53
1:A:212:TYR:C	1:A:214:GLU:N	2.62	0.53
1:A:606:PRO:C	1:A:608:LYS:N	2.61	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:490:VAL:CG2	1:A:491:VAL:N	2.72	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:618:THR:O	1:A:622:ILE:CG1	2.57	0.53
1:A:332:LEU:HD13	1:A:346:VAL:HG22	1.90	0.53
1:A:502:VAL:HG21	1:A:540:LEU:HD21	1.90	0.52
1:A:12:LEU:HD23	1:A:59:MET:HE1	1.91	0.52
1:A:212:TYR:C	1:A:214:GLU:H	2.12	0.52
1:A:417:ILE:CD1	1:A:637:PHE:HZ	2.21	0.52
1:A:595:ILE:O	1:A:595:ILE:HG13	2.10	0.52
1:A:581:GLN:C	1:A:583:ILE:H	2.12	0.52
1:A:674:ILE:O	1:A:674:ILE:HG22	2.10	0.52
1:A:474:TYR:HB3	1:A:477:ASP:OD2	2.10	0.52
1:A:514:SER:OG	1:A:553:GLN:O	2.25	0.52
1:A:602:LYS:HZ1	1:A:602:LYS:HA	1.75	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:590:ASP:C	1:A:592:ARG:N	2.61	0.51
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:430:SER:OG	1:A:431:GLU:N	2.43	0.51
1:A:676:VAL:HG12	1:A:676:VAL:O	2.09	0.51
1:A:588:GLU:C	1:A:590:ASP:N	2.64	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:616:LEU:C	1:A:618:THR:H	2.15	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:616:LEU:O	1:A:620:THR:N	2.30	0.50
1:A:409:TYR:N	1:A:410:PRO:HD3	2.26	0.50
1:A:619:VAL:O	1:A:623:LEU:HD13	2.12	0.50
1:A:653:LYS:CD	1:A:654:PRO:HD2	2.25	0.49
1:A:21:GLN:HB3	1:A:23:GLN:CD	2.32	0.49
1:A:173:ARG:NH1	2:A:862:HOH:O	2.43	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:652:LEU:HD23	1:A:656:MET:SD	2.52	0.49
1:A:492:GLU:O	1:A:496:ASN:OD1	2.30	0.49
1:A:335:ASP:O	1:A:342:VAL:HG23	2.11	0.49
1:A:662:VAL:CG2	1:A:700:LYS:O	2.61	0.49
1:A:641:GLU:CG	1:A:641:GLU:O	2.59	0.49
1:A:248:GLU:O	1:A:248:GLU:OE2	2.30	0.49
1:A:197:ARG:HH12	1:A:216:ASP:CG	2.16	0.49
1:A:694:ASP:OD2	1:A:697:GLU:HG2	2.13	0.49
1:A:408:LYS:HB3	1:A:409:TYR:CD1	2.47	0.48
1:A:362:HIS:CD2	1:A:397:GLU:HB2	2.48	0.48
1:A:49:THR:HG21	1:A:52:LEU:HB2	1.95	0.48
1:A:652:LEU:HA	1:A:656:MET:HE1	1.96	0.48
1:A:527:HIS:O	1:A:528:ARG:C	2.52	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:90:GLU:CD	1:A:90:GLU:H	2.17	0.48
1:A:610:THR:C	1:A:611:ASP:O	2.51	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:223:PRO:HG3	1:A:226:ARG:NE	2.28	0.48
1:A:674:ILE:HD11	1:A:721:LEU:HD21	1.96	0.48
1:A:490:VAL:HG22	1:A:491:VAL:N	2.29	0.48
1:A:658:LEU:H	1:A:658:LEU:HD12	1.78	0.48
1:A:616:LEU:C	1:A:618:THR:N	2.67	0.47
1:A:136:ASP:HB2	2:A:800:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLU:HG3	1:A:83:GLU:N	2.28	0.47
1:A:184:LEU:CD1	1:A:289:LEU:HD13	2.44	0.47
1:A:159:VAL:HG13	1:A:160:LYS:N	2.30	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:708:LYS:HE3	1:A:710:MET:CE	2.45	0.47
1:A:471:VAL:HG22	1:A:475:GLN:HE22	1.80	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: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: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:520:LEU:HA	1:A:523:ASN:HB2	1.96	0.46
