



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:35 PM UTC

PDB ID : 1K1X / pdb_00001k1x
Title : Crystal structure of 4-alpha-glucanotransferase from thermococcus litoralis
Authors : Imamura, H.; Fushinobu, S.; Kumasaka, T.; Yamamoto, M.; Jeon, B.S.; Wakagi, T.; Matsuzawa, H.
Deposited on : 2001-09-26
Resolution : 2.40 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

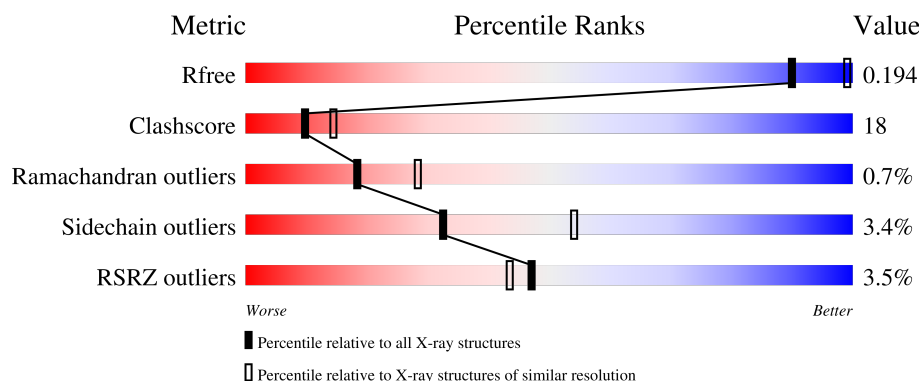
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	659	4% 65% 28% • •
1	B	659	3% 59% 34% • •

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
3	TRS	B	1604	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11205 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.

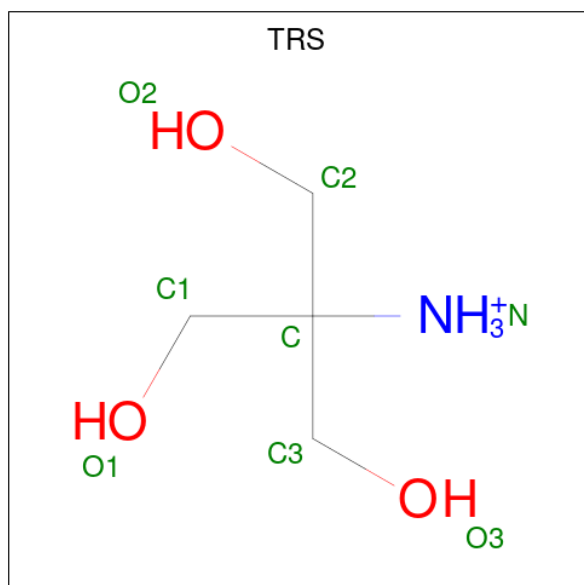
- Molecule 1 is a protein called 4-ALPHA-GLUCANOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	0	0	0
			5348	3498	874	961	15			
1	B	636	Total	C	N	O	S	0	0	0
			5347	3498	874	961	14			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

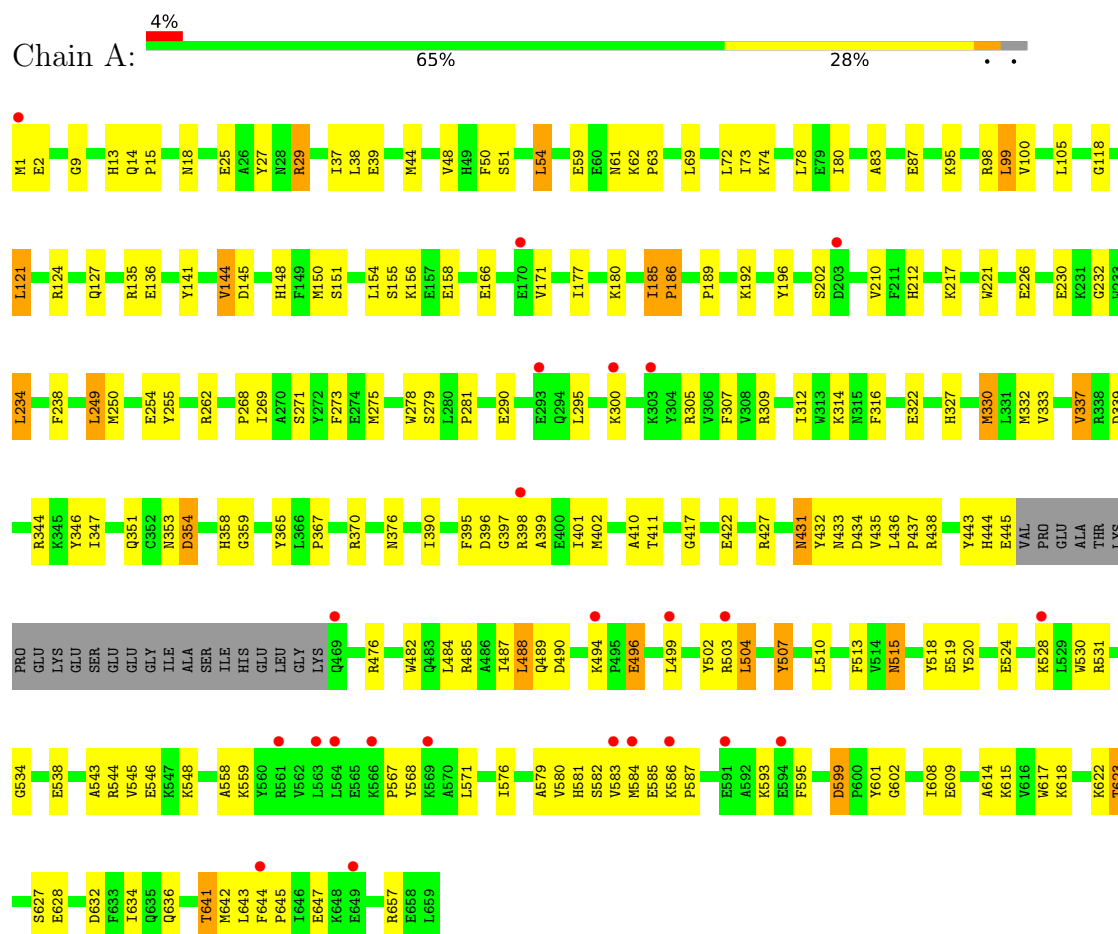
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	290	Total	O	0	0
			290	290		
4	B	209	Total	O	0	0
			209	209		

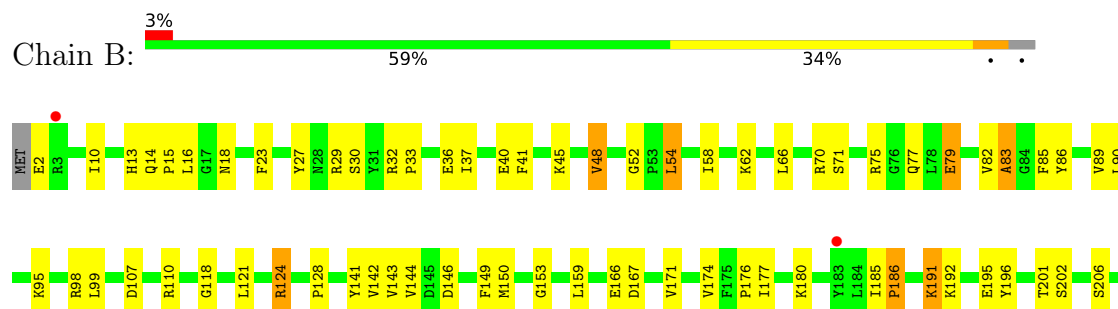
3 Residue-property plots [i](#)

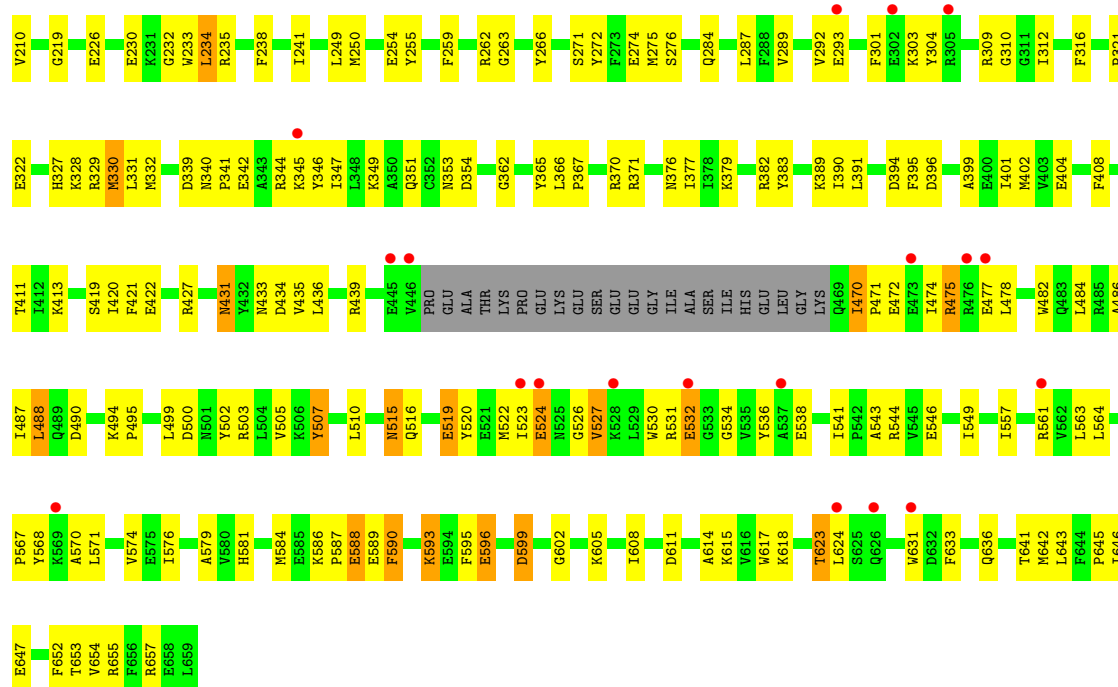
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4-ALPHA-GLUCANOTRANSFERASE



• Molecule 1: 4-ALPHA-GLUCANOTRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.68Å 161.49Å 70.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.40 29.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.00-2.40) 99.6 (29.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.91 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.236 0.197 , 0.194	Depositor DCC
R_{free} test set	3142 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11205	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: CA, TRS

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	0.39	0/5504	0.92	19/7440 (0.3%)
1	B	0.37	0/5503	0.92	26/7440 (0.3%)
All	All	0.38	0/11007	0.92	45/14880 (0.3%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ASN	N-CA-C	9.84	122.00	111.28
1	B	353	ASN	N-CA-C	8.11	120.12	111.28
1	A	484	LEU	N-CA-C	-7.73	100.12	110.55
1	A	504	LEU	N-CA-C	-7.62	99.84	110.35
1	B	599	ASP	CA-C-N	7.61	129.35	119.84
