Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 01:18 PM EDT

PDB ID	:	2AMC
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 (i) 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 (i)) were used in the production of this report:

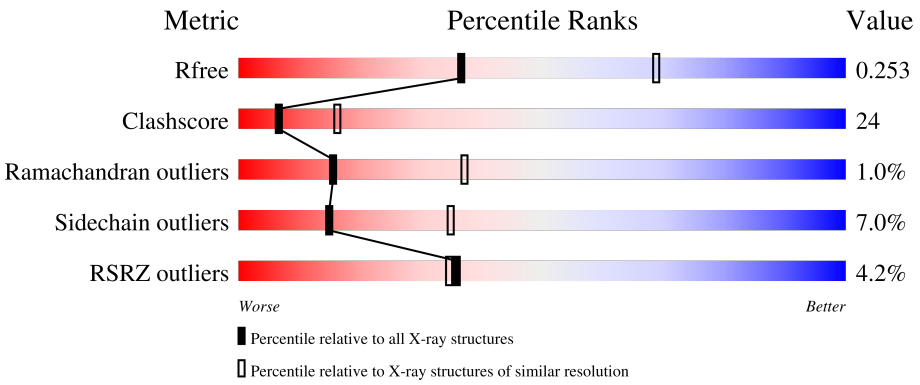
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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% 67% 29% •
2	B	785	5% 57% 39% •

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
			Total	C	N	O	S			
1	A	266	2123	1388	363	365	7	0	0	0

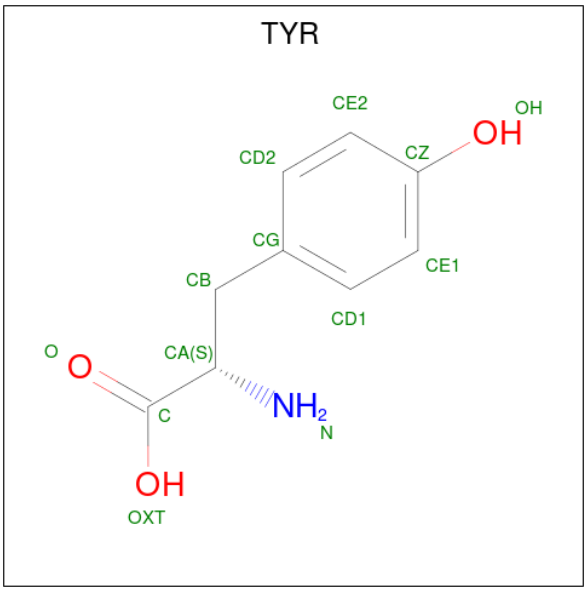
- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

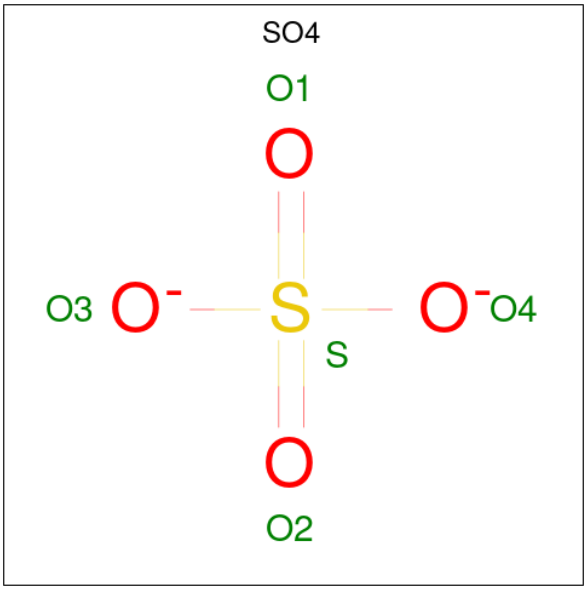
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

- Molecule 4 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

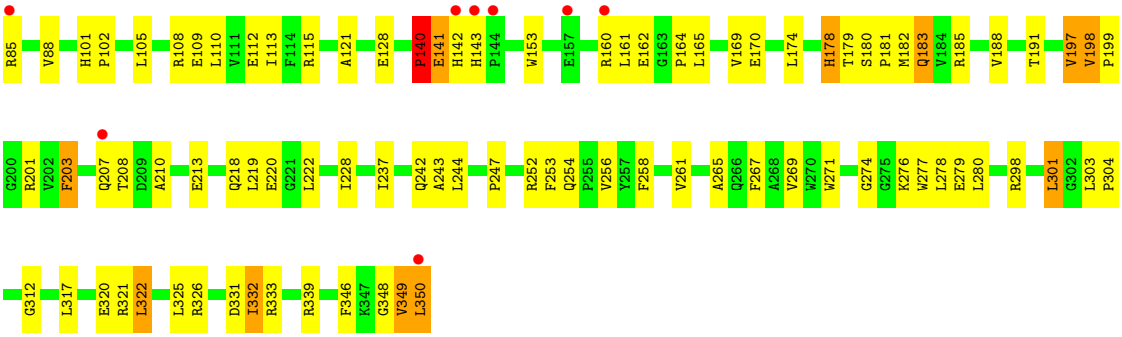
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	46	46	46	0	0
			Total	O		
6	B	186	186	186	0	0

3 Residue-property plots (i)

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.