1:A:643:GLN:C	1:A:645:GLY:N	2.69	0.46
1:A:138:PRO:HA	1:A:273:ALA:HB3	1.96	0.46
1:A:656:MET:HB2	1:A:709:VAL:HG11	1.96	0.46
1:A:417:ILE:HG22	1:A:418:MET:N	2.30	0.46
1:A:49:THR:HG22	1:A:52:LEU:HG	1.97	0.46
1:A:682:VAL:HG11	1:A:723:MET:HE3	1.96	0.46
1:A:391:ASN:ND2	1:A:391:ASN:C	2.68	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:500:VAL:HG11	1:A:510:LEU:HD13	1.98	0.46
1:A:602:LYS:HZ2	1:A:602:LYS:HA	1.80	0.46
1:A:501:ASP:O	1:A:503:ASN:N	2.49	0.46
1:A:125:ALA:HA	1:A:154:LYS:HD3	1.97	0.46
1:A:254:HIS:CD2	1:A:256:CYS:HB2	2.50	0.46
1:A:689:GLU:HA	1:A:689:GLU:OE2	2.15	0.46
1:A:306:GLU:O	1:A:307:ASP:C	2.54	0.45
1:A:116:ARG:HH11	1:A:116:ARG:HG2	1.81	0.45
1:A:588:GLU:HA	1:A:588:GLU:OE1	2.17	0.45
1:A:601:LEU:HD11	1:A:626:LEU:CD2	2.46	0.45
1:A:21:GLN:HB2	1:A:24:GLN:HG3	1.98	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:627:ASP:CB	1:A:628:LYS:HD3	2.43	0.45
1:A:247:GLU:HG3	1:A:248:GLU:C	2.32	0.45
1:A:310:ILE:CG1	1:A:478:VAL:HG11	2.47	0.45
1:A:587:THR:HG23	1:A:587:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:HIS:NE2	1:A:397:GLU:HB2	2.32	0.45
1:A:188:MET:O	1:A:192:ALA:HB3	2.17	0.45
1:A:43:ARG:HB3	1:A:44:TYR:CD1	2.51	0.45
1:A:620:THR:O	1:A:624:LYS:HE2	2.17	0.45
1:A:403:GLY:O	1:A:404:GLU:C	2.54	0.44
1:A:605:ASP:O	1:A:606:PRO:O	2.36	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:339:ARG:HA	1:A:364:PRO:CD	2.46	0.44
1:A:612:GLU:O	1:A:613:THR:CG2	2.59	0.44
1:A:570:SER:C	1:A:572:VAL:H	2.20	0.44
1:A:470:GLY:HA2	1:A:475:GLN:OE1	2.17	0.44
1:A:465:GLU:HG3	1:A:468:SER:OG	2.18	0.44
1:A:421:GLU:HG2	1:A:450:ILE:HD11	1.98	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:585:ALA:O	1:A:586:ASP:HB2	2.18	0.44
1:A:567:LEU:HG	1:A:577:TYR:CE1	2.53	0.44
1:A:120:GLN:OE1	1:A:120:GLN:N	2.50	0.44
1:A:575:GLU:HG2	1:A:614:PHE:CE2	2.51	0.44
1:A:521:ALA:O	1:A:522:GLN:C	2.56	0.44
1:A:627:ASP:OD1	1:A:628:LYS:HD2	2.18	0.44
1:A:38:VAL:N	1:A:39:PRO:HD2	2.32	0.44
1:A:579:LEU:HD13	1:A:609:PHE:HB3	1.99	0.44
1:A:594:LEU:C	1:A:596:GLY:N	2.71	0.44
1:A:708:LYS:HE3	1:A:710:MET:HE1	2.00	0.44
1:A:626:LEU:H	1:A:626:LEU:HD22	1.82	0.43
1:A:498:VAL:O	1:A:498:VAL:HG12	2.18	0.43
1:A:254:HIS:CD2	1:A:256:CYS:H	2.36	0.43
1:A:662:VAL:HG21	1:A:700:LYS:O	2.18	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: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:579:LEU:CD1	1:A:609:PHE:CB	2.94	0.43
1:A:409:TYR:CD2	1:A:412:MET:HE2	2.53	0.43
1:A:232:ARG:O	1:A:236:GLU:HB2	2.19	0.43
1:A:684:ILE:HG23	1:A:685:SER:N	2.34	0.43
1:A:585:ALA:O	1:A:586:ASP:C	2.57	0.43
1:A:619:VAL:O	1:A:622:ILE:HB	2.19	0.43
1:A:254:HIS:HB3	1:A:257:GLU:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:CD2	1:A:487:LEU:HG	2.48	0.43
1:A:67:LEU:O	1:A:70:LEU:HB3	2.19	0.43
1:A:425:SER:O	1:A:426:VAL:C	2.56	0.43
1:A:659:GLU:OE1	1:A:704:ILE:HD11	2.19	0.43
