



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:12 AM UTC

PDB ID : 2AMC / pdb_00002amc
Title : Crystal structure of Phenylalanyl-tRNA synthetase complexed with L-tyrosine
Authors : Kotik-Kogan, O.; Moor, N.; Tworowski, D.; Safro, M.
Deposited on : 2005-08-09
Resolution : 2.70 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

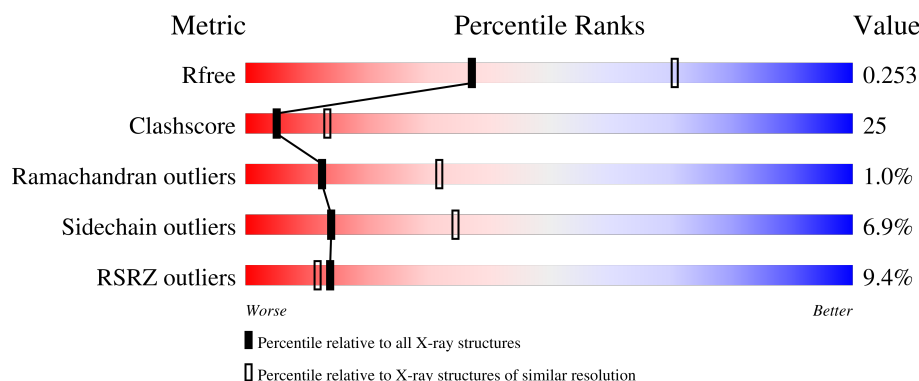
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	4% 64% 31% 5%
2	B	785	11% 55% 40% 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	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8514 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			

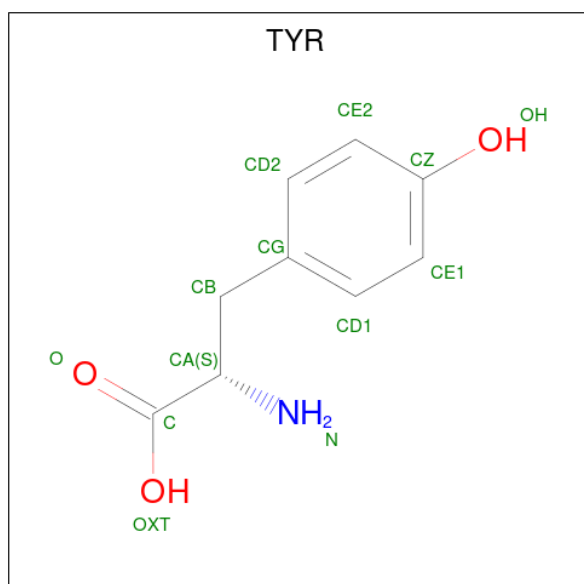
- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

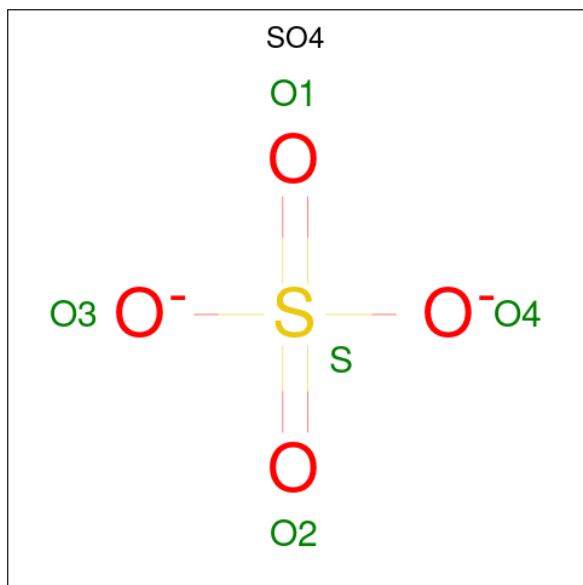
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is TYROSINE (CCD ID: TYR) (formula: C₉H₁₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	9	1	3		
4	B	1	Total	C	N	O	0	0
			13	9	1	3		

- 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		

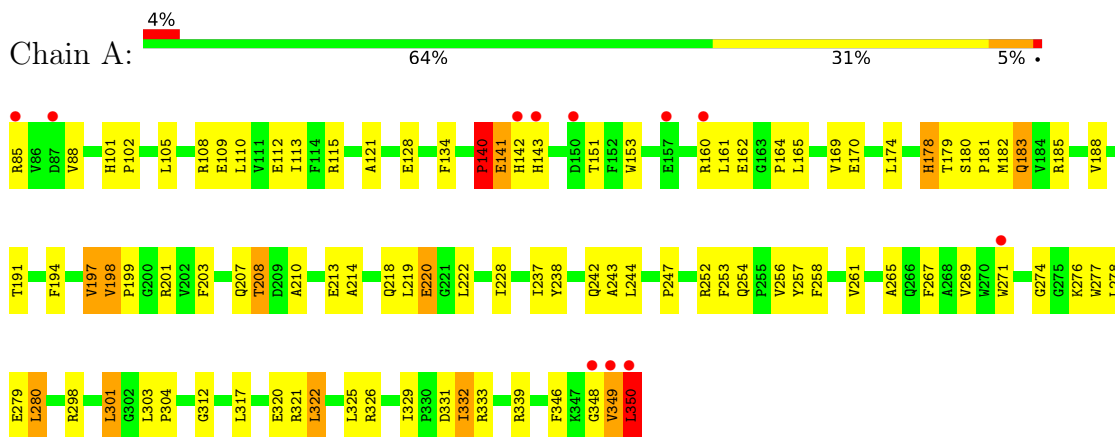
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total	O	0	0
			46	46		
6	B	186	Total	O	0	0
			186	186		