1	B	599	ASP	C-N-CA	7.61	129.35	119.84
1	B	399	ALA	N-CA-C	7.54	120.91	110.35
1	B	538	GLU	N-CA-C	-7.38	103.23	112.90
1	B	482	TRP	N-CA-C	-7.37	104.53	113.97
1	A	316	PHE	N-CA-C	-7.33	103.60	112.54
1	A	232	GLY	N-CA-C	7.15	124.89	114.10
1	B	593	LYS	N-CA-C	-6.84	105.48	114.31
1	B	210	VAL	N-CA-C	6.84	117.69	108.11
1	A	593	LYS	N-CA-C	-6.59	105.37	113.41
1	B	89	VAL	N-CA-C	-6.49	98.17	107.98
1	A	482	TRP	N-CA-C	-6.46	105.14	114.12
1	A	634	ILE	N-CA-C	6.37	117.76	108.53
1	A	210	VAL	N-CA-C	6.14	116.76	108.17
1	B	395	PHE	N-CA-C	5.90	119.53	111.39
1	A	273	PHE	N-CA-C	5.82	118.10	111.11
1	B	48	VAL	N-CA-C	5.65	116.61	108.48
1	B	159	LEU	N-CA-C	5.64	118.94	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ALA	N-CA-C	5.59	118.18	110.35
1	B	377	ILE	N-CA-C	-5.59	105.28	110.53
1	A	185	ILE	N-CA-C	5.58	114.02	107.77
1	B	490	ASP	N-CA-C	5.49	117.17	108.67
1	A	538	GLU	N-CA-C	-5.38	106.89	113.50
1	B	470	ILE	N-CA-C	5.35	114.79	108.96
1	B	484	LEU	N-CA-C	-5.30	102.67	110.52
1	A	48	VAL	N-CA-C	5.30	116.12	108.48
1	B	404	GLU	N-CA-C	5.30	117.14	108.55
1	B	519	GLU	N-CA-C	-5.25	103.47	110.55
1	A	395	PHE	N-CA-C	5.24	118.47	111.24
1	A	490	ASP	N-CA-C	5.22	117.24	109.25
1	B	79	GLU	N-CA-C	-5.15	100.77	109.07
1	B	41	PHE	CA-C-N	5.11	126.23	119.84
1	B	41	PHE	C-N-CA	5.11	126.23	119.84
1	B	329	ARG	N-CA-C	-5.10	105.90	111.82
1	B	232	GLY	N-CA-C	5.08	122.73	114.90
1	A	599	ASP	CA-C-N	5.08	125.11	119.32
1	A	599	ASP	C-N-CA	5.08	125.11	119.32
1	A	354	ASP	N-CA-C	5.08	119.75	111.37
1	B	408	PHE	N-CA-C	5.04	116.84	109.24
1	B	340	ASN	CA-C-N	5.02	124.46	119.24
1	B	340	ASN	C-N-CA	5.02	124.46	119.24

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	5348	0	5250	168	0
1	B	5347	0	5247	214	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	B	8	0	12	0	0
4	A	290	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	209	0	0	7	0
All	All	11205	0	10509	373	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 18.

All (373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:MET:HE1	1:B:316:PHE:HE1	1.19	1.07
1:B:275:MET:HE1	1:B:316:PHE:CE1	2.01	0.95
1:B:166:GLU:HB3	1:B:171:VAL:HG12	1.52	0.92
1:A:503:ARG:HH11	1:A:587:PRO:HG2	1.36	0.90
1:B:82:VAL:CG1	1:B:83:ALA:N	2.48	0.77
1:B:143:VAL:CG1	1:B:177:ILE:HD11	2.16	0.76
1:B:82:VAL:CG1	1:B:83:ALA:H	1.96	0.76
1:A:13:HIS:ND1	1:A:87:GLU:HG3	2.00	0.76