1:A:618:THR:O	1:A:622:ILE:CD1	2.67	0.43
1:A:643:GLN:C	1:A:645:GLY:H	2.20	0.43
1:A:500:VAL:HG13	1:A:505:ALA:HB2	2.01	0.42
1:A:302:ARG:O	1:A:306:GLU:HG3	2.19	0.42
1:A:642:PHE:CD1	1:A:643:GLN:N	2.87	0.42
1:A:310:ILE:HD11	1:A:478:VAL:HG11	2.00	0.42
1:A:93:ARG:O	1:A:97:LEU:HG	2.19	0.42
1:A:388:ALA:HB2	1:A:454:LEU:CD1	2.25	0.42
1:A:313:PHE:CD1	1:A:472:GLY:HA3	2.55	0.42
1:A:646:VAL:CG1	1:A:646:VAL:O	2.67	0.42
1:A:44:TYR:O	1:A:45:ARG:NE	2.53	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:579:LEU:HD12	1:A:579:LEU:C	2.38	0.42
1:A:545:ARG:CB	1:A:545:ARG:HH11	2.33	0.42
1:A:332:LEU:HD21	1:A:375:LEU:HD22	2.02	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:682:VAL:HG11	1:A:723:MET:CE	2.50	0.42
1:A:43:ARG:HB3	1:A:44:TYR:CE1	2.54	0.42
1:A:535:ARG:O	1:A:536:THR:HG23	2.20	0.42
1:A:407:LYS:O	1:A:408:LYS:HD3	2.19	0.42
1:A:641:GLU:CD	1:A:641:GLU:O	2.58	0.42
1:A:392:GLY:N	1:A:421:GLU:OE2	2.50	0.42
1:A:590:ASP:C	1:A:592:ARG:H	2.23	0.42
1:A:353:LEU:HD11	1:A:356:THR:HG22	2.02	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:268:ASN:C	1:A:268:ASN:HD22	2.23	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:90:GLU:N	1:A:90:GLU:OE1	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:VAL:CG1	1:A:479:SER:N	2.83	0.41
1:A:202:LYS:HZ1	1:A:205:GLU:HG2	1.85	0.41
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:577:TYR:N	1:A:578:PRO:CD	2.83	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:604:LEU:O	1:A:605:ASP:C	2.58	0.41
1:A:70:LEU:HD12	1:A:104:LEU:HD22	2.02	0.41
1:A:220:LYS:HG2	1:A:220:LYS:O	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:698:VAL:HG12	1:A:699:VAL:N	2.36	0.41
1:A:641:GLU:O	1:A:641:GLU:HG2	2.20	0.41
1:A:259:MET:HA	1:A:262:GLU:OE2	2.20	0.41
1:A:708:LYS:CG	1:A:710:MET:HE3	2.38	0.41
1:A:331:THR:HG22	1:A:332:LEU:N	2.35	0.41
1:A:632:ASP:C	1:A:634:ARG:H	2.24	0.41
1:A:45:ARG:HA	1:A:45:ARG:HD3	1.82	0.41
1:A:589:ARG:HG3	1:A:589:ARG:H	1.68	0.41
1:A:7:ARG:NH1	2:A:829:HOH:O	2.50	0.41
1:A:496:ASN:HB3	1:A:557:PHE:CD2	2.55	0.41
1:A:19:ARG:HG2	1:A:19:ARG:NH1	2.34	0.41
1:A:215:HIS:C	1:A:216:ASP:OD1	2.59	0.40
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:HE21	1:A:678:GLN:HA	1.87	0.40
1:A:201:GLY:C	1:A:203:GLU:H	2.25	0.40
1:A:576:THR:O	1:A:577:TYR:C	2.57	0.40
1:A:103:ARG:NH1	1:A:103:ARG:HG3	2.35	0.40
1:A:103:ARG:HE	1:A:182:ASP:CG	2.25	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:652:LEU:HA	1:A:656:MET:CE	2.52	0.40
1:A:408:LYS:C	1:A:410:PRO:HD3	2.41	0.40
1:A:501:ASP:C	1:A:503:ASN:N	2.75	0.40
1:A:521:ALA:O	1:A:524:ILE:N	2.53	0.40
1:A:418:MET:HE2	1:A:418:MET:HA	2.03	0.40
1:A:30:ALA:O	1:A:34:GLU:HB2	2.20	0.40
1:A:252:THR:HG22	1:A:253:LEU:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:PRO:HA	1:A:342:VAL:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	727/780 (93%)	593 (82%)	109 (15%)	25 (3%)	5 25