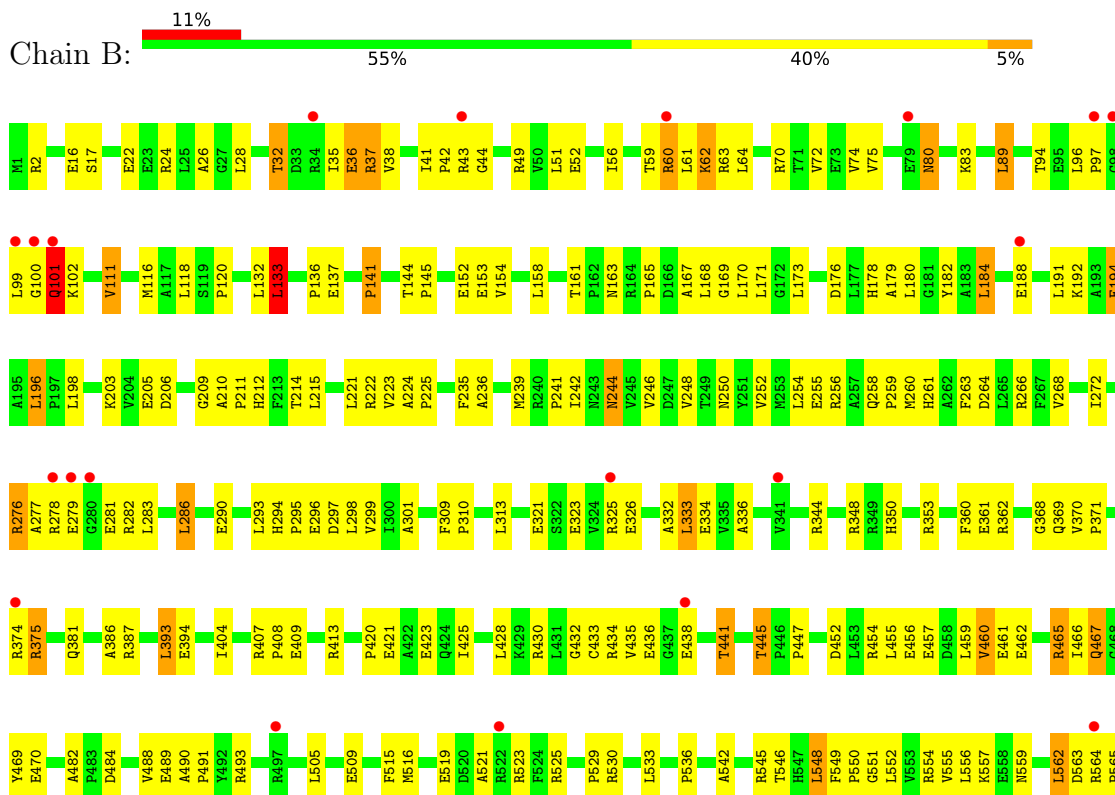
3 Residue-property plots

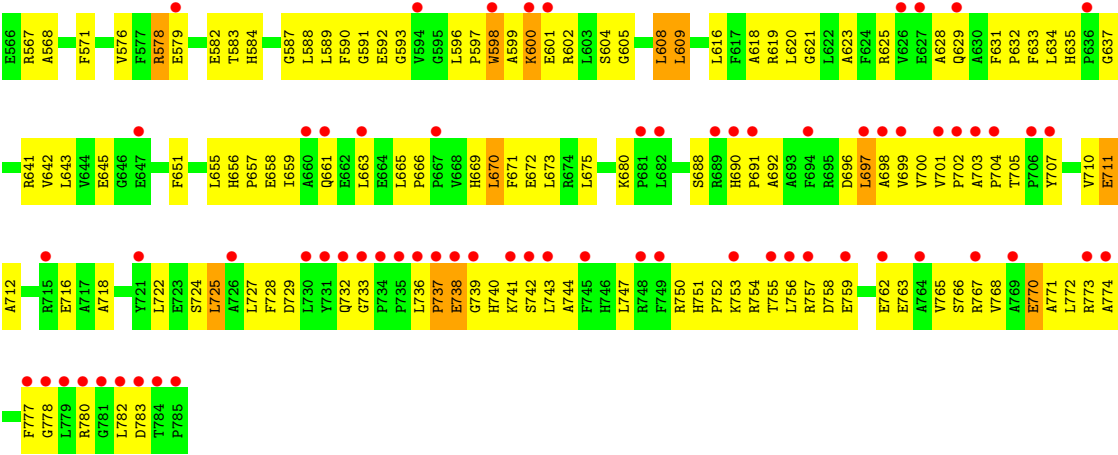
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phenylalanyl-tRNA synthetase alpha chain



- Molecule 2: Phenylalanyl-tRNA synthetase beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.20Å 173.20Å 138.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.41 – 2.70 25.41 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (25.41-2.70) 98.3 (25.41-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.72Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.255 0.228 , 0.253	Depositor DCC
R_{free} test set	3215 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8514	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: SO4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.50	1/2191 (0.0%)	0.99	12/2971 (0.4%)
2	B	0.45	0/6280	1.02	31/8536 (0.4%)
All	All	0.47	1/8471 (0.0%)	1.01	43/11507 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	LEU	N-CA	6.06	1.57	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	VAL	N-CA-C	14.11	127.36	113.53
2	B	101	GLN	OE1-CD-NE2	-10.50	112.10	122.60
1	A	350	LEU	N-CA-CB	-10.49	92.66	110.50
2	B	38	VAL	CA-C-N	-7.60	114.17	123.21
2	B	38	VAL	C-N-CA	-7.60	114.17	123.21
1	A	280	LEU	N-CA-C	7.48	120.90	111.69
2	B	618	ALA	N-CA-C	-7.23	103.48	111.36
1	A	151	THR	N-CA-C	7.09	121.87	109.96
2	B	101	GLN	CG-CD-NE2	6.91	126.76	116.40
1	A	214	ALA	N-CA-C	-6.79	105.16	113.50
2	B	739	GLY	N-CA-C	-6.78	105.87	115.30
2	B	133	LEU	N-CA-C	-6.73	100.31	110.28
1	A	257	TYR	N-CA-C	6.66	120.68	109.76
2	B	332	ALA	N-CA-C	-6.59	97.78	108.52
2	B	521	ALA	N-CA-C	-6.55	104.17	111.71
2	B	60	ARG	N-CA-C	-6.33	104.87	112.59
2	B	608	LEU	N-CA-C	-6.31	103.93	111.69
2	B	482	ALA	CA-C-N	6.27	125.76	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	482	ALA	C-N-CA	6.27	125.76	119.24
1	A	140	PRO	CA-N-CD	-6.21	103.30	112.00
2	B	38	VAL	CB-CA-C	-5.92	104.84	110.65
2	B	141	PRO	N-CA-C	-5.88	103.53	110.70
2	B	118	LEU	N-CA-C	5.87	119.23	110.14
2	B	670	LEU	N-CA-C	5.79	116.95	108.14
2	B	168	LEU	N-CA-C	-5.58	106.68	112.93
1	A	329	ILE	CA-C-N	5.51	125.03	119.19
1	A	329	ILE	C-N-CA	5.51	125.03	119.19
1	A	134	PHE	N-CA-C	5.50	119.49	112.12
2	B	210	ALA	CA-C-N	5.47	125.30	119.28
2	B	210	ALA	C-N-CA	5.47	125.30	119.28
2	B	387	ARG	N-CA-C	-5.46	100.33	109.24
2	B	321	GLU	N-CA-C	5.41	116.86	111.07
2	B	336	ALA	N-CA-C	5.37	116.43	108.86
1	A	350	LEU	N-CA-C	5.34	125.95	111.00
2	B	136	PRO	N-CA-C	-5.30	102.86	111.19
2	B	393	LEU	N-CA-C	-5.25	99.96	108.52
2	B	161	THR	CA-C-N	5.17	126.30	119.84
2	B	161	THR	C-N-CA	5.17	126.30	119.84
2	B	37	ARG	N-CA-C	-5.10	100.99	109.46
2	B	70	ARG	N-CA-C	-5.07	101.60	109.72
2	B	293	LEU	N-CA-C	5.07	117.40	110.55
1	A	238	TYR	N-CA-C	-5.07	105.76	111.28
1	A	208	THR	N-CA-C	5.02	116.37	109.15

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	92	0
2	B	6127	0	6180	324	0
3	A	1	0	0	0	0
4	A	13	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	13	0	8	4	0
5	B	5	0	0	3	0
6	A	46	0	0	3	0
6	B	186	0	0	6	0
All	All	8514	0	8271	409	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 25.

