



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:58 PM UTC

PDB ID : 2AKW / pdb_00002akw
Title : Crystal Structure of T.Thermophilus Phenylalanyl-tRNA synthetase complexed with p-Cl-Phenylalanine
Authors : Kotik-Kogan, O.M.; Moor, N.A.; Tworowski, D.E.; Safro, M.G.
Deposited on : 2005-08-04
Resolution : 2.80 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
Mogul : 2022.3.0, CSD as543be (2022)
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

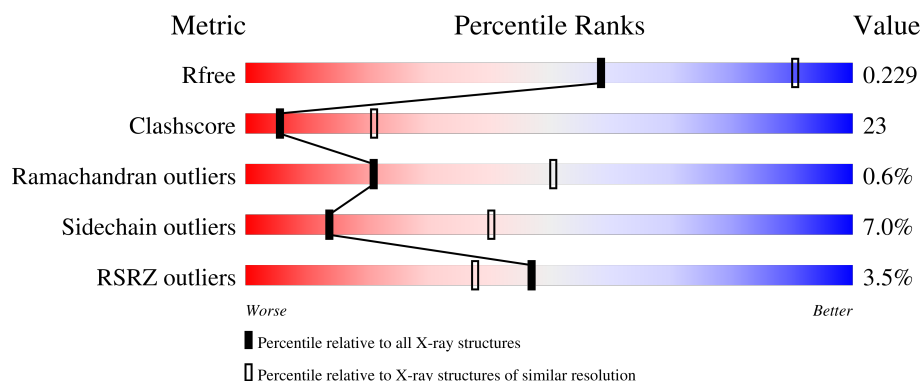
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	266	3% 60% 36% .
2	B	785	4% 56% 38% 5% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	B	786	-	X	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8466 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 Phenylalanyl-tRNA synthetase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2123	1388	363	365	7			

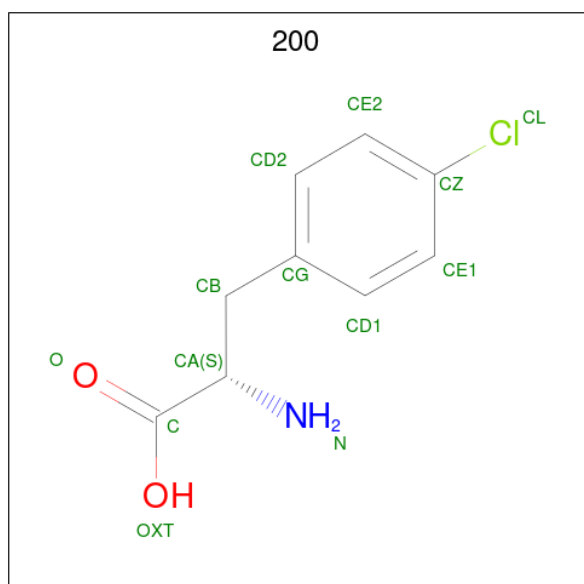
- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	785	Total	C	N	O	S	0	0	0
			6127	3925	1091	1101	10			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 4-CHLORO-L-PHENYLALANINE (CCD ID: 200) (formula: C₉H₁₀ClNO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			13	9	1	1	2		

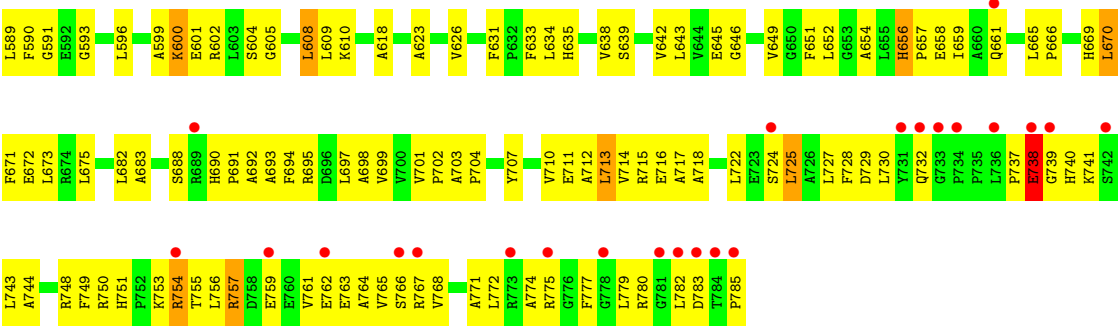
- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total	O	0	0
			41	41		
6	B	156	Total	O	0	0
			156	156		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	172.98Å 172.98Å 138.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.99 – 2.80 9.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (9.99-2.80) 97.0 (9.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.234 0.224 , 0.229	Depositor DCC
R_{free} test set	2918 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8466	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: 200, MN, SO4

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	0.46	0/2191	0.95	14/2971 (0.5%)
2	B	0.53	1/6280 (0.0%)	1.10	41/8536 (0.5%)
All	All	0.52	1/8471 (0.0%)	1.06	55/11507 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	99	LEU	N-CA	21.80	1.75	1.46