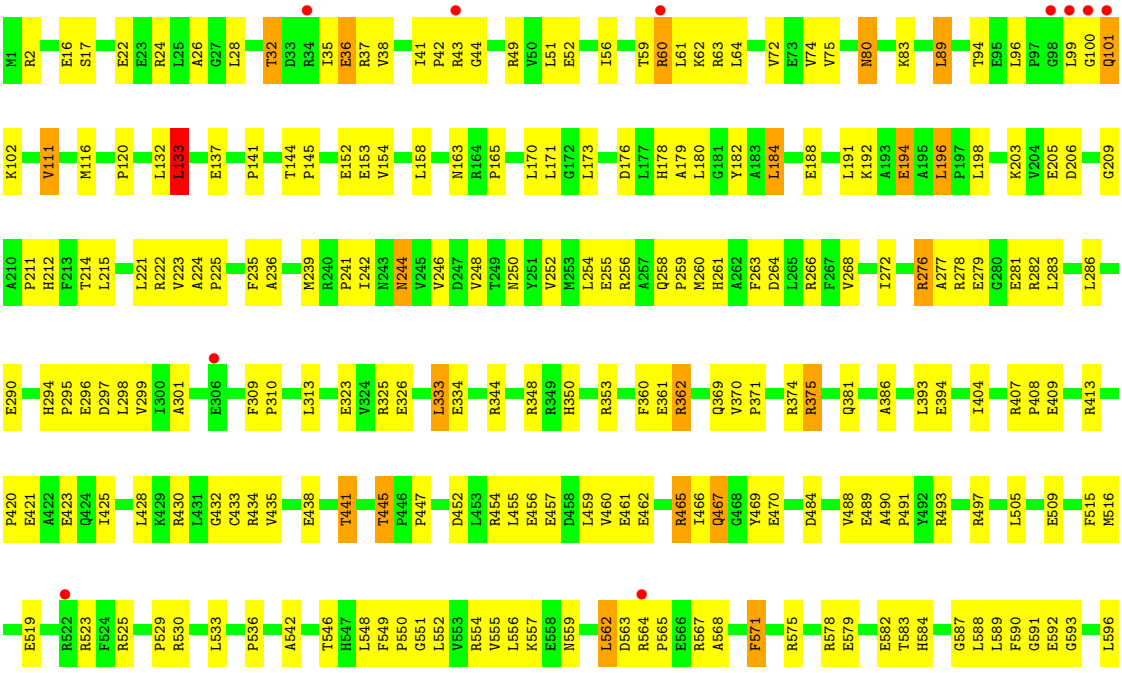
• Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

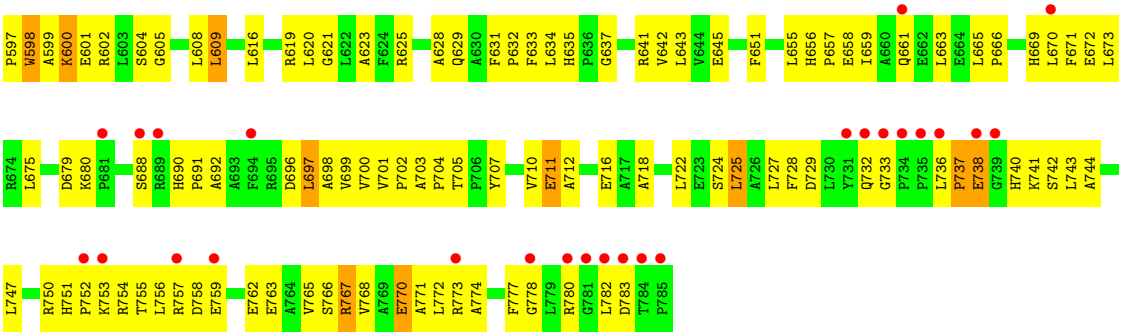
Chain A:



• Molecule 2: Phenylalanyl-tRNA synthetase beta chain

Chain B:




P597 W598 A599 K600 E601 R602 L603 S604 G605 L608 L609 L616 R619 L620 G621 L622 A623 F624 R625 A628 Q629 A630 F631 P632 F633 L634 H635 P636 G637 R641 V642 L643 V644 E645 F651 L655 H656 P657 E658 I659 A660 Q661 E662 L663 E664 L665 P666 H669 L670 F671 E672 L673
R674 L675 D679 K680 P681 S688 R689 H690 P691 A692 A693 F694 R695 D696 L697 A698 V699 V700 V701 P702 A703 P704 T705 P706 Y707 V710 E711 A712 E716 A717 A718 L722 E723 S724 L725 A726 L727 F728 D729 L730 Y731 Q732 G733 P734 P735 L736 P737 E738 G739 H740 K741 S742 L743 A744
L747 R750 H751 P752 K753 R754 T755 L756 R757 D758 E759 E762 E763 A764 V765 S766 R767 V768 A769 E770 A771 L772 R773 A774 F777 G778 L779 R780 G781 L782 D783 T784 P785

4 Data and refinement statistics (i)

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) 98.5 (25.41-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 59.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.45	1/2191 (0.0%)	0.68	3/2971 (0.1%)
2	B	0.38	0/6280	0.66	2/8536 (0.0%)
All	All	0.40	1/8471 (0.0%)	0.66	5/11507 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	LEU	N-CA	5.71	1.57	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	350	LEU	N-CA-CB	-8.87	92.66	110.40
2	B	38	VAL	N-CA-C	6.06	127.36	111.00
1	A	140	PRO	CA-N-CD	-5.86	103.30	111.50
2	B	133	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	350	LEU	N-CA-C	5.54	125.95	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2123	0	2075	90	0
2	B	6127	0	6180	306	0
3	A	1	0	0	0	0
4	A	13	0	8	3	0
4	B	13	0	8	3	0
5	B	5	0	0	2	0
6	A	46	0	0	3	0
6	B	186	0	0	6	0
All	All	8514	0	8271	389	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 24.

All (389) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:407:ARG:NH2	5:B:786:SO4:O1	2.13	0.78
2:B:516:MET:HE3	2:B:546:THR:H	1.49	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: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:712:ALA:O	2:B:716:GLU:HB2	1.95	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: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
2:B:256:ARG:NH2	2:B:375:ARG:HG3	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:99:LEU:HD12	2:B:99:LEU:C	2.19	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: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:239:MET:HE1	2:B:250:ASN:HB3	1.84	0.60
2:B:782:LEU:HD12	2:B:783:ASP:H	1.66	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:702:PRO:C	2:B:704:PRO:HD2	2.22	0.59
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: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:326:GLU:CD	2:B:326:GLU:H	2.07	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
2:B:278:ARG:HG2	2:B:278:ARG:HH11	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PRO:HG2	1:A:188:VAL:HG21	1.86	0.58
1:A:298:ARG:NH1	1:A:304:PRO:O	2.36	0.57
2:B:516:MET:HE3	2:B:546:THR:N	2.17	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
1:A:141:GLU:O	1:A:142:HIS:C	2.44	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: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:239:MET:HE2	2:B:254:LEU:HD11	1.89	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:99:LEU:HD13	2:B:101:GLN:C	2.28	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:MET:CE	2:B:250:ASN:HB3	2.39	0.53
1:A:256:VAL:HG12	1:A:265:ALA:C	2.30	0.53
2:B:120:PRO:HG3	2:B:133:LEU:HD13	1.89	0.53
2:B:353:ARG:C	2:B:353:ARG:HD3	2.30	0.52
2:B:563:ASP:C	2:B:564:ARG:HD2	2.29	0.52
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
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: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
2:B:348:ARG:HH12	2:B:361:GLU:CD	2.13	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: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:456:GLU:HA	2:B:459:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:462:GLU:CD	2:B:465:ARG:NH1	2.66	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: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: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
2:B:642:VAL:C	2:B:643:LEU:HD22	2.33	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: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
1:A:278:LEU:HD11	1:A:325:LEU:CD1	2.45	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ASP:OD2	2:B:266:ARG:HD3	2.14	0.47
2:B:369:GLN:CD	2:B:369:GLN:H	2.19	0.47
2:B:699:VAL:HG22	2:B:772:LEU:HD21	1.97	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
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:697:LEU:HD12	2:B:697:LEU:C	2.35	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: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: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
2:B:101:GLN:O	2:B:102:LYS:C	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:LEU:N	2:B:198:LEU:HD23	2.32	0.45
2:B:209:GLY:C	2:B:211:PRO:HD3	2.37	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: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: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: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:99:LEU:CD1	2:B:99:LEU:C	2.85	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
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
1:A:174:LEU:C	1:A:174:LEU:HD12	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:ALA:N	2:B:704:PRO:CD	2.81	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: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:563:ASP:C	2:B:565:PRO:HD3	2.39	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: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
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:432:GLY:C	2:B:447:PRO:HG3	2.39	0.42
2:B:651:PHE:C	2:B:651:PHE:CD1	2.93	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:261:HIS:HD2	2:B:263:PHE:CE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:VAL:CG1	1:A:280:LEU:HD12	2.51	0.41
2:B:206:ASP:CG	2:B:276:ARG:HH11	2.24	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:407:ARG:HG3	2:B:441:THR:HB	2.03	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:326:GLU:CD	2:B:326:GLU:N	2.72	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
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
1:A:348:GLY:O	1:A:349:VAL:C	2.59	0.40
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: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
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: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: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
1:A:179:THR:C	1:A:181:PRO:HD2	2.42	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%)	19	43
2	B	783/785 (100%)	730 (93%)	45 (6%)	8 (1%)	15	37
All	All	1047/1051 (100%)	980 (94%)	57 (5%)	10 (1%)	15	37