All (409) 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:HD12	2:B:100:GLY:N	1.50	1.27
2:B:467:GLN:HE21	2:B:467:GLN:HA	1.17	1.07
2:B:141:PRO:O	2:B:144:THR:HG23	1.61	0.99
1:A:88:VAL:CG1	6:A:902:HOH:O	2.09	0.99
2:B:99:LEU:HD13	2:B:101:GLN:H	1.27	0.99
1:A:85:ARG:NH1	1:A:85:ARG:HB2	1.81	0.95
2:B:99:LEU:CD1	2:B:101:GLN:H	1.80	0.95
1:A:165:LEU:HD12	1:A:301:LEU:HD23	1.50	0.94
1:A:88:VAL:HG12	6:A:902:HOH:O	1.65	0.94
2:B:602:ARG:HG3	2:B:602:ARG:HH11	1.33	0.93
1:A:183:GLN:HB2	1:A:222:LEU:HD22	1.50	0.93
2:B:99:LEU:HD13	2:B:101:GLN:N	1.82	0.92
2:B:413:ARG:NH2	5:B:786:SO4:O4	2.02	0.92
1:A:350:LEU:HD22	1:A:350:LEU:N	1.85	0.90
1:A:85:ARG:HB2	1:A:85:ARG:HH11	1.35	0.89
2:B:519:GLU:HB3	2:B:523:ARG:HH12	1.37	0.89
2:B:99:LEU:HD12	2:B:100:GLY:H	1.36	0.87
2:B:214:THR:HG22	2:B:394:GLU:HG3	1.56	0.87
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.57	0.87
2:B:286:LEU:HD21	2:B:323:GLU:CG	2.05	0.86
2:B:192:LYS:H	2:B:381:GLN:HE22	1.25	0.82
2:B:628:ALA:HB2	6:B:1180:HOH:O	1.79	0.81
2:B:99:LEU:CD1	2:B:101:GLN:N	2.40	0.81
2:B:282:ARG:HH12	2:B:290:GLU:HG3	1.43	0.81
1:A:350:LEU:HD22	1:A:350:LEU:H	1.43	0.81
2:B:74:VAL:HG21	2:B:116:MET:HA	1.64	0.79
2:B:255:GLU:OE2	2:B:375:ARG:HD2	1.83	0.79
2:B:325:ARG:NH1	2:B:325:ARG:HB2	1.97	0.79
2:B:37:ARG:HH11	2:B:37:ARG:HB3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:ARG:NH2	5:B:786:SO4:O1	2.13	0.78
2:B:467:GLN:HA	2:B:467:GLN:NE2	1.99	0.78
2:B:152:GLU:HG3	6:B:1082:HOH:O	1.83	0.77
2:B:590:PHE:HA	6:B:1178:HOH:O	1.85	0.77
2:B:404:ILE:HD12	2:B:454:ARG:O	1.84	0.76
2:B:600:LYS:HD3	2:B:600:LYS:N	2.00	0.76
2:B:37:ARG:HB3	2:B:37:ARG:NH1	2.02	0.75
2:B:413:ARG:NH2	5:B:786:SO4:S	2.61	0.73
1:A:160:ARG:NH1	2:B:579:GLU:HB3	2.04	0.73
2:B:596:LEU:HB2	2:B:599:ALA:HB3	1.71	0.73
1:A:280:LEU:HD21	1:A:322:LEU:HD23	1.70	0.72
1:A:108:ARG:O	1:A:112:GLU:HG2	1.88	0.72
2:B:282:ARG:HH11	2:B:282:ARG:HB3	1.53	0.72
2:B:266:ARG:NH1	2:B:325:ARG:HH22	1.87	0.72
2:B:80:ASN:H	2:B:80:ASN:HD22	1.38	0.71
2:B:99:LEU:CD1	2:B:100:GLY:N	2.44	0.71
2:B:80:ASN:HD21	2:B:132:LEU:H	1.35	0.70
2:B:261:HIS:HD2	2:B:263:PHE:CZ	2.10	0.70
1:A:115:ARG:CZ	2:B:493:ARG:HH21	2.05	0.69
2:B:224:ALA:H	2:B:244:ASN:ND2	1.91	0.69
1:A:350:LEU:N	1:A:350:LEU:CD2	2.52	0.69
2:B:762:GLU:O	2:B:765:VAL:HG22	1.93	0.67
2:B:239:MET:HE2	2:B:254:LEU:HD11	1.77	0.67
2:B:268:VAL:HG13	2:B:272:ILE:HD12	1.76	0.67
2:B:701:VAL:HG22	2:B:777:PHE:CD1	2.29	0.67
2:B:757:ARG:HD2	2:B:759:GLU:OE1	1.94	0.67
2:B:516:MET:HE3	2:B:545:ARG:HA	1.75	0.67
2:B:712:ALA:O	2:B:716:GLU:HB2	1.95	0.66
2:B:99:LEU:HD12	2:B:99:LEU:C	2.19	0.66
2:B:767:ARG:HE	2:B:767:ARG:N	1.93	0.66
2:B:279:GLU:HG2	2:B:295:PRO:HD3	1.76	0.65
2:B:282:ARG:HB3	2:B:282:ARG:NH1	2.10	0.65
1:A:191:THR:HG23	2:B:484:ASP:OD2	1.97	0.65
2:B:223:VAL:HA	2:B:244:ASN:HD22	1.61	0.65
2:B:432:GLY:O	2:B:447:PRO:HG3	1.97	0.65
1:A:320:GLU:HG2	1:A:332:ILE:HD11	1.79	0.65
2:B:286:LEU:HD21	2:B:323:GLU:HG3	1.77	0.64
1:A:109:GLU:O	1:A:113:ILE:HG12	1.97	0.64
2:B:702:PRO:C	2:B:704:PRO:HD2	2.22	0.64
2:B:710:VAL:HG11	2:B:743:LEU:HD12	1.78	0.64
2:B:192:LYS:N	2:B:381:GLN:HE22	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ARG:NH2	2:B:375:ARG:HG3	2.13	0.64
2:B:766:SER:HB3	2:B:767:ARG:HH21	1.63	0.64
2:B:457:GLU:HA	2:B:460:VAL:HG13	1.79	0.64
2:B:587:GLY:HA3	2:B:671:PHE:CE1	2.32	0.64
2:B:409:GLU:OE2	2:B:413:ARG:HD3	1.98	0.63
2:B:409:GLU:OE1	2:B:413:ARG:NH1	2.31	0.63
2:B:178:HIS:O	2:B:430:ARG:NH1	2.31	0.63
2:B:286:LEU:HD21	2:B:323:GLU:HG2	1.81	0.63
2:B:326:GLU:CD	2:B:326:GLU:H	2.07	0.63
1:A:242:GLN:OE1	1:A:247:PRO:HA	1.98	0.63
2:B:28:LEU:HD13	2:B:176:ASP:HB3	1.81	0.62
2:B:224:ALA:N	2:B:244:ASN:ND2	2.46	0.62
1:A:213:GLU:HG3	1:A:332:ILE:HD12	1.81	0.62
2:B:203:LYS:HE3	2:B:205:GLU:OE2	1.99	0.62
1:A:258:PHE:HB2	1:A:261:VAL:HG22	1.80	0.62
2:B:408:PRO:HG2	2:B:421:GLU:HG3	1.81	0.62
2:B:697:LEU:O	2:B:697:LEU:HD12	2.00	0.61
2:B:602:ARG:HG3	2:B:602:ARG:NH1	2.07	0.61
2:B:763:GLU:O	2:B:767:ARG:HG2	2.01	0.61
2:B:74:VAL:CG2	2:B:116:MET:HA	2.29	0.61
1:A:141:GLU:O	1:A:142:HIS:C	2.44	0.60
1:A:179:THR:OG1	1:A:220:GLU:HG3	2.00	0.60
2:B:530:ARG:HH11	2:B:530:ARG:HB2	1.66	0.60
2:B:732:GLN:HB3	2:B:741:LYS:HB3	1.83	0.60
2:B:407:ARG:HD3	2:B:456:GLU:OE2	2.01	0.60
2:B:578:ARG:O	2:B:579:GLU:HB2	2.02	0.60
2:B:782:LEU:HD12	2:B:783:ASP:H	1.66	0.60
1:A:182:MET:HE3	1:A:182:MET:O	2.01	0.60
1:A:271:TRP:CZ3	1:A:274:GLY:HA3	2.36	0.60
2:B:489:GLU:HG3	2:B:493:ARG:HD2	1.84	0.60
2:B:519:GLU:CB	2:B:523:ARG:HH12	2.13	0.60
2:B:703:ALA:N	2:B:704:PRO:HD2	2.16	0.60
2:B:707:TYR:OH	2:B:711:GLU:HG3	2.02	0.59