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	99	LEU	N-CA-CB	-22.11	75.95	110.44
2	B	99	LEU	N-CA-C	18.62	136.32	113.23
2	B	38	VAL	N-CA-C	15.83	129.05	113.53
2	B	98	GLY	CA-C-N	-13.61	97.72	121.66
2	B	98	GLY	C-N-CA	-13.61	97.72	121.66
2	B	133	LEU	N-CA-C	-7.51	99.16	110.28
2	B	739	GLY	N-CA-C	-7.36	105.05	115.43
2	B	670	LEU	N-CA-C	7.36	118.25	107.88
2	B	332	ALA	N-CA-C	-7.14	97.26	108.90
2	B	38	VAL	CA-C-N	-7.05	114.24	123.34
2	B	38	VAL	C-N-CA	-7.05	114.24	123.34
2	B	38	VAL	CB-CA-C	-6.68	104.10	110.65
2	B	168	LEU	N-CA-C	-6.67	105.46	112.93
1	A	280	LEU	N-CA-C	6.64	119.50	111.40
2	B	12	VAL	CA-C-N	6.49	126.71	119.32
2	B	12	VAL	C-N-CA	6.49	126.71	119.32
1	A	214	ALA	N-CA-C	-6.36	105.68	113.50
2	B	141	PRO	N-CA-C	-6.32	102.99	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70	ARG	N-CA-C	-6.30	100.88	110.14
2	B	563	ASP	N-CA-C	-6.25	100.94	109.95
1	A	151	THR	N-CA-C	6.01	119.70	110.20
1	A	163	GLY	CA-C-N	5.98	125.46	119.24
1	A	163	GLY	C-N-CA	5.98	125.46	119.24
2	B	387	ARG	N-CA-C	-5.98	98.98	108.73
2	B	118	LEU	N-CA-C	5.98	119.37	110.52
1	A	319	VAL	N-CA-C	5.96	116.60	110.82
1	A	184	VAL	N-CA-C	-5.91	105.95	111.45
2	B	416	GLY	N-CA-C	-5.87	106.64	115.32
2	B	656	HIS	CA-C-N	5.83	125.30	119.24
2	B	656	HIS	C-N-CA	5.83	125.30	119.24
1	A	257	TYR	N-CA-C	5.80	119.27	109.76
2	B	39	PHE	N-CA-C	5.74	119.42	108.97
2	B	608	LEU	N-CA-C	-5.74	104.40	111.40
2	B	521	ALA	N-CA-C	-5.68	105.09	111.28
2	B	618	ALA	N-CA-C	-5.66	105.11	111.28
2	B	256	ARG	N-CA-C	5.61	117.63	110.61
1	A	326	ARG	N-CA-C	5.49	117.07	111.14
2	B	245	VAL	N-CA-C	5.46	115.67	110.42
2	B	123	LEU	N-CA-C	-5.41	105.55	111.82
2	B	37	ARG	N-CA-C	-5.39	100.51	109.46
2	B	467	GLN	N-CA-C	-5.33	105.52	112.23
1	A	246	GLY	CA-C-N	5.30	124.97	119.56
1	A	246	GLY	C-N-CA	5.30	124.97	119.56
1	A	197	VAL	N-CA-C	-5.30	100.44	108.17
1	A	128	GLU	N-CA-C	5.28	117.44	109.41
2	B	785	PRO	CB-CA-C	5.23	120.03	110.10
2	B	336	ALA	N-CA-C	5.22	116.22	108.86
2	B	16	GLU	N-CA-C	5.20	117.03	111.36
2	B	66	LEU	N-CA-C	5.15	117.89	109.59
2	B	69	GLY	N-CA-C	-5.14	100.99	113.18
2	B	155	VAL	N-CA-C	5.13	115.25	107.75
2	B	393	LEU	N-CA-C	-5.10	100.20	108.52
2	B	309	PHE	CA-C-N	5.06	124.82	119.76
2	B	309	PHE	C-N-CA	5.06	124.82	119.76
1	A	208	THR	N-CA-C	5.06	116.51	108.67

There are no chirality outliers.

There are no planarity outliers.

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	2123	0	2075	94	0
2	B	6127	0	6180	298	0
3	A	1	0	0	0	0
4	A	13	0	9	2	0
5	B	5	0	0	2	0
6	A	41	0	0	1	0
6	B	156	0	0	0	0
All	All	8466	0	8264	387	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 23.

