Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 03:23 PM EDT

PDB ID	:	2AKW
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:

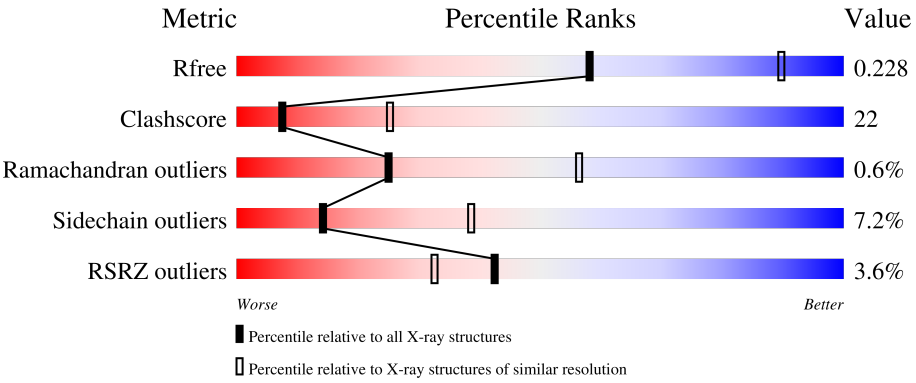
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	2% 66% 32% ·
2	B	785	4% 59% 37% ·

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

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			

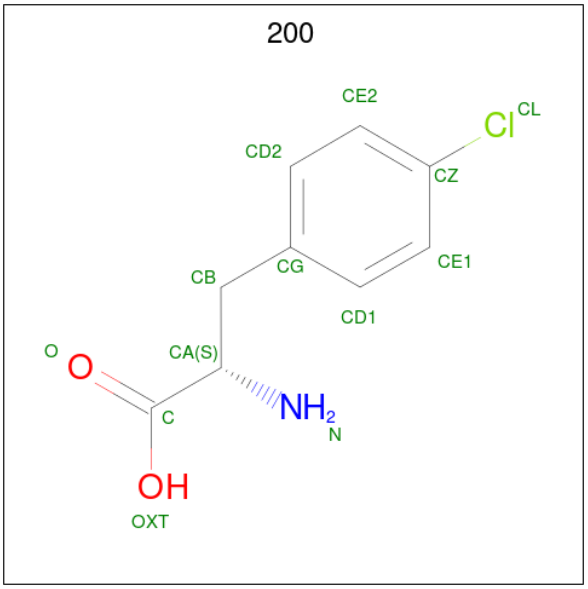
- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

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 (three-letter code: MN) (formula: Mn).

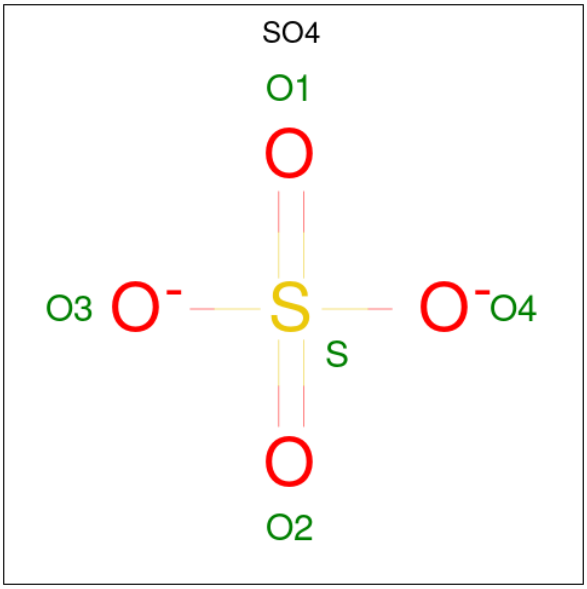
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 4-CHLORO-L-PHENYLALANINE (three-letter code: 200) (formula: $C_9H_{10}ClNO_2$).