2:B:60:ARG:NE	2:B:60:ARG:O	2.35	0.59
2:B:751:HIS:HB3	2:B:754:ARG:O	2.01	0.59
2:B:99:LEU:HD13	2:B:101:GLN:C	2.28	0.59
2:B:530:ARG:HB2	2:B:530:ARG:NH1	2.18	0.59
1:A:162:GLU:O	1:A:185:ARG:NH2	2.36	0.58
2:B:49:ARG:HG3	2:B:137:GLU:HG3	1.84	0.58
2:B:699:VAL:CG1	2:B:772:LEU:HD11	2.33	0.58
2:B:266:ARG:HH11	2:B:325:ARG:HH22	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:ARG:HG2	2:B:278:ARG:HH11	1.69	0.58
1:A:164:PRO:HG2	1:A:188:VAL:HG21	1.86	0.58
1:A:256:VAL:HG12	1:A:265:ALA:C	2.30	0.57
1:A:298:ARG:NH1	1:A:304:PRO:O	2.36	0.57
2:B:353:ARG:C	2:B:353:ARG:HD3	2.30	0.57
2:B:325:ARG:HB2	2:B:325:ARG:CZ	2.32	0.57
2:B:773:ARG:NH1	2:B:778:GLY:HA2	2.19	0.57
1:A:88:VAL:HG13	6:A:902:HOH:O	1.87	0.57
2:B:773:ARG:HH12	2:B:778:GLY:HA2	1.70	0.56
2:B:546:THR:HG21	6:B:1183:HOH:O	2.05	0.56
2:B:563:ASP:C	2:B:564:ARG:HD2	2.29	0.56
2:B:516:MET:HE3	2:B:546:THR:H	1.71	0.56
1:A:178:HIS:HB2	1:A:218:GLN:HE22	1.71	0.55
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.87	0.55
1:A:185:ARG:O	1:A:188:VAL:HG22	2.06	0.55
2:B:782:LEU:HD12	2:B:783:ASP:N	2.20	0.55
2:B:51:LEU:O	2:B:83:LYS:HD2	2.06	0.55
2:B:222:ARG:O	2:B:222:ARG:HG3	2.05	0.55
2:B:282:ARG:HH12	2:B:290:GLU:CG	2.18	0.55
2:B:462:GLU:OE1	2:B:465:ARG:NH1	2.38	0.55
2:B:348:ARG:HH12	2:B:361:GLU:CD	2.13	0.55
2:B:699:VAL:HG11	2:B:772:LEU:HD11	1.89	0.55
2:B:564:ARG:HD2	2:B:564:ARG:N	2.21	0.55
1:A:332:ILE:HD13	1:A:332:ILE:O	2.07	0.54
2:B:515:PHE:CE1	2:B:533:LEU:HD21	2.43	0.54
2:B:44:GLY:HA3	2:B:94:THR:OG1	2.07	0.54
2:B:551:GLY:O	2:B:555:VAL:HG13	2.07	0.54
2:B:178:HIS:CD2	2:B:430:ARG:HH12	2.24	0.54
2:B:605:GLY:HA2	2:B:669:HIS:CD2	2.42	0.54
2:B:32:THR:HG23	6:B:1004:HOH:O	2.08	0.54
2:B:462:GLU:CD	2:B:465:ARG:NH1	2.66	0.54
2:B:583:THR:HG22	2:B:675:LEU:HD12	1.90	0.54
2:B:699:VAL:HG12	2:B:701:VAL:HG23	1.88	0.54
2:B:625:ARG:HA	6:B:1177:HOH:O	2.06	0.54
2:B:699:VAL:O	2:B:742:SER:HA	2.08	0.54
2:B:188:GLU:HG3	2:B:188:GLU:O	2.08	0.53
2:B:221:LEU:HD23	2:B:386:ALA:HB2	1.89	0.53
2:B:642:VAL:C	2:B:643:LEU:HD22	2.33	0.53
2:B:62:LYS:HB2	2:B:62:LYS:NZ	2.24	0.53
2:B:212:HIS:HE1	2:B:394:GLU:OE2	1.91	0.53
2:B:701:VAL:HG13	2:B:702:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:688:SER:HB2	2:B:752:PRO:HA	1.90	0.53
2:B:732:GLN:O	2:B:732:GLN:HG3	2.08	0.53
1:A:271:TRP:CE3	1:A:274:GLY:HA3	2.44	0.53
1:A:271:TRP:CE3	1:A:325:LEU:HD11	2.44	0.53
2:B:239:MET:CE	2:B:250:ASN:HB3	2.39	0.53
2:B:120:PRO:HG3	2:B:133:LEU:HD13	1.89	0.53
1:A:252:ARG:HB2	1:A:277:TRP:CZ3	2.44	0.52
2:B:690:HIS:CE1	2:B:753:LYS:O	2.62	0.52
2:B:771:ALA:HA	2:B:774:ALA:HB3	1.91	0.52
2:B:96:LEU:HB2	2:B:99:LEU:HG	1.91	0.52
2:B:655:LEU:HD11	2:B:659:ILE:HG21	1.91	0.52
1:A:228:ILE:HG21	1:A:312:GLY:HA2	1.92	0.52
2:B:99:LEU:HD12	2:B:100:GLY:CA	2.35	0.52
2:B:260:MET:O	4:B:999:TYR:HD2	1.92	0.52
2:B:702:PRO:HB2	2:B:704:PRO:HD2	1.92	0.52
2:B:736:LEU:HD11	2:B:742:SER:HB3	1.92	0.52
2:B:56:ILE:HD11	2:B:63:ARG:HB2	1.91	0.52
2:B:516:MET:SD	2:B:529:PRO:HG3	2.50	0.52
2:B:718:ALA:HB3	2:B:722:LEU:HD22	1.91	0.51
1:A:182:MET:HG2	1:A:198:VAL:HG21	1.92	0.51
2:B:80:ASN:HD22	2:B:80:ASN:N	2.00	0.51
2:B:141:PRO:HD2	2:B:144:THR:HG21	1.91	0.51
2:B:369:GLN:CD	2:B:369:GLN:H	2.19	0.51
1:A:128:GLU:OE2	1:A:185:ARG:HD2	2.10	0.51
2:B:701:VAL:HG13	2:B:777:PHE:CE1	2.45	0.51
2:B:697:LEU:HD12	2:B:697:LEU:C	2.35	0.51
2:B:178:HIS:CD2	2:B:184:LEU:HB2	2.46	0.51
2:B:16:GLU:O	2:B:17:SER:HB3	2.11	0.51
2:B:428:LEU:O	2:B:433:CYS:HB2	2.11	0.51
2:B:56:ILE:HB	2:B:59:THR:OG1	2.10	0.51
2:B:523:ARG:HG3	2:B:523:ARG:HH11	1.76	0.51
2:B:462:GLU:OE2	2:B:465:ARG:NH1	2.44	0.50
2:B:692:ALA:HB2	2:B:750:ARG:HD2	1.93	0.50
2:B:263:PHE:HE2	2:B:334:GLU:OE2	1.94	0.50
1:A:161:LEU:O	1:A:169:VAL:HG12	2.11	0.50
2:B:60:ARG:HD3	2:B:61:LEU:HD23	1.93	0.50
2:B:277:ALA:O	2:B:295:PRO:HA	2.11	0.50
2:B:656:HIS:HB3	2:B:659:ILE:HG12	1.94	0.50
2:B:24:ARG:NE	2:B:182:TYR:OH	2.41	0.50
2:B:22:GLU:OE1	2:B:35:ILE:HD11	2.12	0.50
2:B:209:GLY:C	2:B:211:PRO:HD3	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:GLY:O	2:B:736:LEU:HB2	2.11	0.50
2:B:582:GLU:OE2	2:B:584:HIS:HE1	1.95	0.50
2:B:101:GLN:O	2:B:102:LYS:C	2.56	0.49
2:B:456:GLU:HA	2:B:459:LEU:HD23	1.93	0.49
2:B:707:TYR:CE1	2:B:727:LEU:HD22	2.46	0.49
1:A:160:ARG:HH12	2:B:579:GLU:HB3	1.77	0.49
2:B:99:LEU:HD12	2:B:101:GLN:N	2.22	0.49
2:B:604:SER:HA	2:B:608:LEU:HD22	1.95	0.49
2:B:286:LEU:CD1	4:B:999:TYR:O	2.60	0.49
2:B:516:MET:CE	2:B:546:THR:H	2.24	0.49
2:B:616:LEU:O	2:B:620:LEU:HG	2.12	0.49
1:A:278:LEU:CD1	1:A:325:LEU:HD13	2.43	0.49
2:B:772:LEU:O	2:B:777:PHE:HB2	2.13	0.49
2:B:99:LEU:CD1	2:B:99:LEU:C	2.85	0.49