All (387) 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)
2:B:99:LEU:N	2:B:99:LEU:CA	1.75	1.45
1:A:167:GLU:OE2	1:A:301:LEU:HD21	1.10	1.25
2:B:99:LEU:N	2:B:99:LEU:CB	2.02	1.20
1:A:167:GLU:OE2	1:A:301:LEU:CD2	2.05	1.03
2:B:282:ARG:HH11	2:B:282:ARG:HB3	1.25	1.01
2:B:98:GLY:C	2:B:99:LEU:CA	2.33	1.00
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.43	0.99
1:A:183:GLN:HB2	1:A:222:LEU:HD22	1.44	0.98
2:B:467:GLN:HE21	2:B:467:GLN:HA	1.30	0.95
1:A:165:LEU:HD12	1:A:301:LEU:HD23	1.49	0.95
2:B:656:HIS:HB3	2:B:659:ILE:HD13	1.51	0.89
2:B:192:LYS:H	2:B:381:GLN:HE22	1.21	0.87
2:B:407:ARG:NH2	5:B:786:SO4:O1	2.08	0.85
2:B:557:LYS:HG2	2:B:665:LEU:HD21	1.58	0.85
2:B:713:LEU:HD11	2:B:775:ARG:HG3	1.57	0.85
2:B:176:ASP:OD2	2:B:465:ARG:NH2	2.10	0.84
2:B:99:LEU:N	2:B:99:LEU:HB2	1.91	0.84
2:B:602:ARG:HG3	2:B:602:ARG:HH11	1.46	0.80
2:B:782:LEU:HD23	2:B:783:ASP:N	1.95	0.80
2:B:282:ARG:HB3	2:B:282:ARG:NH1	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:596:LEU:HB2	2:B:599:ALA:HB3	1.66	0.78
2:B:80:ASN:H	2:B:80:ASN:HD22	1.33	0.77
2:B:600:LYS:HD3	2:B:600:LYS:N	2.00	0.75
1:A:160:ARG:HH21	2:B:579:GLU:HB3	1.52	0.75
2:B:214:THR:HG22	2:B:394:GLU:HG3	1.69	0.75
2:B:461:GLU:O	2:B:465:ARG:HG2	1.87	0.74
2:B:767:ARG:HE	2:B:767:ARG:N	1.85	0.74
2:B:710:VAL:HG11	2:B:743:LEU:HD12	1.68	0.74
1:A:179:THR:OG1	1:A:220:GLU:HG2	1.88	0.74
2:B:649:VAL:HG23	2:B:673:LEU:HD22	1.70	0.74
2:B:255:GLU:OE2	2:B:375:ARG:HD2	1.89	0.73
2:B:98:GLY:O	2:B:99:LEU:CA	2.37	0.73
2:B:56:ILE:HB	2:B:59:THR:OG1	1.89	0.72
2:B:427:ILE:HD12	2:B:466:ILE:CG2	2.19	0.72
2:B:693:ALA:HB3	2:B:749:PHE:HB2	1.71	0.71
2:B:374:ARG:HG2	2:B:374:ARG:HH11	1.55	0.71
1:A:317:LEU:O	1:A:317:LEU:HD12	1.90	0.71
2:B:407:ARG:HD3	2:B:456:GLU:OE2	1.90	0.71
2:B:764:ALA:HA	2:B:767:ARG:HG2	1.71	0.71
2:B:761:VAL:O	2:B:765:VAL:HG13	1.90	0.71
1:A:198:VAL:HG13	1:A:220:GLU:HB2	1.73	0.71
2:B:604:SER:HA	2:B:608:LEU:HD22	1.72	0.70
1:A:280:LEU:HD21	1:A:322:LEU:HD23	1.71	0.70
2:B:192:LYS:N	2:B:381:GLN:HE22	1.89	0.70
2:B:176:ASP:CG	2:B:465:ARG:HH22	2.00	0.69
2:B:99:LEU:CB	2:B:99:LEU:H	2.05	0.69
2:B:294:HIS:CE1	2:B:296:GLU:HB2	2.28	0.69
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.75	0.69
1:A:169:VAL:HG22	1:A:170:GLU:H	1.59	0.68
2:B:279:GLU:HG2	2:B:295:PRO:HD3	1.73	0.68
1:A:165:LEU:HD11	1:A:303:LEU:HD11	1.76	0.68
2:B:427:ILE:HD12	2:B:466:ILE:HG21	1.77	0.67
2:B:697:LEU:O	2:B:697:LEU:HD12	1.94	0.67
2:B:763:GLU:OE2	2:B:767:ARG:HD2	1.94	0.67
2:B:519:GLU:HB3	2:B:523:ARG:NH1	2.11	0.66
2:B:353:ARG:C	2:B:353:ARG:HD3	2.21	0.66
2:B:63:ARG:HD2	2:B:73:GLU:OE2	1.96	0.66
2:B:631:PHE:HB2	2:B:634:LEU:HD12	1.77	0.66
1:A:271:TRP:CZ3	1:A:274:GLY:HA3	2.31	0.65
2:B:413:ARG:NH2	5:B:786:SO4:O4	2.29	0.65
1:A:329:ILE:HD11	1:A:346:PHE:HZ	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:VAL:HG13	2:B:702:PRO:HD2	1.79	0.65
2:B:258:GLN:HE22	2:B:369:GLN:NE2	1.94	0.65
1:A:210:ALA:HA	1:A:331:ASP:OD1	1.98	0.64
2:B:701:VAL:HG22	2:B:777:PHE:CD1	2.32	0.64
2:B:28:LEU:HD13	2:B:176:ASP:HB3	1.80	0.64
2:B:277:ALA:O	2:B:295:PRO:HA	1.98	0.64
2:B:702:PRO:HA	2:B:740:HIS:HA	1.79	0.64
2:B:703:ALA:N	2:B:704:PRO:HD2	2.13	0.63
1:A:160:ARG:NH2	2:B:579:GLU:HB3	2.12	0.63
2:B:209:GLY:C	2:B:211:PRO:HD3	2.23	0.63
1:A:169:VAL:HG22	1:A:170:GLU:N	2.13	0.63
2:B:732:GLN:HB3	2:B:741:LYS:HB3	1.81	0.62
2:B:751:HIS:HB3	2:B:754:ARG:O	1.98	0.62
1:A:329:ILE:HD11	1:A:346:PHE:CZ	2.34	0.62
1:A:109:GLU:O	1:A:113:ILE:HG12	2.00	0.62