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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

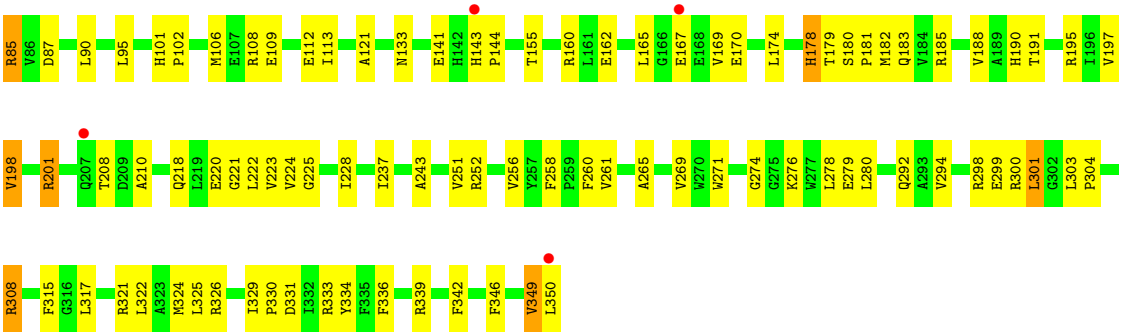
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total	O	0	0
			41	41		
6	B	156	Total	O	0	0
			156	156		

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.

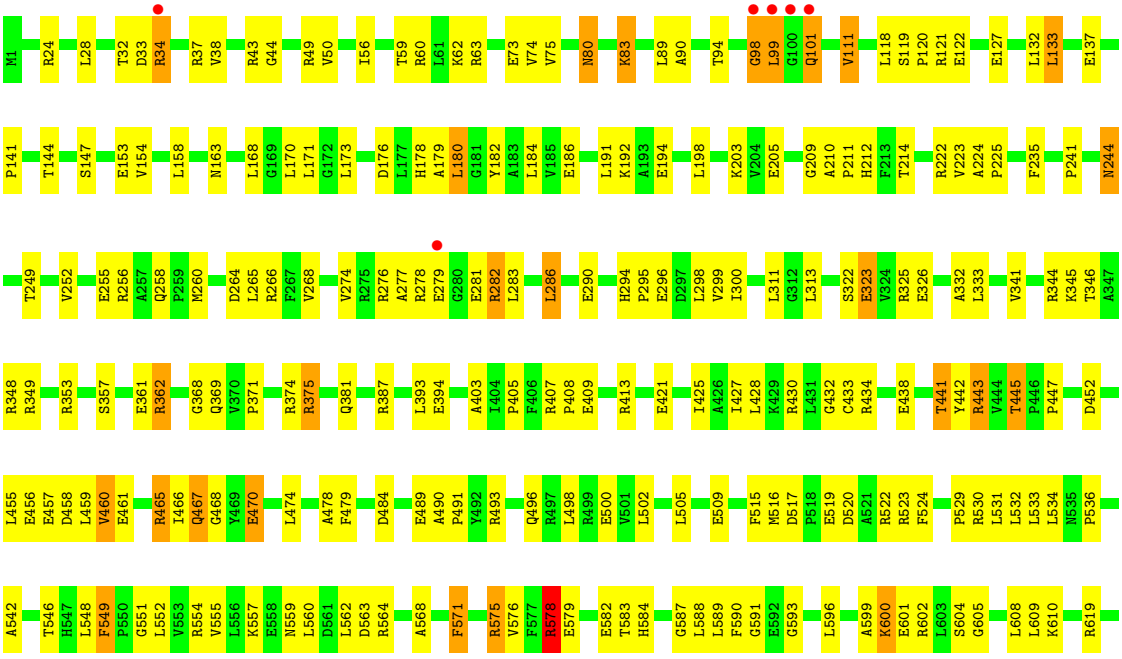
• Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