2:B:294:HIS:CE1	2:B:296:GLU:HB2	2.47	0.49
1:A:208:THR:HG22	1:A:333:ARG:HD3	1.94	0.49
1:A:317:LEU:O	1:A:317:LEU:HD12	2.12	0.49
2:B:99:LEU:HD13	2:B:101:GLN:CA	2.41	0.49
2:B:600:LYS:HD3	2:B:600:LYS:H	1.74	0.49
2:B:515:PHE:HE1	2:B:533:LEU:HD21	1.78	0.48
2:B:242:ILE:HD12	2:B:246:VAL:HG11	1.95	0.48
2:B:589:LEU:HD21	2:B:608:LEU:HB3	1.95	0.48
1:A:85:ARG:HH11	1:A:85:ARG:CB	2.17	0.48
1:A:203:PHE:CD1	1:A:203:PHE:N	2.80	0.48
1:A:178:HIS:CB	1:A:218:GLN:HE22	2.26	0.48
2:B:657:PRO:O	2:B:661:GLN:OE1	2.32	0.48
2:B:728:PHE:CZ	2:B:744:ALA:HB1	2.49	0.48
2:B:420:PRO:HG2	2:B:423:GLU:HG3	1.95	0.48
2:B:700:VAL:HB	2:B:778:GLY:HA3	1.96	0.48
1:A:174:LEU:C	1:A:174:LEU:HD12	2.39	0.48
1:A:271:TRP:HZ3	1:A:276:LYS:HE2	1.79	0.48
2:B:552:LEU:O	2:B:555:VAL:HG22	2.13	0.48
1:A:180:SER:HA	1:A:220:GLU:OE2	2.14	0.47
2:B:600:LYS:N	2:B:600:LYS:CD	2.75	0.47
2:B:509:GLU:HB2	2:B:571:PHE:CE1	2.49	0.47
1:A:237:ILE:HD12	1:A:253:PHE:CZ	2.49	0.47
1:A:237:ILE:HD13	1:A:267:PHE:CG	2.50	0.47
1:A:258:PHE:CZ	4:A:888:TYR:HD2	2.32	0.47
2:B:629:GLN:OE1	2:B:641:ARG:HD3	2.14	0.47
2:B:563:ASP:C	2:B:565:PRO:HD3	2.39	0.47
1:A:278:LEU:HD11	1:A:325:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:VAL:CG1	2:B:705:THR:HB	2.45	0.47
1:A:213:GLU:CG	1:A:332:ILE:HD12	2.44	0.47
2:B:344:ARG:O	2:B:348:ARG:HD3	2.15	0.47
2:B:755:THR:HG22	2:B:756:LEU:N	2.29	0.47
1:A:210:ALA:HA	1:A:331:ASP:OD1	2.14	0.47
1:A:280:LEU:HD21	1:A:322:LEU:CD2	2.44	0.47
2:B:264:ASP:OD2	2:B:266:ARG:HD3	2.14	0.47
2:B:699:VAL:HG22	2:B:772:LEU:HD21	1.97	0.47
2:B:432:GLY:C	2:B:447:PRO:HG3	2.39	0.47
1:A:180:SER:N	1:A:181:PRO:HD2	2.30	0.46
2:B:165:PRO:HB3	2:B:362:ARG:HB3	1.96	0.46
2:B:214:THR:HA	2:B:393:LEU:O	2.15	0.46
2:B:651:PHE:C	2:B:651:PHE:CD1	2.93	0.46
1:A:254:GLN:NE2	2:B:26:ALA:HB1	2.31	0.46
2:B:281:GLU:HG2	2:B:310:PRO:HG2	1.97	0.46
2:B:434:ARG:HB3	2:B:445:THR:HG23	1.96	0.46
2:B:261:HIS:HB2	4:B:999:TYR:CD2	2.50	0.46
2:B:623:ALA:HB3	2:B:645:GLU:HA	1.96	0.46
2:B:75:VAL:HG23	2:B:111:VAL:HG22	1.97	0.46
2:B:589:LEU:HB2	2:B:609:LEU:HG	1.96	0.46
2:B:656:HIS:HE1	2:B:658:GLU:HG3	1.81	0.46
1:A:326:ARG:NH1	1:A:326:ARG:HG3	2.31	0.46
2:B:261:HIS:CD2	2:B:263:PHE:CZ	2.98	0.46
2:B:525:ARG:HG3	2:B:659:ILE:HD11	1.98	0.46
2:B:737:PRO:O	2:B:738:GLU:O	2.33	0.46
2:B:635:HIS:CE1	2:B:637:GLY:H	2.34	0.46
1:A:258:PHE:CE1	4:A:888:TYR:HD2	2.34	0.46
2:B:325:ARG:HB2	2:B:325:ARG:HH11	1.74	0.46
2:B:596:LEU:HD13	2:B:598:TRP:CH2	2.51	0.45
2:B:206:ASP:CG	2:B:276:ARG:HH11	2.24	0.45
2:B:239:MET:HE2	2:B:254:LEU:CD1	2.45	0.45
2:B:248:VAL:O	2:B:252:VAL:HG23	2.16	0.45
2:B:407:ARG:NH1	2:B:456:GLU:OE1	2.49	0.45
2:B:747:LEU:N	2:B:747:LEU:HD12	2.31	0.45
2:B:549:PHE:CG	2:B:550:PRO:HD3	2.51	0.45
2:B:602:ARG:NH1	2:B:602:ARG:CG	2.74	0.45
2:B:732:GLN:HB2	2:B:740:HIS:O	2.17	0.45
1:A:348:GLY:O	1:A:349:VAL:C	2.59	0.45
1:A:349:VAL:HG12	1:A:350:LEU:HD23	1.97	0.45
2:B:194:GLU:O	2:B:196:LEU:HD22	2.17	0.45
2:B:326:GLU:CD	2:B:326:GLU:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:GLU:O	2:B:465:ARG:HG2	2.16	0.45
2:B:631:PHE:HB2	2:B:634:LEU:HD12	1.99	0.45
2:B:75:VAL:CG2	2:B:111:VAL:HG22	2.47	0.45
1:A:165:LEU:CD1	1:A:301:LEU:HD23	2.33	0.45
1:A:339:ARG:NE	2:B:562:LEU:HD13	2.30	0.45
2:B:767:ARG:O	2:B:770:GLU:HB3	2.16	0.45
2:B:215:LEU:HA	2:B:333:LEU:O	2.17	0.45
2:B:751:HIS:HB2	2:B:756:LEU:HD21	1.99	0.45
1:A:140:PRO:HB2	1:A:143:HIS:HB2	1.99	0.45
1:A:179:THR:C	1:A:181:PRO:HD2	2.42	0.45
2:B:198:LEU:N	2:B:198:LEU:HD23	2.32	0.45
2:B:690:HIS:HB3	2:B:691:PRO:HD2	1.98	0.45
2:B:179:ALA:HA	2:B:430:ARG:HB3	1.99	0.45
2:B:266:ARG:NH1	2:B:325:ARG:NH2	2.60	0.45
2:B:434:ARG:HH12	2:B:436:GLU:CD	2.25	0.45
2:B:567:ARG:HA	2:B:591:GLY:HA3	1.99	0.44
2:B:633:PHE:CD1	2:B:634:LEU:HG	2.52	0.44
2:B:722:LEU:HD11	2:B:724:SER:O	2.17	0.44
2:B:43:ARG:HG3	2:B:43:ARG:HH11	1.82	0.44
2:B:523:ARG:HG3	2:B:523:ARG:NH1	2.31	0.44
2:B:559:ASN:O	2:B:563:ASP:O	2.35	0.44
1:A:101:HIS:ND1	1:A:102:PRO:HD2	2.32	0.44
1:A:102:PRO:HG3	1:A:346:PHE:CD1	2.53	0.44
1:A:198:VAL:O	1:A:198:VAL:HG22	2.18	0.44
2:B:264:ASP:CG	2:B:266:ARG:HD3	2.42	0.44
2:B:578:ARG:O	2:B:578:ARG:HG3	2.18	0.44
1:A:269:VAL:HG13	1:A:280:LEU:HD12	2.00	0.44
2:B:72:VAL:HG21	2:B:89:LEU:HD11	2.00	0.44
2:B:239:MET:HE1	2:B:250:ASN:HB3	2.00	0.44
2:B:737:PRO:O	2:B:738:GLU:C	2.61	0.44
2:B:163:ASN:O	2:B:452:ASP:HB3	2.18	0.44
2:B:635:HIS:ND1	2:B:637:GLY:N	2.54	0.44
2:B:24:ARG:HD2	2:B:182:TYR:HE1	1.83	0.44
2:B:259:PRO:HB2	2:B:360:PHE:CE2	2.53	0.44
2:B:536:PRO:HB3	2:B:542:ALA:HA	2.00	0.44
2:B:557:LYS:HE2	2:B:663:LEU:O	2.18	0.44
2:B:696:ASP:O	2:B:697:LEU:HB3	2.17	0.44