1:A:27:TYR:CZ	1:A:62:LYS:HG2	2.20	0.76
1:A:365:TYR:CD2	1:A:623:THR:HG21	2.21	0.76
1:B:382:ARG:HD2	4:B:1693:HOH:O	1.85	0.75
1:B:477:GLU:CD	1:B:503:ARG:HH22	1.94	0.75
1:B:599:ASP:OD2	1:B:602:GLY:HA3	1.87	0.74
1:A:307:PHE:HE1	1:B:287:LEU:HD22	1.51	0.74
1:B:82:VAL:HG12	1:B:83:ALA:N	2.03	0.73
1:A:250:MET:HE2	1:A:255:TYR:HA	1.69	0.73
1:A:254:GLU:OE1	4:A:1779:HOH:O	2.06	0.73
1:B:557:ILE:HD11	1:B:653:THR:HG22	1.71	0.73
1:A:585:GLU:O	1:A:586:LYS:HD2	1.88	0.72
1:A:1:MET:HE2	1:A:202:SER:HA	1.71	0.72
1:B:142:VAL:CG1	1:B:174:VAL:HG12	2.20	0.71
1:B:121:LEU:HD12	1:B:144:VAL:HG12	1.72	0.71
1:A:69:LEU:O	1:A:73:ILE:HG12	1.90	0.71
1:A:496:GLU:CD	1:A:496:GLU:H	1.99	0.70
1:B:142:VAL:HG13	1:B:174:VAL:HG12	1.73	0.70
1:B:557:ILE:HD11	1:B:653:THR:CG2	2.22	0.70
1:B:118:GLY:HA3	1:B:141:TYR:CZ	2.28	0.69
1:B:571:LEU:HD23	1:B:645:PRO:HA	1.75	0.69
1:B:435:VAL:HG12	1:B:436:LEU:N	2.07	0.68
1:B:365:TYR:CD2	1:B:623:THR:HG21	2.29	0.68
1:A:262:ARG:NH1	4:A:1891:HOH:O	2.26	0.68
1:A:25:GLU:O	1:A:29:ARG:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLN:HE21	1:A:18:ASN:ND2	1.93	0.67
1:A:370:ARG:HD2	1:A:434:ASP:OD1	1.94	0.66
1:A:494:LYS:HB3	1:A:496:GLU:OE2	1.95	0.66
1:A:2:GLU:HB2	1:A:202:SER:O	1.94	0.66
1:A:27:TYR:CE2	1:A:62:LYS:HG2	2.31	0.66
1:B:327:HIS:ND1	1:B:328:LYS:HE3	2.11	0.66
1:B:82:VAL:HG13	1:B:83:ALA:H	1.59	0.66
1:A:166:GLU:HB3	1:A:171:VAL:HG12	1.79	0.65
1:B:614:ALA:HB1	1:B:643:LEU:O	1.97	0.65
1:B:586:LYS:HG3	1:B:587:PRO:HD2	1.78	0.65
1:B:191:LYS:O	1:B:195:GLU:HG3	1.96	0.64
1:B:342:GLU:HG2	1:B:383:TYR:OH	1.97	0.64
1:A:502:TYR:CE2	1:A:641:THR:HG21	2.33	0.63
1:B:327:HIS:O	1:B:330:MET:HG3	1.97	0.63
1:A:623:THR:HG22	4:A:1697:HOH:O	1.98	0.63
1:A:37:ILE:HG21	1:A:234:LEU:HD12	1.79	0.63
1:A:365:TYR:CE2	1:A:623:THR:HG21	2.34	0.63
1:B:532:GLU:CD	1:B:532:GLU:H	2.07	0.62
1:A:226:GLU:HA	1:A:230:GLU:HG3	1.82	0.62
1:A:13:HIS:CE1	1:A:87:GLU:HG3	2.35	0.62
1:A:275:MET:HE3	1:A:278:TRP:HE3	1.63	0.62
1:B:274:GLU:H	1:B:274:GLU:CD	2.07	0.62
1:B:568:TYR:O	1:B:647:GLU:HA	2.00	0.62
1:B:250:MET:HE2	1:B:255:TYR:HA	1.81	0.61
1:B:144:VAL:HG23	1:B:149:PHE:HE1	1.65	0.61
1:B:431:ASN:ND2	1:B:433:ASN:H	1.97	0.61
1:A:305:ARG:HG3	1:A:305:ARG:HH11	1.66	0.61
1:B:474:ILE:HG23	1:B:633:PHE:CE2	2.36	0.61
1:B:37:ILE:HG21	1:B:234:LEU:HD12	1.83	0.60
1:A:435:VAL:HG12	1:A:436:LEU:N	2.17	0.60
1:B:617:TRP:HB2	1:B:641:THR:HG23	1.84	0.60