1:A:165:LEU:CD1	1:A:301:LEU:HD23	2.28	0.62
2:B:49:ARG:HD2	2:B:137:GLU:HG3	1.82	0.62
2:B:99:LEU:N	2:B:99:LEU:HB3	2.13	0.62
2:B:583:THR:HG22	2:B:675:LEU:HD12	1.81	0.62
2:B:698:ALA:HB3	2:B:780:ARG:HB3	1.81	0.62
1:A:300:ARG:NH1	1:A:300:ARG:HB2	2.14	0.61
1:A:113:ILE:HD12	1:A:243:ALA:HB1	1.83	0.61
2:B:224:ALA:N	2:B:244:ASN:ND2	2.48	0.61
2:B:457:GLU:HA	2:B:460:VAL:HG13	1.81	0.61
2:B:582:GLU:OE2	2:B:584:HIS:HE1	1.83	0.61
1:A:308:ARG:HE	1:A:308:ARG:HA	1.66	0.60
2:B:62:LYS:HB2	2:B:62:LYS:NZ	2.15	0.60
2:B:80:ASN:HD21	2:B:132:LEU:H	1.47	0.60
1:A:223:VAL:HG12	1:A:228:ILE:HD13	1.83	0.60
2:B:530:ARG:HD2	2:B:579:GLU:H	1.66	0.60
2:B:516:MET:HE3	2:B:545:ARG:HA	1.81	0.60
2:B:782:LEU:HD23	2:B:783:ASP:HB2	1.84	0.60
2:B:98:GLY:O	2:B:99:LEU:HA	2.00	0.60
2:B:557:LYS:HA	2:B:560:LEU:HD12	1.83	0.60
2:B:643:LEU:HD12	2:B:646:GLY:O	2.02	0.60
2:B:80:ASN:H	2:B:80:ASN:ND2	2.00	0.60
2:B:563:ASP:C	2:B:564:ARG:HD2	2.26	0.60
2:B:282:ARG:HH11	2:B:282:ARG:CB	2.10	0.60
2:B:767:ARG:HE	2:B:767:ARG:CA	2.14	0.60
2:B:44:GLY:HA3	2:B:94:THR:OG1	2.02	0.59
2:B:589:LEU:HD21	2:B:608:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:LEU:HD23	2:B:268:VAL:HG21	1.84	0.59
2:B:530:ARG:HB2	2:B:530:ARG:NH1	2.17	0.59
2:B:642:VAL:C	2:B:643:LEU:HD22	2.29	0.58
2:B:732:GLN:HB2	2:B:740:HIS:O	2.04	0.58
2:B:605:GLY:HA2	2:B:669:HIS:CD2	2.39	0.57
2:B:256:ARG:NH2	2:B:375:ARG:HG3	2.18	0.57
2:B:520:ASP:HA	2:B:523:ARG:HB2	1.86	0.57
2:B:589:LEU:HD12	2:B:590:PHE:H	1.70	0.57
1:A:155:THR:HB	2:B:534:LEU:HD21	1.87	0.57
2:B:101:GLN:N	2:B:101:GLN:NE2	2.52	0.57
2:B:223:VAL:HA	2:B:244:ASN:HD22	1.69	0.57
2:B:690:HIS:HB3	2:B:691:PRO:HD2	1.85	0.57
2:B:688:SER:HB3	2:B:750:ARG:HD3	1.87	0.57
1:A:271:TRP:HZ3	1:A:276:LYS:HE2	1.69	0.57
2:B:587:GLY:HA3	2:B:671:PHE:CE1	2.39	0.57
1:A:162:GLU:O	1:A:185:ARG:NH2	2.38	0.57
1:A:298:ARG:NH1	1:A:304:PRO:O	2.37	0.57
1:A:165:LEU:HB2	1:A:167:GLU:OE1	2.04	0.57
1:A:223:VAL:HG12	1:A:228:ILE:CD1	2.35	0.57
1:A:174:LEU:C	1:A:174:LEU:HD12	2.30	0.56
2:B:224:ALA:H	2:B:244:ASN:ND2	2.03	0.56
2:B:697:LEU:HD12	2:B:697:LEU:C	2.31	0.56
2:B:762:GLU:O	2:B:765:VAL:HG22	2.05	0.56
2:B:212:HIS:HE1	2:B:394:GLU:OE2	1.89	0.56
2:B:530:ARG:HB2	2:B:530:ARG:HH11	1.70	0.56
2:B:692:ALA:HB2	2:B:750:ARG:NH1	2.21	0.56
1:A:256:VAL:HG12	1:A:265:ALA:C	2.31	0.56
1:A:349:VAL:HG12	1:A:350:LEU:HD23	1.87	0.56
2:B:141:PRO:O	2:B:144:THR:HG23	2.06	0.56
2:B:593:GLY:HA3	2:B:604:SER:HB3	1.88	0.56
2:B:596:LEU:HB2	2:B:599:ALA:CB	2.34	0.56
2:B:120:PRO:HG3	2:B:133:LEU:HD13	1.87	0.56
2:B:163:ASN:O	2:B:452:ASP:HB3	2.07	0.55
2:B:588:LEU:C	2:B:588:LEU:HD23	2.32	0.55
2:B:701:VAL:CG1	2:B:702:PRO:HD2	2.36	0.55
2:B:702:PRO:C	2:B:704:PRO:HD2	2.30	0.55
1:A:292:GLN:HA	1:A:308:ARG:HH22	1.71	0.55
1:A:261:VAL:HG11	4:A:999:200:CL	2.44	0.55
1:A:85:ARG:N	1:A:85:ARG:HD2	2.21	0.55
2:B:610:LYS:HZ3	2:B:626:VAL:HB	1.72	0.55
2:B:49:ARG:CD	2:B:137:GLU:HG3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ASP:OD1	2:B:266:ARG:HG3	2.07	0.55
1:A:182:MET:HE3	1:A:182:MET:O	2.07	0.55
2:B:56:ILE:HD11	2:B:63:ARG:HB2	1.89	0.55
1:A:182:MET:HG2	1:A:198:VAL:HG21	1.88	0.54
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.87	0.54
2:B:578:ARG:O	2:B:579:GLU:HB2	2.08	0.54
2:B:602:ARG:HG3	2:B:602:ARG:NH1	2.17	0.54
1:A:178:HIS:HB2	1:A:218:GLN:HE22	1.73	0.54
1:A:324:MET:HG2	1:A:329:ILE:HB	1.89	0.54
2:B:516:MET:SD	2:B:529:PRO:HG3	2.47	0.54
2:B:509:GLU:HB2	2:B:571:PHE:CE1	2.42	0.54
1:A:87:ASP:O	1:A:90:LEU:HB2	2.07	0.54