2:B:64:LEU:HB2	2:B:74:VAL:HG12	2.00	0.44
2:B:192:LYS:H	2:B:381:GLN:NE2	2.05	0.43
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.48	0.43
2:B:556:LEU:HD22	2:B:588:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:OG1	1:A:220:GLU:CG	2.66	0.43
1:A:252:ARG:NH2	1:A:279:GLU:OE2	2.51	0.43
1:A:110:LEU:HD13	1:A:317:LEU:HD11	2.01	0.43
2:B:763:GLU:HG2	2:B:767:ARG:HD2	1.99	0.43
1:A:178:HIS:HB3	4:A:888:TYR:OXT	2.17	0.43
2:B:212:HIS:HD2	2:B:369:GLN:OE1	2.01	0.43
2:B:601:GLU:O	2:B:602:ARG:HG3	2.18	0.43
2:B:96:LEU:HB2	2:B:99:LEU:CD2	2.49	0.43
2:B:593:GLY:HA3	2:B:604:SER:HB3	2.00	0.43
2:B:52:GLU:HA	2:B:83:LYS:HB2	2.00	0.43
2:B:455:LEU:O	2:B:459:LEU:HD22	2.19	0.43
2:B:703:ALA:N	2:B:704:PRO:CD	2.81	0.43
2:B:239:MET:HE3	2:B:250:ASN:HB3	2.00	0.43
1:A:278:LEU:HB3	1:A:321:ARG:HH12	1.84	0.43
2:B:554:ARG:HG2	2:B:554:ARG:HH11	1.84	0.43
1:A:207:GLN:OE1	1:A:207:GLN:HA	2.19	0.42
2:B:260:MET:C	4:B:999:TYR:HD2	2.27	0.42
2:B:301:ALA:HB1	2:B:309:PHE:O	2.19	0.42
2:B:235:PHE:CZ	2:B:241:PRO:HD2	2.54	0.42
2:B:665:LEU:HA	2:B:666:PRO:HD3	1.92	0.42
2:B:699:VAL:HG13	2:B:772:LEU:HD11	2.00	0.42
1:A:85:ARG:HB2	1:A:85:ARG:CZ	2.47	0.42
2:B:698:ALA:HB3	2:B:780:ARG:HB3	2.02	0.42
2:B:758:ASP:O	2:B:762:GLU:HG2	2.20	0.42
2:B:277:ALA:HB2	2:B:299:VAL:HG21	2.00	0.42
2:B:278:ARG:O	2:B:281:GLU:HB2	2.19	0.42
2:B:408:PRO:CG	2:B:421:GLU:HG3	2.48	0.42
2:B:751:HIS:HB2	2:B:756:LEU:CD2	2.50	0.42
1:A:121:ALA:HA	1:A:197:VAL:O	2.19	0.42
2:B:167:ALA:C	2:B:169:GLY:H	2.28	0.42
2:B:294:HIS:ND1	2:B:296:GLU:HB2	2.35	0.42
2:B:462:GLU:O	2:B:466:ILE:HG12	2.20	0.42
2:B:763:GLU:O	2:B:766:SER:HB2	2.19	0.42
1:A:252:ARG:O	1:A:267:PHE:HA	2.19	0.42
2:B:99:LEU:HD13	2:B:101:GLN:O	2.19	0.42
2:B:533:LEU:N	2:B:533:LEU:HD12	2.34	0.42
2:B:268:VAL:CG1	2:B:272:ILE:HD12	2.46	0.42
2:B:621:GLY:O	2:B:680:LYS:HE2	2.20	0.42
2:B:724:SER:O	2:B:725:LEU:HB2	2.19	0.42
1:A:101:HIS:CG	1:A:102:PRO:HD2	2.55	0.42
1:A:128:GLU:OE2	1:A:185:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:HA	1:A:199:PRO:HD2	1.98	0.42
2:B:36:GLU:O	2:B:154:VAL:HA	2.19	0.42
2:B:370:VAL:HB	2:B:371:PRO:HD3	2.01	0.42
2:B:409:GLU:CD	2:B:413:ARG:HH11	2.27	0.42
2:B:725:LEU:C	2:B:725:LEU:HD23	2.45	0.42
1:A:153:TRP:CZ3	1:A:174:LEU:HD23	2.54	0.42
2:B:549:PHE:HB2	2:B:670:LEU:HD22	2.02	0.42
2:B:80:ASN:H	2:B:80:ASN:ND2	2.12	0.41
2:B:224:ALA:H	2:B:244:ASN:HD22	1.64	0.41
2:B:297:ASP:OD2	2:B:350:HIS:HE1	2.04	0.41
2:B:596:LEU:HA	2:B:597:PRO:HD3	1.93	0.41
2:B:600:LYS:HG2	2:B:601:GLU:OE2	2.20	0.41
2:B:601:GLU:CD	2:B:601:GLU:H	2.27	0.41
2:B:261:HIS:HD2	2:B:263:PHE:CE2	2.36	0.41
1:A:269:VAL:CG1	1:A:280:LEU:HD12	2.51	0.41
2:B:656:HIS:HB3	2:B:659:ILE:CG1	2.50	0.41
2:B:309:PHE:HA	2:B:310:PRO:HD3	1.87	0.41
2:B:369:GLN:CD	2:B:369:GLN:N	2.78	0.41
2:B:407:ARG:HG3	2:B:441:THR:HB	2.03	0.41
2:B:516:MET:HE1	2:B:546:THR:OG1	2.20	0.41
1:A:113:ILE:CD1	1:A:243:ALA:HB1	2.51	0.41
2:B:43:ARG:NH1	2:B:145:PRO:HG2	2.35	0.41
2:B:96:LEU:HB2	2:B:99:LEU:CG	2.50	0.41
2:B:768:VAL:O	2:B:772:LEU:HB2	2.19	0.41
2:B:2:ARG:NH1	2:B:236:ALA:O	2.54	0.41
2:B:286:LEU:CD2	2:B:323:GLU:HG3	2.49	0.41
2:B:425:ILE:HD12	2:B:435:VAL:HG11	2.01	0.41
1:A:197:VAL:HG13	1:A:219:LEU:HD11	2.03	0.41
1:A:265:ALA:HB2	2:B:469:TYR:HE2	1.86	0.41
2:B:49:ARG:CD	2:B:137:GLU:HG3	2.51	0.41
2:B:258:GLN:HE22	2:B:369:GLN:HE21	1.69	0.41
2:B:548:LEU:H	2:B:672:GLU:CD	2.28	0.41
1:A:169:VAL:HG22	1:A:170:GLU:N	2.35	0.41
1:A:213:GLU:HG3	1:A:332:ILE:CD1	2.50	0.41
2:B:672:GLU:C	2:B:673:LEU:HD23	2.46	0.41
2:B:41:ILE:HA	2:B:42:PRO:HD3	1.93	0.40
2:B:530:ARG:HH11	2:B:530:ARG:CB	2.33	0.40
2:B:549:PHE:CD1	2:B:549:PHE:C	2.99	0.40
2:B:592:GLU:O	2:B:604:SER:HB3	2.21	0.40
2:B:656:HIS:HA	2:B:657:PRO:HD3	1.94	0.40
2:B:729:ASP:HB3	2:B:744:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:LEU:CD2	2:B:386:ALA:HB2	2.51	0.40
2:B:224:ALA:N	2:B:244:ASN:HD22	2.17	0.40
2:B:368:GLY:C	2:B:371:PRO:HD2	2.46	0.40
2:B:672:GLU:O	2:B:673:LEU:HD23	2.21	0.40
2:B:718:ALA:CB	2:B:722:LEU:HD22	2.50	0.40
2:B:153:GLU:HG3	2:B:154:VAL:N	2.37	0.40
1:A:101:HIS:CE1	1:A:102:PRO:HD2	2.56	0.40
1:A:194:PHE:CD1	1:A:194:PHE:C	3.00	0.40
1:A:298:ARG:HB3	1:A:303:LEU:HB2	2.02	0.40
1:A:178:HIS:O	1:A:181:PRO:HD2	2.21	0.40
2:B:700:VAL:HB	2:B:778:GLY:CA	2.52	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	264/266 (99%)	250 (95%)	12 (4%)	2 (1%)	16	37
2	B	783/785 (100%)	730 (93%)	45 (6%)	8 (1%)	12	32
All	All	1047/1051 (100%)	980 (94%)	57 (5%)	10 (1%)	12	32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	738	GLU
1	A	349	VAL
2	B	244	ASN
2	B	725	LEU
2	B	770	GLU
2	B	737	PRO
2	B	568	ALA