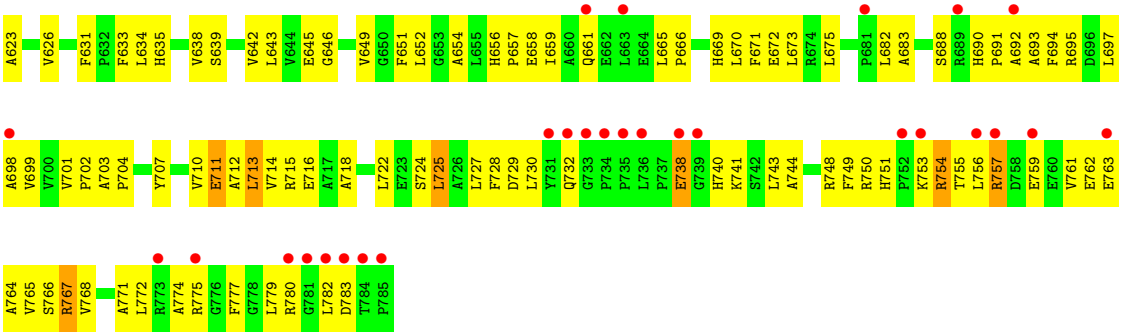
Chain A:



• Molecule 2: Phenylalanyl-tRNA synthetase beta chain

Chain B:




A623 V626 F631 P632 F633 L634 H635 V638 S639 V642 L643 V644 E645 G646 V649 G650 F651 L652 G653 A654 L655 H656 P657 E658 I659 A660 Q661 E662 L663 E664 L665 P666 H669 L670 F671 E672 L673 R674 L675 P681 L682 A683 S688 R689 H690 P691 A692 A693 F694 R695 D696 L697
A698 V699 V700 V701 P702 A703 P704 Y707 V710 E711 A712 L713 V714 R715 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 R748 F749 R750 H751 P752 K753 R754 T755 L756 R757 D758 E759 E760 V761 E762 E763
A764 V765 S766 R767 V768 A771 L772 R773 A774 R775 G776 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	172.98Å 172.98Å 138.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.99 – 2.80 29.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (9.99-2.80) 99.3 (29.96-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.234 0.220 , 0.228	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)	0.36 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	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.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MN, 200

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	0.41	0/2191	0.63	0/2971
2	B	0.42	1/6280 (0.0%)	0.70	6/8536 (0.1%)
All	All	0.42	1/8471 (0.0%)	0.69	6/11507 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	99	LEU	N-CA	14.35	1.75	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	99	LEU	N-CA-CB	-17.22	75.95	110.40
2	B	98	GLY	C-N-CA	-9.59	97.72	121.70
2	B	99	LEU	N-CA-C	9.38	136.32	111.00
2	B	38	VAL	N-CA-C	6.68	129.05	111.00
2	B	133	LEU	CA-CB-CG	5.35	127.61	115.30
2	B	332	ALA	N-CA-C	-5.09	97.26	111.00

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	87	0
2	B	6127	0	6180	283	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	365	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 22.