2:B:203:LYS:HE3	2:B:205:GLU:OE2	2.06	0.54
2:B:326:GLU:CD	2:B:326:GLU:H	2.16	0.54
2:B:755:THR:HG22	2:B:756:LEU:N	2.23	0.54
2:B:554:ARG:HG2	2:B:554:ARG:HH11	1.72	0.53
2:B:768:VAL:O	2:B:772:LEU:HB2	2.08	0.53
2:B:730:LEU:HD13	2:B:743:LEU:HD23	1.91	0.53
2:B:519:GLU:HB3	2:B:523:ARG:HH12	1.72	0.53
2:B:710:VAL:O	2:B:714:VAL:HG23	2.08	0.53
2:B:368:GLY:O	2:B:371:PRO:HD2	2.09	0.52
1:A:237:ILE:HG22	1:A:251:VAL:HG11	1.90	0.52
1:A:252:ARG:NH2	1:A:279:GLU:OE2	2.43	0.52
2:B:604:SER:HA	2:B:608:LEU:HB2	1.92	0.52
2:B:49:ARG:CG	2:B:137:GLU:HG3	2.40	0.52
2:B:258:GLN:HE22	2:B:369:GLN:HE21	1.58	0.52
2:B:282:ARG:HH12	2:B:290:GLU:HG3	1.74	0.52
2:B:552:LEU:O	2:B:555:VAL:HG22	2.10	0.52
2:B:718:ALA:CB	2:B:722:LEU:HD22	2.40	0.52
2:B:178:HIS:CD2	2:B:430:ARG:HH12	2.28	0.51
2:B:408:PRO:HG2	2:B:421:GLU:HG3	1.90	0.51
2:B:409:GLU:OE1	2:B:413:ARG:HD3	2.10	0.51
2:B:549:PHE:CD1	2:B:549:PHE:C	2.88	0.51
2:B:178:HIS:O	2:B:430:ARG:NH1	2.43	0.51
2:B:474:LEU:HD12	2:B:474:LEU:N	2.25	0.51
2:B:516:MET:HE3	2:B:546:THR:H	1.76	0.51
2:B:730:LEU:HD13	2:B:743:LEU:CD2	2.39	0.51
1:A:102:PRO:HG3	1:A:346:PHE:CD1	2.46	0.51
1:A:113:ILE:HD12	1:A:243:ALA:CB	2.40	0.51
1:A:174:LEU:HD12	1:A:174:LEU:O	2.10	0.51
1:A:188:VAL:HG12	1:A:294:VAL:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:HIS:HE1	2:B:658:GLU:HG3	1.75	0.51
2:B:711:GLU:CD	2:B:715:ARG:HH12	2.18	0.51
2:B:49:ARG:HD2	2:B:137:GLU:CG	2.41	0.51
2:B:600:LYS:HG2	2:B:601:GLU:OE2	2.10	0.51
2:B:49:ARG:HG3	2:B:137:GLU:HG3	1.93	0.51
2:B:718:ALA:HB3	2:B:722:LEU:HD22	1.93	0.51
2:B:407:ARG:HG3	2:B:441:THR:HB	1.92	0.50
2:B:657:PRO:O	2:B:661:GLN:OE1	2.29	0.50
2:B:757:ARG:HG2	2:B:757:ARG:HH11	1.77	0.50
1:A:191:THR:HG23	2:B:484:ASP:OD2	2.12	0.49
1:A:201:ARG:HD2	1:A:336:PHE:HZ	1.77	0.49
2:B:368:GLY:C	2:B:371:PRO:HD2	2.36	0.49
2:B:583:THR:CG2	2:B:675:LEU:HD12	2.43	0.49
2:B:693:ALA:O	2:B:748:ARG:HA	2.12	0.49
2:B:690:HIS:CE1	2:B:753:LYS:O	2.65	0.49
1:A:271:TRP:CZ3	1:A:325:LEU:HD11	2.47	0.49
1:A:269:VAL:CG1	1:A:280:LEU:HD12	2.42	0.49
2:B:762:GLU:OE2	2:B:783:ASP:OD2	2.31	0.49
2:B:374:ARG:HG2	2:B:374:ARG:NH1	2.26	0.49
2:B:651:PHE:C	2:B:651:PHE:CD1	2.91	0.49
2:B:699:VAL:CG1	2:B:772:LEU:HD11	2.43	0.49
2:B:62:LYS:HB2	2:B:62:LYS:HZ2	1.76	0.49
2:B:638:VAL:HB	2:B:654:ALA:HB3	1.95	0.49
2:B:701:VAL:HG22	2:B:777:PHE:HD1	1.78	0.49
1:A:269:VAL:HG13	1:A:280:LEU:HD12	1.96	0.48
1:A:108:ARG:O	1:A:112:GLU:HG2	2.13	0.48
1:A:113:ILE:CD1	1:A:243:ALA:HB1	2.43	0.48
2:B:369:GLN:CD	2:B:369:GLN:H	2.21	0.48
2:B:610:LYS:NZ	2:B:626:VAL:HB	2.28	0.48
1:A:85:ARG:HG3	1:A:85:ARG:HH11	1.79	0.48
1:A:85:ARG:HG3	1:A:85:ARG:NH1	2.28	0.48
1:A:190:HIS:HB3	2:B:484:ASP:OD1	2.14	0.48
2:B:767:ARG:CA	2:B:767:ARG:NE	2.76	0.48
2:B:578:ARG:O	2:B:579:GLU:CB	2.62	0.48
2:B:755:THR:HG22	2:B:756:LEU:H	1.79	0.48
1:A:179:THR:OG1	1:A:220:GLU:CG	2.61	0.47
2:B:357:SER:O	2:B:361:GLU:HG3	2.14	0.47
2:B:362:ARG:HH11	2:B:362:ARG:HG2	1.79	0.47
2:B:729:ASP:HB3	2:B:744:ALA:CB	2.44	0.47
1:A:350:LEU:HD22	1:A:350:LEU:N	2.30	0.47
2:B:341:VAL:HG12	2:B:345:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HD12	1:A:317:LEU:C	2.40	0.47
2:B:300:ILE:O	2:B:311:LEU:HB2	2.14	0.47
2:B:762:GLU:CD	2:B:783:ASP:OD2	2.57	0.47
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.45	0.47
2:B:489:GLU:HG3	2:B:493:ARG:HD2	1.97	0.47
2:B:775:ARG:NH1	2:B:777:PHE:HE2	2.11	0.47
1:A:101:HIS:CG	1:A:102:PRO:HD2	2.50	0.47
2:B:101:GLN:CD	2:B:101:GLN:H	2.22	0.47
2:B:224:ALA:N	2:B:244:ASN:HD22	2.13	0.47