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Mol	Chain	Res	Type
2	B	697	LEU
1	A	140	PRO
2	B	632	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	214/214 (100%)	200 (94%)	14 (6%)	15	37
2	B	630/630 (100%)	586 (93%)	44 (7%)	14	34
All	All	844/844 (100%)	786 (93%)	58 (7%)	14	34

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	140	PRO
1	A	141	GLU
1	A	178	HIS
1	A	183	GLN
1	A	197	VAL
1	A	198	VAL
1	A	201	ARG
1	A	220	GLU
1	A	244	LEU
1	A	301	LEU
1	A	322	LEU
1	A	332	ILE
1	A	350	LEU
2	B	32	THR
2	B	36	GLU
2	B	62	LYS
2	B	80	ASN
2	B	89	LEU
2	B	97	PRO

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Mol	Chain	Res	Type
2	B	101	GLN
2	B	111	VAL
2	B	133	LEU
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	194	GLU
2	B	196	LEU
2	B	276	ARG
2	B	283	LEU
2	B	286	LEU
2	B	298	LEU
2	B	313	LEU
2	B	333	LEU
2	B	374	ARG
2	B	375	ARG
2	B	438	GLU
2	B	441	THR
2	B	445	THR
2	B	460	VAL
2	B	465	ARG
2	B	467	GLN
2	B	470	GLU
2	B	488	VAL
2	B	505	LEU
2	B	548	LEU
2	B	562	LEU
2	B	576	VAL
2	B	578	ARG
2	B	598	TRP
2	B	600	LYS
2	B	609	LEU
2	B	619	ARG
2	B	711	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	190	HIS
1	A	218	GLN
1	A	254	GLN
1	A	266	GLN
2	B	54	HIS
2	B	80	ASN
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	485	ASN
2	B	584	HIS
2	B	661	GLN
2	B	669	HIS
2	B	685	GLN
2	B	732	GLN
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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	TYR	A	888	-	12,13,13	1.02	0	13,17,17	0.38	0
4	TYR	B	999	-	12,13,13	1.10	1 (8%)	13,17,17	0.69	0
5	SO4	B	786	-	4,4,4	1.06	0	6,6,6	3.01	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	TYR	A	888	-	-	2/8/8/8	0/1/1/1
4	TYR	B	999	-	-	2/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	TYR	CE2-CD2	2.10	1.42	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	786	SO4	O4-S-O1	6.43	143.18	109.56
5	B	786	SO4	O4-S-O3	-2.17	96.56	108.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	999	TYR	C-CA-CB-CG
4	B	999	TYR	N-CA-CB-CG
4	A	888	TYR	O-C-CA-CB
4	A	888	TYR	OXT-C-CA-CB