All (365) 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: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:98:GLY:C	2:B:99:LEU:CA	2.33	0.95
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
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:516:MET:HE3	2:B:546:THR:H	1.50	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:B:701:VAL:HG13	2:B:702:PRO:HD2	1.79	0.65
2:B:176:ASP:CG	2:B:465:ARG:HH22	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:353:ARG:C	2:B:353:ARG:HD3	2.21	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: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: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
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:209:GLY:C	2:B:211:PRO:HD3	2.23	0.58
2:B:467:GLN:HA	2:B:467:GLN:NE2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:224:ALA:H	2:B:244:ASN:ND2	2.03	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: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:701:VAL:CG1	2:B:702:PRO:HD2	2.36	0.55
1:A:292:GLN:HA	1:A:308:ARG:HH22	1.71	0.55
2:B:563:ASP:C	2:B:564:ARG:HD2	2.26	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:49:ARG:CD	2:B:137:GLU:HG3	2.37	0.55
2:B:264:ASP:OD1	2:B:266:ARG:HG3	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:755:THR:HG22	2:B:756:LEU:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:642:VAL:C	2:B:643:LEU:HD22	2.29	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
1:A:174:LEU:C	1:A:174:LEU:HD12	2.30	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: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: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
2:B:656:HIS:HE1	2:B:658:GLU:HG3	1.75	0.51
1:A:256:VAL:HG12	1:A:265:ALA:C	2.31	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:702:PRO:C	2:B:704:PRO:HD2	2.30	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:588:LEU:C	2:B:588:LEU:HD23	2.32	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
2:B:697:LEU:HD12	2:B:697:LEU:C	2.31	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:583:THR:CG2	2:B:675:LEU:HD12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:326:GLU:CD	2:B:326:GLU:H	2.16	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:699:VAL:CG1	2:B:772:LEU:HD11	2.43	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: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
2:B:300:ILE:O	2:B:311:LEU:HB2	2.14	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: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:516:MET:HE3	2:B:546:THR:N	2.24	0.47
2:B:549:PHE:CD1	2:B:549:PHE:C	2.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:711:GLU:CD	2:B:715:ARG:HH12	2.18	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
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:772:LEU:O	2:B:777:PHE:HB2	2.17	0.45
1:A:339:ARG:O	1:A:342:PHE:HB3	2.17	0.45
2:B:33:ASP:O	2:B:34:ARG:HB2	2.16	0.45
2:B:368:GLY:C	2:B:371:PRO:HD2	2.36	0.45
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: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
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
2:B:651:PHE:C	2:B:651:PHE:CD1	2.91	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:62:LYS:HB2	2:B:62:LYS:HZ3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:369:GLN:CD	2:B:369:GLN:H	2.21	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: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
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:286:LEU:HD21	2:B:323:GLU:CG	2.49	0.43
2:B:757:ARG:HD2	2:B:759:GLU:OE1	2.18	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: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:762:GLU:CD	2:B:783:ASP:OD2	2.57	0.43
2:B:707:TYR:OH	2:B:711:GLU:HG3	2.19	0.42
1:A:141:GLU:C	1:A:143:HIS:N	2.73	0.42
1:A:317:LEU:HD12	1:A:317:LEU:C	2.40	0.42
2:B:694:PHE:CD1	2:B:694:PHE:N	2.87	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:143:HIS:ND1	1:A:144:PRO:HD2	2.34	0.42
1:A:179:THR:C	1:A:181:PRO:HD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:192:LYS:H	2:B:381:GLN:NE2	2.03	0.41
2:B:252:VAL:HG11	2:B:260:MET:HE1	2.01	0.41
2:B:101:GLN:CD	2:B:101:GLN:H	2.22	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
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:725:LEU:C	2:B:725:LEU:HD23	2.40	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
2:B:409:GLU:CD	2:B:413:ARG:HD3	2.41	0.41
1:A:165:LEU:HD12	1:A:301:LEU:CD2	2.35	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:95:LEU:HD22	1:A:95:LEU:H	1.86	0.40
1:A:315:PHE:CD1	1:A:315:PHE:C	2.94	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:141:GLU:C	1:A:143:HIS:H	2.25	0.40
2:B:548:LEU:H	2:B:672:GLU:CD	2.24	0.40
2:B:699:VAL:HG12	2:B:701:VAL:HG23	2.03	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:751:HIS:HB2	2:B:756:LEU:CD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:601:GLU:CD	2:B:601:GLU:H	2.24	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 (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%)	249 (94%)	14 (5%)	1 (0%)	34	66
2	B	783/785 (100%)	725 (93%)	53 (7%)	5 (1%)	25	56
All	All	1047/1051 (100%)	974 (93%)	67 (6%)	6 (1%)	25	56

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 (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%)	205 (96%)	9 (4%)	30 63
2	B	630/630 (100%)	578 (92%)	52 (8%)	11 32
All	All	844/844 (100%)	783 (93%)	61 (7%)	14 38