1:A:431:ASN:ND2	1:A:433:ASN:H	1.99	0.60
1:B:143:VAL:HG12	1:B:177:ILE:HD11	1.82	0.60
1:B:124:ARG:HD3	1:B:124:ARG:N	2.17	0.60
1:A:397:GLY:C	1:A:398:ARG:HG2	2.26	0.59
1:A:583:VAL:O	1:A:585:GLU:N	2.35	0.59
1:A:499:LEU:HD23	1:A:617:TRP:CG	2.38	0.59
1:B:435:VAL:HG12	1:B:436:LEU:H	1.69	0.58
1:A:250:MET:HE2	1:A:255:TYR:CA	2.34	0.58
1:A:250:MET:HE3	1:A:254:GLU:HG2	1.84	0.58
1:A:339:ASP:HB2	4:A:1847:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:GLU:O	1:B:589:GLU:HG3	2.02	0.58
1:A:444:HIS:O	1:A:445:GLU:HB2	2.02	0.58
1:A:548:LYS:O	1:A:558:ALA:HA	2.03	0.58
1:A:13:HIS:CG	1:A:87:GLU:HG3	2.38	0.58
1:A:581:HIS:HE1	4:A:1815:HOH:O	1.85	0.57
1:B:478:LEU:C	1:B:478:LEU:HD23	2.29	0.57
1:B:590:PHE:HD1	1:B:590:PHE:H	1.51	0.57
1:B:272:TYR:CZ	1:B:275:MET:HG2	2.39	0.57
1:B:275:MET:HE3	1:B:275:MET:O	2.04	0.57
1:B:470:ILE:HG12	1:B:631:TRP:CE2	2.39	0.57
1:B:234:LEU:HD11	1:B:238:PHE:CZ	2.39	0.57
1:B:478:LEU:HD11	1:B:624:LEU:HD11	1.87	0.57
1:B:534:GLY:HA2	1:B:543:ALA:H	1.68	0.57
1:A:124:ARG:HG2	1:A:145:ASP:OD2	2.05	0.57
1:A:599:ASP:OD2	1:A:602:GLY:HA3	2.05	0.57
1:B:124:ARG:O	1:B:271:SER:HA	2.05	0.57
1:B:32:ARG:HB3	1:B:33:PRO:HD3	1.86	0.56
1:B:522:MET:SD	1:B:527:VAL:CG1	2.93	0.56
1:A:431:ASN:C	1:A:431:ASN:HD22	2.12	0.56
1:A:614:ALA:HB2	1:A:644:PHE:CE2	2.40	0.56
1:B:420:ILE:O	1:B:486:ALA:HB1	2.05	0.56
1:A:121:LEU:HB3	1:A:124:ARG:HA	1.88	0.56
1:B:617:TRP:HB2	1:B:641:THR:CG2	2.35	0.56
1:A:144:VAL:HG13	1:A:145:ASP:N	2.20	0.56
1:A:615:LYS:HB3	1:A:643:LEU:HB2	1.86	0.56
1:B:191:LYS:HD2	1:B:192:LYS:N	2.21	0.56
1:B:596:GLU:HG2	1:B:605:LYS:NZ	2.21	0.56
1:B:587:PRO:O	1:B:588:GLU:HB2	2.04	0.56
1:A:515:ASN:H	1:A:515:ASN:HD22	1.54	0.55
1:B:303:LYS:HE3	1:B:304:TYR:CZ	2.41	0.55
1:A:61:ASN:C	1:A:63:PRO:HD3	2.32	0.55
1:B:371:ARG:HH11	1:B:371:ARG:CB	2.19	0.55
1:B:27:TYR:CZ	1:B:62:LYS:HG2	2.42	0.55
1:A:519:GLU:HB2	1:A:530:TRP:CE2	2.41	0.55
1:B:431:ASN:C	1:B:431:ASN:HD22	2.15	0.54
1:A:124:ARG:NH1	1:A:177:ILE:HD12	2.22	0.54
1:A:410:ALA:HA	1:A:422:GLU:O	2.07	0.54
1:A:180:LYS:HD2	1:A:196:TYR:CE1	2.42	0.54
1:A:307:PHE:CE1	1:B:287:LEU:HD22	2.39	0.54
1:B:29:ARG:O	1:B:219:GLY:HA3	2.07	0.54
1:A:38:LEU:HD23	1:A:72:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ARG:HB2	4:A:1785:HOH:O	2.07	0.54
1:B:370:ARG:NH2	1:B:636:GLN:OE1	2.40	0.54
1:B:226:GLU:HG3	1:B:230:GLU:OE2	2.06	0.54