2:B:286:LEU:HD21	2:B:323:GLU:HG3	1.96	0.47
2:B:478:ALA:O	2:B:479:PHE:HB3	2.14	0.47
2:B:604:SER:HA	2:B:608:LEU:CD2	2.44	0.47
2:B:564:ARG:HD2	2:B:564:ARG:N	2.30	0.47
2:B:775:ARG:CZ	2:B:775:ARG:HB3	2.43	0.47
1:A:179:THR:C	1:A:181:PRO:HD2	2.40	0.47
2:B:724:SER:H	2:B:748:ARG:HB2	1.80	0.47
2:B:496:GLN:O	2:B:500:GLU:HG3	2.15	0.46
2:B:519:GLU:HG3	2:B:522:ARG:NH2	2.30	0.46
2:B:695:ARG:HD2	2:B:765:VAL:HG11	1.97	0.46
2:B:763:GLU:O	2:B:766:SER:HB2	2.15	0.46
1:A:271:TRP:CE3	1:A:274:GLY:HA3	2.50	0.46
2:B:235:PHE:CZ	2:B:241:PRO:HD2	2.50	0.46
2:B:515:PHE:CE1	2:B:533:LEU:HD21	2.50	0.46
2:B:557:LYS:CG	2:B:665:LEU:HD21	2.38	0.46
1:A:180:SER:N	1:A:181:PRO:HD2	2.30	0.46
2:B:50:VAL:HG12	2:B:83:LYS:HA	1.98	0.46
2:B:771:ALA:HA	2:B:774:ALA:HB3	1.98	0.46
2:B:24:ARG:NE	2:B:182:TYR:OH	2.46	0.46
2:B:562:LEU:HD22	2:B:563:ASP:OD1	2.15	0.46
2:B:725:LEU:C	2:B:725:LEU:HD23	2.40	0.46
1:A:106:MET:SD	1:A:322:LEU:HD12	2.56	0.46
1:A:133:ASN:HA	1:A:181:PRO:HB3	1.96	0.46
2:B:296:GLU:HB3	2:B:349:ARG:HH12	1.81	0.46
2:B:344:ARG:O	2:B:348:ARG:HD3	2.16	0.46
2:B:409:GLU:CD	2:B:413:ARG:HD3	2.41	0.46
2:B:772:LEU:O	2:B:777:PHE:HB2	2.17	0.45
1:A:141:GLU:C	1:A:143:HIS:H	2.25	0.45
1:A:315:PHE:CD1	1:A:315:PHE:C	2.94	0.45
1:A:339:ARG:O	1:A:342:PHE:HB3	2.17	0.45
2:B:548:LEU:H	2:B:672:GLU:CD	2.24	0.45
2:B:33:ASP:O	2:B:34:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:VAL:CG1	1:A:350:LEU:HD23	2.46	0.45
2:B:153:GLU:HG3	2:B:154:VAL:N	2.32	0.45
2:B:516:MET:CE	2:B:546:THR:H	2.30	0.45
2:B:782:LEU:CD2	2:B:783:ASP:HB2	2.47	0.45
2:B:121:ARG:HG3	2:B:121:ARG:HH11	1.82	0.45
2:B:601:GLU:CD	2:B:601:GLU:H	2.24	0.45
1:A:208:THR:HG22	1:A:333:ARG:HD3	1.98	0.45
2:B:432:GLY:O	2:B:447:PRO:HG3	2.16	0.45
2:B:210:ALA:HB2	2:B:274:VAL:HG11	1.98	0.45
1:A:330:PRO:HG2	1:A:334:TYR:HE2	1.82	0.45
2:B:428:LEU:O	2:B:433:CYS:HB2	2.16	0.45
2:B:554:ARG:HG2	2:B:554:ARG:NH1	2.30	0.45
2:B:698:ALA:O	2:B:779:LEU:HD12	2.16	0.45
2:B:707:TYR:CE1	2:B:727:LEU:HD22	2.51	0.45
2:B:702:PRO:HB2	2:B:704:PRO:HD2	1.99	0.44
2:B:168:LEU:HD23	2:B:168:LEU:HA	1.85	0.44
2:B:699:VAL:HG11	2:B:772:LEU:HD11	1.99	0.44
2:B:75:VAL:HG23	2:B:111:VAL:HG22	1.99	0.44
1:A:141:GLU:C	1:A:143:HIS:N	2.73	0.44
2:B:516:MET:HG2	2:B:517:ASP:N	2.33	0.44
1:A:101:HIS:ND1	1:A:102:PRO:HD2	2.33	0.44
2:B:279:GLU:HG2	2:B:295:PRO:CD	2.46	0.44
1:A:224:VAL:HG12	1:A:225:GLY:N	2.33	0.44
2:B:24:ARG:HD2	2:B:182:TYR:HE1	1.83	0.44
1:A:271:TRP:CZ3	1:A:276:LYS:HE2	2.50	0.44
2:B:278:ARG:HB2	2:B:281:GLU:HG3	2.00	0.44
2:B:455:LEU:O	2:B:458:ASP:HB2	2.17	0.44
2:B:652:LEU:HD12	2:B:670:LEU:O	2.18	0.44
2:B:43:ARG:HG3	2:B:43:ARG:HH11	1.82	0.43
2:B:623:ALA:HB3	2:B:645:GLU:HA	1.99	0.43
2:B:425:ILE:HD11	2:B:442:TYR:CZ	2.53	0.43
2:B:656:HIS:HB3	2:B:659:ILE:CD1	2.35	0.43
1:A:271:TRP:HB2	1:A:278:LEU:HD11	1.99	0.43
1:A:300:ARG:HB2	1:A:300:ARG:HH11	1.82	0.43
2:B:194:GLU:OE1	2:B:387:ARG:NH2	2.49	0.43
2:B:264:ASP:CG	2:B:328:THR:HG23	2.43	0.43
2:B:455:LEU:O	2:B:459:LEU:HD22	2.18	0.43
2:B:635:HIS:O	2:B:639:SER:HB2	2.18	0.43
2:B:249:THR:HB	2:B:260:MET:HG3	2.00	0.43
2:B:498:LEU:O	2:B:502:LEU:HG	2.18	0.43
2:B:779:LEU:CD2	2:B:782:LEU:HD12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ALA:HA	1:A:197:VAL:O	2.19	0.43
2:B:409:GLU:OE2	2:B:413:ARG:NH1	2.43	0.43
2:B:703:ALA:N	2:B:704:PRO:CD	2.80	0.43
2:B:280:GLY:O	2:B:281:GLU:C	2.60	0.43
2:B:286:LEU:HD21	2:B:323:GLU:CG	2.49	0.43
2:B:737:PRO:O	2:B:738:GLU:C	2.60	0.43
2:B:757:ARG:HD2	2:B:759:GLU:OE1	2.18	0.43