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ARG
1	A	178	HIS
1	A	198	VAL
1	A	201	ARG
1	A	260	PHE
1	A	299	GLU
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	60	ARG
2	B	74	VAL
2	B	80	ASN
2	B	83	LYS
2	B	89	LEU
2	B	101	GLN
2	B	111	VAL
2	B	127	GLU
2	B	147	SER
2	B	158	LEU
2	B	170	LEU
2	B	171	LEU
2	B	173	LEU
2	B	180	LEU
2	B	191	LEU

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Mol	Chain	Res	Type
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	362	ARG
2	B	375	ARG
2	B	438	GLU
2	B	441	THR
2	B	443	ARG
2	B	445	THR
2	B	460	VAL
2	B	465	ARG
2	B	467	GLN
2	B	470	GLU
2	B	505	LEU
2	B	549	PHE
2	B	571	PHE
2	B	575	ARG
2	B	576	VAL
2	B	578	ARG
2	B	600	LYS
2	B	609	LEU
2	B	619	ARG
2	B	711	GLU
2	B	713	LEU
2	B	738	GLU
2	B	754	ARG
2	B	757	ARG
2	B	767	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	183	GLN
1	A	207	GLN
1	A	218	GLN

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Mol	Chain	Res	Type
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	350	HIS
2	B	381	GLN
2	B	467	GLN
2	B	584	HIS
2	B	661	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 monosaccharides 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	2.01	6 (50%)	16,17,17	0.71	0
5	SO4	B	786	-	4,4,4	2.24	3 (75%)	6,6,6	2.06	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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	200	CD1-CG	3.51	1.46	1.38
4	A	999	200	CE2-CZ	2.92	1.43	1.38
5	B	786	SO4	O1-S	2.66	1.60	1.46
4	A	999	200	CD2-CG	2.52	1.44	1.38
4	A	999	200	CE2-CD2	2.47	1.43	1.38
4	A	999	200	CE1-CZ	2.38	1.42	1.38
4	A	999	200	CE1-CD1	2.28	1.42	1.38
5	B	786	SO4	O3-S	-2.25	1.29	1.47
5	B	786	SO4	O2-S	-2.09	1.34	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	786	SO4	O3-S-O2	3.96	129.97	109.31
5	B	786	SO4	O2-S-O1	-2.23	92.94	109.43

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, 95^{th} 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%)	-0.24	4 (1%)	73	68	25, 41, 73, 86	0
2	B	785/785 (100%)	-0.13	34 (4%)	35	25	22, 46, 87, 87	0
All	All	1051/1051 (100%)	-0.15	38 (3%)	42	32	22, 44, 86, 87	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	782	LEU	6.7
2	B	781	GLY	5.9
2	B	783	ASP	5.9
2	B	739	GLY	4.8
2	B	98	GLY	4.7
2	B	736	LEU	4.4
2	B	732	GLN	4.0
2	B	784	THR	4.0
2	B	785	PRO	3.9
2	B	731	TYR	3.9
2	B	756	LEU	3.2
2	B	759	GLU	3.2
1	A	350	LEU	3.2
2	B	733	GLY	2.9
1	A	167	GLU	2.9
2	B	738	GLU	2.9
2	B	698	ALA	2.8
2	B	780	ARG	2.8
2	B	101	GLN	2.7
2	B	99	LEU	2.7
2	B	663	LEU	2.6
2	B	689	ARG	2.5
2	B	681	PRO	2.5
2	B	279	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	753	LYS	2.4
2	B	773	ARG	2.3
2	B	734	PRO	2.3
1	A	207	GLN	2.3
2	B	661	GLN	2.2
2	B	775	ARG	2.2
1	A	143	HIS	2.2
2	B	757	ARG	2.2
2	B	752	PRO	2.2
2	B	100	GLY	2.2
2	B	763	GLU	2.2
2	B	34	ARG	2.2
2	B	692	ALA	2.1
2	B	735	PRO	2.1

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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
3	MN	A	901	1/1	0.82	0.11	42,42,42,42	0
4	200	A	999	13/13	0.88	0.18	8,12,18,54	0
5	SO4	B	786	5/5	0.94	0.34	7,7,7,18	0

6.5 Other polymers (i)

There are no such residues in this entry.