1:B:541:ILE:HD12	1:B:541:ILE:N	2.22	0.54
1:A:144:VAL:HG22	1:A:148:HIS:CE1	2.43	0.54
1:B:365:TYR:HD2	1:B:623:THR:HG21	1.71	0.54
1:A:370:ARG:NH2	1:A:636:GLN:OE1	2.40	0.53
1:B:519:GLU:HB2	1:B:530:TRP:CE2	2.43	0.53
1:A:502:TYR:HE2	1:A:641:THR:HG21	1.71	0.53
1:A:234:LEU:HD11	1:A:238:PHE:CZ	2.43	0.53
1:A:295:LEU:HD23	1:A:300:LYS:HE3	1.89	0.53
1:A:627:SER:HB3	1:A:632:ASP:OD2	2.07	0.53
1:B:655:ARG:HE	1:B:657:ARG:CZ	2.22	0.53
1:B:144:VAL:O	1:B:176:PRO:HA	2.08	0.53
1:A:438:ARG:HH21	1:A:485:ARG:HH21	1.57	0.53
1:A:513:PHE:CD2	1:A:531:ARG:HD3	2.44	0.53
1:B:500:ASP:HA	1:B:503:ARG:HD3	1.92	0.52
1:A:83:ALA:H	1:A:105:LEU:HD23	1.73	0.52
1:B:615:LYS:NZ	4:B:1777:HOH:O	2.42	0.52
1:A:435:VAL:HG12	1:A:436:LEU:H	1.74	0.52
1:A:615:LYS:HE2	1:A:617:TRP:NE1	2.25	0.52
1:B:499:LEU:HD13	1:B:503:ARG:HD2	1.91	0.52
1:B:54:LEU:HD22	1:B:58:ILE:HD11	1.92	0.51
1:B:532:GLU:O	1:B:532:GLU:HG2	2.10	0.51
1:B:563:LEU:C	1:B:563:LEU:HD23	2.34	0.51
1:B:107:ASP:HA	1:B:110:ARG:NH1	2.24	0.51
1:B:328:LYS:HD3	1:B:331:LEU:HD12	1.93	0.51
1:B:470:ILE:HB	1:B:475:ARG:NH1	2.24	0.51
1:A:580:VAL:CG1	1:A:583:VAL:HB	2.40	0.51
1:B:250:MET:HE2	1:B:255:TYR:CA	2.40	0.51
1:A:503:ARG:NH1	1:A:587:PRO:HG2	2.16	0.51
1:B:2:GLU:HB3	1:B:201:THR:HG23	1.92	0.51
1:A:100:VAL:HG21	1:A:344:ARG:NH1	2.26	0.50
1:B:390:ILE:HD12	1:B:401:ILE:HG12	1.93	0.50
1:B:608:ILE:HG21	1:B:642:MET:HE3	1.94	0.50
1:A:118:GLY:HA3	1:A:141:TYR:CZ	2.46	0.50
1:B:180:LYS:HD3	1:B:196:TYR:CE1	2.46	0.50
1:B:234:LEU:HD11	1:B:238:PHE:CE2	2.47	0.50
1:A:567:PRO:HA	1:A:647:GLU:O	2.12	0.50
1:A:582:SER:HB3	1:A:601:TYR:HB2	1.93	0.50
1:B:411:THR:HB	1:B:422:GLU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:PHE:HD2	1:A:54:LEU:HD13	1.77	0.49
1:B:379:LYS:HA	1:B:382:ARG:HG2	1.93	0.49
1:B:435:VAL:CG1	1:B:436:LEU:N	2.74	0.49
1:A:579:ALA:HB1	1:A:581:HIS:CE1	2.48	0.49
1:A:628:GLU:CD	1:A:628:GLU:H	2.21	0.49
4:A:1641:HOH:O	1:B:284:GLN:HG2	2.12	0.49
1:A:513:PHE:HB3	1:A:518:TYR:OH	2.12	0.49
1:A:568:TYR:O	1:A:647:GLU:HA	2.12	0.49
1:B:413:LYS:HD2	1:B:421:PHE:CD1	2.47	0.49
1:B:371:ARG:HB3	1:B:371:ARG:NH1	2.27	0.49
1:B:390:ILE:HD11	1:B:522:MET:SD	2.52	0.49
1:A:234:LEU:HD11	1:A:238:PHE:CE2	2.48	0.49
1:A:73:ILE:HD11	1:A:80:ILE:HD11	1.95	0.49
1:B:487:ILE:O	1:B:488:LEU:HB2	2.12	0.49
1:B:54:LEU:HD22	1:B:58:ILE:CD1	2.43	0.49
1:B:502:TYR:HA	1:B:507:TYR:CD2	2.47	0.49