1:A:348:GLY:O	1:A:349:VAL:C	2.62	0.43
2:B:264:ASP:CG	2:B:266:ARG:HD3	2.44	0.43
2:B:403:ALA:CB	2:B:443:ARG:HD3	2.48	0.43
1:A:322:LEU:HD13	1:A:322:LEU:O	2.19	0.43
2:B:326:GLU:CD	2:B:326:GLU:N	2.77	0.43
2:B:405:PRO:HA	2:B:442:TYR:O	2.19	0.43
2:B:695:ARG:NH1	2:B:761:VAL:HG12	2.34	0.43
2:B:782:LEU:HD23	2:B:782:LEU:C	2.43	0.43
2:B:369:GLN:CD	2:B:369:GLN:N	2.77	0.42
2:B:707:TYR:OH	2:B:711:GLU:HG3	2.19	0.42
2:B:467:GLN:HA	2:B:467:GLN:NE2	2.11	0.42
2:B:694:PHE:CD1	2:B:694:PHE:N	2.87	0.42
2:B:782:LEU:O	2:B:783:ASP:C	2.62	0.42
2:B:43:ARG:HG3	2:B:43:ARG:NH1	2.34	0.42
2:B:222:ARG:O	2:B:222:ARG:HG3	2.19	0.42
2:B:509:GLU:HB2	2:B:571:PHE:CZ	2.54	0.42
1:A:313:PHE:CD1	1:A:313:PHE:C	2.98	0.42
2:B:516:MET:HE1	2:B:546:THR:OG1	2.19	0.42
1:A:143:HIS:ND1	1:A:144:PRO:HD2	2.34	0.42
1:A:221:GLY:HA3	1:A:315:PHE:CZ	2.54	0.42
2:B:119:SER:OG	2:B:122:GLU:HG3	2.20	0.42
2:B:277:ALA:HB2	2:B:299:VAL:HG21	2.02	0.42
2:B:184:LEU:HD11	2:B:186:GLU:HG3	2.02	0.42
1:A:258:PHE:CZ	4:A:999:200:HD2	2.55	0.42
1:A:321:ARG:HD3	6:A:1021:HOH:O	2.18	0.42
1:A:329:ILE:CD1	1:A:346:PHE:HZ	2.29	0.42
2:B:206:ASP:CG	2:B:276:ARG:HH11	2.28	0.42
2:B:192:LYS:H	2:B:381:GLN:NE2	2.03	0.41
2:B:434:ARG:HB3	2:B:445:THR:HG23	2.01	0.41
2:B:552:LEU:HA	2:B:555:VAL:HG22	2.02	0.41
2:B:560:LEU:HD21	2:B:590:PHE:CZ	2.55	0.41
2:B:665:LEU:HA	2:B:666:PRO:HD3	1.91	0.41
2:B:712:ALA:O	2:B:716:GLU:HB2	2.21	0.41
2:B:732:GLN:HB3	2:B:741:LYS:CB	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:ALA:HB2	2:B:118:LEU:HD11	2.03	0.41
2:B:728:PHE:CZ	2:B:744:ALA:HB1	2.55	0.41
2:B:99:LEU:HG	2:B:101:GLN:HG2	2.01	0.41
2:B:311:LEU:HD23	2:B:311:LEU:HA	1.90	0.41
2:B:652:LEU:HD13	2:B:671:PHE:HB3	2.02	0.41
2:B:690:HIS:ND1	2:B:690:HIS:N	2.68	0.41
2:B:1:MET:HE1	2:B:168:LEU:C	2.45	0.41
2:B:119:SER:C	2:B:133:LEU:HD22	2.46	0.41
2:B:551:GLY:O	2:B:555:VAL:HG13	2.21	0.41
1:A:195:ARG:HG2	1:A:223:VAL:HG13	2.03	0.41
2:B:255:GLU:OE1	2:B:375:ARG:NH1	2.54	0.41
1:A:165:LEU:HD12	1:A:301:LEU:CD2	2.35	0.41
1:A:285:MET:O	1:A:286:VAL:C	2.64	0.41
2:B:214:THR:HA	2:B:393:LEU:O	2.21	0.41
2:B:224:ALA:HB1	2:B:225:PRO:HD2	2.03	0.41
2:B:524:PHE:O	2:B:633:PHE:HB3	2.20	0.41
1:A:92:GLY:O	1:A:93:ALA:C	2.63	0.40
1:A:95:LEU:HD22	1:A:95:LEU:H	1.86	0.40
2:B:531:LEU:O	2:B:532:LEU:HD23	2.21	0.40
2:B:600:LYS:HD3	2:B:600:LYS:H	1.80	0.40
1:A:128:GLU:CD	1:A:185:ARG:HH11	2.29	0.40
2:B:699:VAL:HG12	2:B:701:VAL:HG23	2.03	0.40
1:A:260:PHE:C	1:A:287:HIS:HB2	2.46	0.40
2:B:179:ALA:HA	2:B:430:ARG:HB3	2.03	0.40
2:B:468:GLY:HA3	2:B:470:GLU:OE2	2.21	0.40
2:B:533:LEU:N	2:B:533:LEU:HD12	2.36	0.40
2:B:590:PHE:CD1	2:B:591:GLY:N	2.89	0.40
2:B:717:ALA:C	2:B:768:VAL:HG22	2.46	0.40
2:B:751:HIS:HB2	2:B:756:LEU:CD2	2.51	0.40
1:A:308:ARG:HE	1:A:308:ARG:CA	2.33	0.40
2:B:101:GLN:N	2:B:101:GLN:HE21	2.18	0.40
2:B:252:VAL:HG11	2:B:260:MET:HE1	2.03	0.40
2:B:313:LEU:HD22	2:B:346:THR:HG21	2.03	0.40
2:B:557:LYS:HG2	2:B:665:LEU:CD2	2.39	0.40
2:B:575:ARG:HD2	2:B:583:THR:OG1	2.21	0.40
2:B:682:LEU:HD12	2:B:683:ALA:H	1.87	0.40
2:B:121:ARG:HG3	2:B:121:ARG:NH1	2.37	0.40
2:B:180:LEU:HD12	2:B:180:LEU:HA	1.95	0.40
2:B:559:ASN:O	2:B:563:ASP:O	2.39	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	264/266 (99%)	249 (94%)	14 (5%)	1 (0%)	30	60
2	B	783/785 (100%)	725 (93%)	53 (7%)	5 (1%)	21	51
All	All	1047/1051 (100%)	974 (93%)	67 (6%)	6 (1%)	21	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	VAL
2	B	244	ASN
2	B	578	ARG
2	B	738	GLU
2	B	725	LEU
2	B	568	ALA