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	888	TYR	3	0
4	B	999	TYR	4	0
5	B	786	SO4	3	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%)	0.13	11 (4%) 41 37	22, 38, 70, 82	0
2	B	785/785 (100%)	0.36	88 (11%) 10 8	20, 43, 84, 84	0
All	All	1051/1051 (100%)	0.30	99 (9%) 14 12	20, 41, 82, 84	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	782	LEU	7.6
1	A	350	LEU	7.5
2	B	98	GLY	6.2
2	B	781	GLY	6.2
2	B	731	TYR	5.6
2	B	785	PRO	5.3
2	B	783	ASP	5.3
2	B	689	ARG	5.2
2	B	99	LEU	4.9
2	B	736	LEU	4.9
2	B	739	GLY	4.9
2	B	101	GLN	4.7
2	B	784	THR	4.6
2	B	738	GLU	4.6
2	B	733	GLY	4.1
1	A	143	HIS	4.1
2	B	564	ARG	4.0
1	A	142	HIS	4.0
2	B	759	GLU	3.9
2	B	734	PRO	3.9
2	B	737	PRO	3.8
2	B	100	GLY	3.7
1	A	85	ARG	3.5
2	B	778	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	60	ARG	3.4
2	B	757	ARG	3.4
1	A	87	ASP	3.3
2	B	732	GLN	3.2
1	A	349	VAL	3.2
2	B	726	ALA	3.1
2	B	667	PRO	3.1
2	B	745	PHE	3.1
2	B	694	PHE	3.0
2	B	701	VAL	3.0
2	B	749	PHE	2.9
2	B	742	SER	2.9
2	B	769	ALA	2.9
2	B	755	THR	2.9
2	B	730	LEU	2.9
1	A	348	GLY	2.8
2	B	661	GLN	2.8
2	B	325	ARG	2.8
2	B	735	PRO	2.8
2	B	743	LEU	2.8
2	B	721	TYR	2.8
2	B	774	ALA	2.7
2	B	280	GLY	2.6
2	B	579	GLU	2.6
2	B	681	PRO	2.6
2	B	780	ARG	2.6
2	B	600	LYS	2.6
2	B	594	VAL	2.6
2	B	753	LYS	2.6
2	B	762	GLU	2.6
2	B	43	ARG	2.5
2	B	374	ARG	2.5
2	B	691	PRO	2.5
2	B	682	LEU	2.5
2	B	598	TRP	2.4
1	A	157	GLU	2.4
2	B	601	GLU	2.4
2	B	706	PRO	2.4
2	B	279	GLU	2.4
2	B	699	VAL	2.4
2	B	707	TYR	2.4
2	B	660	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	698	ALA	2.4
2	B	748	ARG	2.4
2	B	34	ARG	2.4
2	B	627	GLU	2.3
1	A	271	TRP	2.3
2	B	497	ARG	2.3
2	B	663	LEU	2.3
2	B	756	LEU	2.3
2	B	777	PHE	2.3
2	B	79	GLU	2.3
1	A	150	ASP	2.3
2	B	341	VAL	2.3
2	B	697	LEU	2.3
2	B	438	GLU	2.2
1	A	160	ARG	2.2
2	B	626	VAL	2.2
2	B	636	PRO	2.2
2	B	773	ARG	2.2
2	B	647	GLU	2.2
2	B	690	HIS	2.2
2	B	522	ARG	2.1
2	B	629	GLN	2.1
2	B	703	ALA	2.1
2	B	764	ALA	2.1
2	B	188	GLU	2.1
2	B	704	PRO	2.1
2	B	278	ARG	2.1
2	B	715	ARG	2.1
2	B	767	ARG	2.1
2	B	702	PRO	2.1
2	B	779	LEU	2.1
2	B	97	PRO	2.1
2	B	741	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

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	TYR	B	999	13/13	0.73	0.30	7,12,46,53	0
4	TYR	A	888	13/13	0.89	0.24	5,9,16,51	0
3	MG	A	901	1/1	0.91	0.31	41,41,41,41	0
5	SO4	B	786	5/5	0.95	0.40	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.