1:B:30:SER:C	1:B:33:PRO:HD2	2.38	0.48
1:A:151:SER:HA	1:A:309:ARG:NH2	2.27	0.48
1:A:398:ARG:HD3	4:A:1657:HOH:O	2.13	0.48
1:A:417:GLY:HA2	1:A:518:TYR:CE1	2.48	0.48
1:B:27:TYR:CE2	1:B:62:LYS:HG2	2.47	0.48
1:B:332:MET:HE1	1:B:402:MET:HE1	1.95	0.48
1:B:330:MET:CE	1:B:351:GLN:HG2	2.43	0.48
1:A:487:ILE:O	1:A:488:LEU:HB2	2.13	0.48
1:B:29:ARG:HH11	1:B:29:ARG:HG3	1.78	0.48
1:A:275:MET:HE3	1:A:275:MET:HA	1.94	0.48
1:B:345:LYS:NZ	1:B:349:LYS:HE2	2.28	0.48
1:B:121:LEU:CD1	1:B:144:VAL:HG12	2.43	0.48
1:B:564:LEU:HD12	1:B:564:LEU:N	2.28	0.48
1:B:202:SER:HB2	4:B:1687:HOH:O	2.13	0.48
1:B:586:LYS:HG3	1:B:587:PRO:CD	2.43	0.48
1:A:346:TYR:O	1:A:376:ASN:HB3	2.13	0.47
1:A:327:HIS:O	1:A:330:MET:HG3	2.14	0.47
1:A:571:LEU:HD23	1:A:645:PRO:HA	1.96	0.47
1:B:557:ILE:HD12	1:B:654:VAL:O	2.14	0.47
1:B:32:ARG:HD2	1:B:36:GLU:CD	2.39	0.47
1:B:570:ALA:O	1:B:646:ILE:HG22	2.14	0.47
1:A:37:ILE:CG2	1:A:234:LEU:HD12	2.43	0.47
1:A:515:ASN:H	1:A:515:ASN:ND2	2.11	0.47
1:B:250:MET:HE3	1:B:254:GLU:HG2	1.96	0.47
1:A:14:GLN:HE21	1:A:18:ASN:HD22	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:CD1	1:A:401:ILE:HG12	2.44	0.47
1:A:544:ARG:HH11	1:A:546:GLU:CD	2.23	0.47
1:B:371:ARG:CB	1:B:371:ARG:NH1	2.78	0.47
1:B:596:GLU:HG2	1:B:605:LYS:HZ1	1.79	0.47
1:A:502:TYR:O	1:A:504:LEU:O	2.33	0.47
1:B:18:ASN:HB3	1:B:23:PHE:CE1	2.49	0.47
1:B:146:ASP:O	1:B:150:MET:HG3	2.14	0.47
1:B:526:GLY:HA3	1:B:549:ILE:O	2.14	0.47
1:A:309:ARG:HG3	1:B:309:ARG:HB2	1.96	0.47
1:A:581:HIS:CE1	4:A:1815:HOH:O	2.63	0.47
1:B:641:THR:HG22	4:B:1700:HOH:O	2.15	0.47
1:A:275:MET:CE	1:A:278:TRP:HE3	2.28	0.47
1:B:401:ILE:HD13	1:B:527:VAL:HG11	1.97	0.47
1:A:332:MET:HE1	1:A:402:MET:HE1	1.97	0.46
1:B:272:TYR:HD1	1:B:274:GLU:OE2	1.98	0.46
1:B:95:LYS:HA	1:B:98:ARG:HD2	1.97	0.46
1:A:530:TRP:HA	1:A:545:VAL:O	2.14	0.46
1:B:262:ARG:HG2	1:B:262:ARG:O	2.16	0.46
1:B:419:SER:HB3	1:B:488:LEU:O	2.15	0.46
1:A:51:SER:HB2	1:A:87:GLU:HG2	1.97	0.46
1:A:150:MET:HE3	1:A:156:LYS:HD3	1.97	0.46
1:B:499:LEU:HD23	1:B:617:TRP:CG	2.49	0.46
1:A:431:ASN:ND2	1:A:431:ASN:C	2.74	0.46
1:A:437:PRO:HG3	4:A:1628:HOH:O	2.14	0.46
1:B:45:LYS:H	1:B:249:LEU:HD21	1.80	0.46
1:B:71:SER:O	1:B:75:ARG:HG2	2.16	0.46
1:B:289:VAL:O	1:B:293:GLU:HG2	2.16	0.46
1:B:128:PRO:HB2	1:B:167:ASP:OD2	2.16	0.46
1:B:32:ARG:HG3	1:B:32:ARG:HH11	1.81	0.46