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	214/214 (100%)	204 (95%)	10 (5%)	23	57
2	B	630/630 (100%)	581 (92%)	49 (8%)	11	35
All	All	844/844 (100%)	785 (93%)	59 (7%)	14	40

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

Mol	Chain	Res	Type
1	A	85	ARG
1	A	105	LEU
1	A	157	GLU
1	A	178	HIS
1	A	197	VAL
1	A	198	VAL
1	A	260	PHE
1	A	301	LEU
1	A	308	ARG
1	A	326	ARG
2	B	32	THR
2	B	34	ARG
2	B	37	ARG
2	B	62	LYS
2	B	74	VAL
2	B	80	ASN
2	B	89	LEU
2	B	101	GLN
2	B	111	VAL
2	B	127	GLU
2	B	147	SER
2	B	153	GLU
2	B	158	LEU
2	B	170	LEU
2	B	171	LEU
2	B	173	LEU
2	B	180	LEU
2	B	184	LEU
2	B	191	LEU
2	B	276	ARG
2	B	282	ARG
2	B	283	LEU
2	B	286	LEU
2	B	298	LEU
2	B	322	SER
2	B	323	GLU
2	B	325	ARG
2	B	333	LEU
2	B	375	ARG
2	B	393	LEU
2	B	438	GLU
2	B	441	THR
2	B	443	ARG

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Mol	Chain	Res	Type
2	B	445	THR
2	B	459	LEU
2	B	460	VAL
2	B	467	GLN
2	B	470	GLU
2	B	505	LEU
2	B	548	LEU
2	B	557	LYS
2	B	576	VAL
2	B	578	ARG
2	B	600	LYS
2	B	609	LEU
2	B	713	LEU
2	B	738	GLU
2	B	754	ARG
2	B	757	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	A	207	GLN
1	A	218	GLN
2	B	54	HIS
2	B	80	ASN
2	B	101	GLN
2	B	178	HIS
2	B	212	HIS
2	B	231	GLN
2	B	244	ASN
2	B	258	GLN
2	B	261	HIS
2	B	350	HIS
2	B	381	GLN
2	B	467	GLN
2	B	584	HIS
2	B	669	HIS
2	B	746	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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$
4	200	A	999	-	12,13,13	2.15	6 (50%)	13,17,17	0.62	0
5	SO4	B	786	-	4,4,4	2.15	2 (50%)	6,6,6	2.01	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	200	A	999	-	-	2/8/8/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	200	CD1-CG	3.80	1.46	1.38
4	A	999	200	CE2-CZ	2.99	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	200	CE2-CD2	2.74	1.43	1.38
4	A	999	200	CD2-CG	2.71	1.44	1.38
5	B	786	SO4	O1-S	2.62	1.60	1.44
4	A	999	200	CE1-CD1	2.53	1.42	1.38
4	A	999	200	CE1-CZ	2.43	1.42	1.38
5	B	786	SO4	O3-S	-2.28	1.29	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	786	SO4	O3-S-O2	3.90	129.97	109.56
5	B	786	SO4	O2-S-O1	-2.29	92.94	109.06

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	200	O-C-CA-CB
4	A	999	200	OXT-C-CA-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	200	2	0
5	B	786	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	266/266 (100%)	-0.35	8 (3%) 52 42	25, 41, 73, 86	0
2	B	785/785 (100%)	-0.18	29 (3%) 45 36	22, 46, 87, 87	0
All	All	1051/1051 (100%)	-0.22	37 (3%) 47 38	22, 44, 86, 87	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	98	GLY	7.6
1	A	167	GLU	6.1
2	B	783	ASP	5.7
2	B	785	PRO	5.7
2	B	781	GLY	5.6
2	B	784	THR	5.5
1	A	299	GLU	5.0
2	B	101	GLN	5.0
2	B	759	GLU	4.7
2	B	739	GLY	4.7
2	B	661	GLN	4.4
2	B	782	LEU	4.2
1	A	350	LEU	3.9
2	B	736	LEU	3.9
2	B	731	TYR	3.4
1	A	348	GLY	3.4
2	B	733	GLY	3.4
2	B	100	GLY	3.3
2	B	738	GLU	3.2
2	B	762	GLU	3.2
2	B	689	ARG	3.0
2	B	732	GLN	2.9
2	B	734	PRO	2.8
2	B	778	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	775	ARG	2.7
2	B	742	SER	2.6
2	B	99	LEU	2.6
2	B	773	ARG	2.5
2	B	564	ARG	2.4
2	B	767	ARG	2.2
1	A	87	ASP	2.2
2	B	724	SER	2.2
1	A	300	ARG	2.1
2	B	766	SER	2.1
1	A	143	HIS	2.1
2	B	754	ARG	2.0
1	A	349	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	200	A	999	13/13	0.80	0.17	8,12,18,54	0
3	MN	A	901	1/1	0.81	0.12	42,42,42,42	0
5	SO4	B	786	5/5	0.95	0.34	7,7,7,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.