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

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Mol	Chain	Res	Type
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 (i)

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%)	524 (88%)	70 (12%)	6	25

All (70) 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	64	LEU
1	A	82	GLU
1	A	86	LYS
1	A	88	THR
1	A	91	LEU
1	A	94	ASP
1	A	107	LEU
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	235	ASN
1	A	236	GLU
1	A	247	GLU
1	A	248	GLU
1	A	263	ARG

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Mol	Chain	Res	Type
1	A	268	ASN
1	A	269	GLN
1	A	280	VAL
1	A	286	LYS
1	A	315	ARG
1	A	358	THR
1	A	391	ASN
1	A	396	ARG
1	A	404	GLU
1	A	406	ILE
1	A	408	LYS
1	A	418	MET
1	A	442	VAL
1	A	458	LEU
1	A	480	GLN
1	A	481	LEU
1	A	486	SER
1	A	488	ASP
1	A	490	VAL
1	A	492	GLU
1	A	495	VAL
1	A	504	THR
1	A	512	ARG
1	A	531	ASN
1	A	538	ASP
1	A	546	LEU
1	A	549	LYS
1	A	553	GLN
1	A	567	LEU
1	A	579	LEU
1	A	597	ASP
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	628	LYS
1	A	631	ARG
1	A	639	THR

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Mol	Chain	Res	Type
1	A	649	LEU
1	A	658	LEU
1	A	659	GLU
1	A	661	VAL
1	A	679	ASP
1	A	703	ASP
1	A	725	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

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

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5　Carbohydrates ⓘ

There are no carbohydrates 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%)	-0.25	11 (1%)	76	58	10, 29, 69, 70	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	PHE	3.7
1	A	205	GLU	3.1
1	A	612	GLU	2.7
1	A	590	ASP	2.6
1	A	338	LEU	2.6
1	A	586	ASP	2.4
1	A	603	ARG	2.3
1	A	250	PRO	2.3
1	A	605	ASP	2.3
1	A	363	ALA	2.1
1	A	613	THR	2.1

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 carbohydrates 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.