1:B:328:LYS:HG3	1:B:394:ASP:HA	1.98	0.46
1:B:435:VAL:CG1	1:B:436:LEU:H	2.29	0.46
1:B:470:ILE:O	1:B:475:ARG:NH1	2.49	0.46
1:B:487:ILE:HG23	1:B:576:ILE:HG23	1.98	0.46
1:B:505:VAL:HG12	1:B:505:VAL:O	2.15	0.46
1:B:515:ASN:H	1:B:515:ASN:ND2	2.14	0.46
1:B:40:GLU:OE2	1:B:235:ARG:NH1	2.49	0.45
1:B:86:TYR:CE2	1:B:349:LYS:HG2	2.51	0.45
1:A:347:ILE:O	1:A:351:GLN:HG3	2.15	0.45
1:A:548:LYS:HD3	1:A:559:LYS:HD2	1.98	0.45
1:B:546:GLU:HB2	1:B:561:ARG:HB3	1.99	0.45
1:A:314:LYS:HB3	1:B:266:TYR:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:GLU:C	1:B:474:ILE:H	2.23	0.45
1:B:32:ARG:O	1:B:36:GLU:HG3	2.16	0.45
1:B:185:ILE:HA	1:B:186:PRO:HA	1.75	0.45
1:A:515:ASN:HD22	1:A:515:ASN:N	2.11	0.45
1:A:358:HIS:HE1	1:A:443:TYR:OH	1.99	0.45
1:B:66:LEU:O	1:B:70:ARG:HG3	2.16	0.45
1:A:502:TYR:HA	1:A:507:TYR:CD2	2.52	0.45
1:B:52:GLY:HA3	1:B:85:PHE:O	2.16	0.45
1:B:646:ILE:HG12	1:B:647:GLU:N	2.32	0.45
1:B:191:LYS:HE2	1:B:192:LYS:NZ	2.32	0.44
1:A:305:ARG:HH11	1:A:305:ARG:CG	2.30	0.44
1:B:339:ASP:O	1:B:341:PRO:HD3	2.17	0.44
1:B:14:GLN:HE21	1:B:18:ASN:ND2	2.15	0.44
1:B:515:ASN:ND2	1:B:516:GLN:HE21	2.16	0.44
1:A:74:LYS:HE3	1:A:74:LYS:HB2	1.89	0.44
1:A:166:GLU:CB	1:A:171:VAL:HG12	2.44	0.44
1:A:520:TYR:HA	1:A:528:LYS:O	2.18	0.44
1:A:595:PHE:CZ	1:A:608:ILE:HD12	2.52	0.44
1:B:275:MET:HE3	1:B:275:MET:CA	2.48	0.44
1:B:75:ARG:HD2	1:B:77:GLN:OE1	2.18	0.44
1:A:268:PRO:HB3	1:B:312:ILE:HG21	1.99	0.44
1:A:489:GLN:HG2	4:A:1691:HOH:O	2.17	0.44
1:B:371:ARG:HH11	1:B:371:ARG:HB2	1.80	0.44
1:B:420:ILE:HB	1:B:487:ILE:HB	1.99	0.44
1:A:44:MET:SD	1:A:249:LEU:HD21	2.58	0.44
1:A:99:LEU:HD21	1:A:136:GLU:HB2	2.00	0.44
1:A:185:ILE:HA	1:A:186:PRO:HA	1.65	0.44
1:A:499:LEU:HD13	1:A:499:LEU:C	2.42	0.44
1:B:494:LYS:HG3	1:B:510:LEU:HD11	2.00	0.44
1:B:495:PRO:HA	1:B:571:LEU:CD1	2.48	0.44
1:B:584:MET:HE3	1:B:584:MET:HA	2.00	0.44
1:B:185:ILE:HG23	1:B:233:TRP:CH2	2.53	0.43
1:A:9:GLY:O	1:A:212:HIS:HA	2.18	0.43
1:B:2:GLU:HB3	1:B:201:THR:CG2	2.48	0.43
1:B:27:TYR:CD2	1:B:62:LYS:HE3	2.53	0.43
1:B:499:LEU:HD23	1:B:617:TRP:HB3	2.00	0.43
1:A:609:GLU:OE1	1:A:657:ARG:HD2	2.19	0.43
1:B:322:GLU:H	1:B:322:GLU:CD	2.25	0.43
1:B:536:TYR:N	1:B:536:TYR:CD1	2.87	0.43
1:B:593:LYS:HE3	1:B:611:ASP:C	2.43	0.43
1:B:276:SER:HB2	1:B:310:GLY:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:TYR:O	1:B:367:PRO:HD3	2.18	0.43
1:A:61:ASN:C	1:A:62:LYS:HD2	2.43	0.43