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
2	B	697	LEU
1	A	140	PRO
2	B	632	PRO

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	214/214 (100%)	201 (94%)	13 (6%)	18	41
2	B	630/630 (100%)	585 (93%)	45 (7%)	14	34
All	All	844/844 (100%)	786 (93%)	58 (7%)	15	35

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	203	PHE
1	A	244	LEU
1	A	301	LEU
1	A	322	LEU
1	A	332	ILE
2	B	32	THR
2	B	36	GLU
2	B	60	ARG
2	B	80	ASN
2	B	89	LEU
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	298	LEU
2	B	313	LEU
2	B	333	LEU
2	B	362	ARG
2	B	374	ARG
2	B	375	ARG
2	B	438	GLU
2	B	441	THR
2	B	445	THR
2	B	465	ARG

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Mol	Chain	Res	Type
2	B	467	GLN
2	B	470	GLU
2	B	488	VAL
2	B	497	ARG
2	B	505	LEU
2	B	548	LEU
2	B	562	LEU
2	B	571	PHE
2	B	575	ARG
2	B	598	TRP
2	B	600	LYS
2	B	609	LEU
2	B	619	ARG
2	B	679	ASP
2	B	711	GLU
2	B	767	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	120	GLN
1	A	183	GLN
1	A	218	GLN
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	584	HIS
2	B	661	GLN
2	B	669	HIS
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 monosaccharides 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	0.98	0	16,17,17	0.77	0
5	SO4	B	786	2	4,4,4	1.16	0	6,6,6	3.13	2 (33%)
4	TYR	B	999	-	12,13,13	1.03	0	16,17,17	0.73	0

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	786	SO4	O4-S-O1	6.49	143.18	109.31
5	B	786	SO4	O4-S-O3	-2.93	96.56	109.06

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 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	888	TYR	3	0
5	B	786	SO4	2	0
4	B	999	TYR	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 (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	266/266 (100%)	-0.25	8 (3%)	50	51	22, 38, 70, 82	0
2	B	785/785 (100%)	-0.05	36 (4%)	32	31	20, 43, 84, 84	0
All	All	1051/1051 (100%)	-0.10	44 (4%)	36	35	20, 41, 82, 84	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	785	PRO	5.3
2	B	98	GLY	5.1
2	B	731	TYR	5.1
2	B	783	ASP	5.0
2	B	781	GLY	4.9
2	B	736	LEU	4.6
2	B	782	LEU	4.6
2	B	101	GLN	4.2
2	B	99	LEU	3.9
2	B	732	GLN	3.9
2	B	689	ARG	3.9
2	B	738	GLU	3.7
2	B	780	ARG	3.7
2	B	734	PRO	3.7
2	B	759	GLU	3.6
2	B	739	GLY	3.6
1	A	142	HIS	3.5
2	B	735	PRO	3.5
2	B	733	GLY	3.2
2	B	753	LYS	3.1
2	B	757	ARG	3.0
1	A	143	HIS	2.9
2	B	306	GLU	2.9
1	A	350	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	85	ARG	2.7
2	B	773	ARG	2.7
2	B	34	ARG	2.7
2	B	752	PRO	2.6
2	B	694	PHE	2.5
1	A	157	GLU	2.4
2	B	784	THR	2.4
1	A	207	GLN	2.4
2	B	60	ARG	2.3
1	A	144	PRO	2.3
2	B	564	ARG	2.3
2	B	688	SER	2.3
2	B	661	GLN	2.3
2	B	43	ARG	2.2
2	B	100	GLY	2.2
2	B	681	PRO	2.2
2	B	778	GLY	2.2
1	A	160	ARG	2.1
2	B	522	ARG	2.1
2	B	670	LEU	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 monosaccharides 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(Å^2)	Q<0.9
4	TYR	B	999	13/13	0.80	0.30	7,12,46,53	0
4	TYR	A	888	13/13	0.91	0.26	5,9,16,51	0
3	MG	A	901	1/1	0.95	0.50	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	B	786	5/5	0.96	0.44	5,5,5,5	0

6.5 Other polymers (i)

There are no such residues in this entry.