1:A:95:LYS:HA	1:A:98:ARG:HD2	2.01	0.43
1:A:124:ARG:HD3	1:A:124:ARG:N	2.33	0.43
1:B:153:GLY:HA2	4:B:1774:HOH:O	2.18	0.43
1:B:389:LYS:HG3	1:B:391:LEU:HD22	2.01	0.43
1:A:155:SER:O	1:A:158:GLU:HG2	2.18	0.43
1:A:476:ARG:NH1	1:A:476:ARG:CB	2.82	0.43
1:B:515:ASN:H	1:B:515:ASN:HD22	1.67	0.43
1:B:370:ARG:HD2	1:B:434:ASP:OD1	2.18	0.43
1:B:495:PRO:HG3	1:B:571:LEU:HG	2.00	0.43
1:A:390:ILE:HD12	1:A:401:ILE:HG12	2.00	0.43
1:A:396:ASP:HA	1:B:263:GLY:HA2	2.01	0.43
1:A:476:ARG:NH1	1:A:476:ARG:HB2	2.34	0.43
1:A:59:GLU:O	1:A:63:PRO:HG3	2.19	0.43
1:A:189:PRO:HG2	1:A:192:LYS:HG2	2.01	0.43
1:B:166:GLU:CB	1:B:171:VAL:HG12	2.34	0.43
1:B:328:LYS:HD3	1:B:328:LYS:HA	1.80	0.43
1:B:413:LYS:HD2	1:B:421:PHE:CG	2.54	0.43
1:A:275:MET:HE3	1:A:278:TRP:CE3	2.49	0.42
1:A:390:ILE:CD1	1:A:401:ILE:HG23	2.49	0.42
1:A:411:THR:HB	1:A:422:GLU:HB3	2.00	0.42
1:B:396:ASP:OD1	1:B:396:ASP:C	2.61	0.42
1:B:531:ARG:HH11	1:B:531:ARG:HG3	1.84	0.42
1:A:494:LYS:HG3	1:A:510:LEU:HD11	2.01	0.42
1:B:10:ILE:HG13	1:B:48:VAL:HG23	2.00	0.42
1:B:275:MET:HE3	1:B:275:MET:C	2.43	0.42
1:B:499:LEU:HD13	1:B:499:LEU:C	2.45	0.42
1:A:367:PRO:HG3	1:A:636:GLN:OE1	2.19	0.42
1:B:45:LYS:H	1:B:249:LEU:CD2	2.33	0.42
1:A:217:LYS:HG2	1:A:221:TRP:CE3	2.54	0.42
1:B:523:ILE:HG13	1:B:524:GLU:H	1.83	0.42
1:B:595:PHE:CZ	1:B:608:ILE:HD12	2.55	0.42
1:A:73:ILE:HD13	1:A:78:LEU:HB2	2.02	0.42
1:A:156:LYS:HA	1:A:156:LYS:HD2	1.90	0.42
1:A:431:ASN:HD22	1:A:432:TYR:N	2.17	0.42
1:B:13:HIS:CG	1:B:14:GLN:N	2.87	0.42
1:B:201:THR:HG21	4:B:1736:HOH:O	2.20	0.42
1:B:347:ILE:HD12	1:B:347:ILE:HA	1.95	0.42
1:B:401:ILE:HG21	1:B:527:VAL:HG11	2.02	0.42
1:A:124:ARG:O	1:A:271:SER:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:LEU:CD1	1:B:624:LEU:HD11	2.49	0.42
1:B:532:GLU:O	1:B:532:GLU:CG	2.68	0.42
1:B:579:ALA:HB1	1:B:581:HIS:CE1	2.55	0.42
1:B:586:LYS:HE2	1:B:586:LYS:HB2	1.91	0.42
1:A:290:GLU:HG2	1:B:304:TYR:OH	2.20	0.42
1:A:496:GLU:CD	1:A:496:GLU:N	2.73	0.42
1:A:595:PHE:CE1	1:A:608:ILE:HD12	2.54	0.42
1:B:371:ARG:NH2	4:B:1801:HOH:O	2.44	0.42
1:B:367:PRO:O	1:B:371:ARG:HG3	2.19	0.41
1:A:622:LYS:HB2	4:A:1609:HOH:O	2.19	0.41
1:B:499:LEU:O	1:B:503:ARG:HG2	2.21	0.41
1:B:522:MET:SD	1:B:527:VAL:HG13	2.61	0.41
1:B:574:VAL:HG21	1:B:652:PHE:HZ	1.86	0.41
1:A:15:PRO:HD2	1:A:18:ASN:ND2	2.34	0.41
1:A:503:ARG:HH11	1:A:587:PRO:CG	2.21	0.41
1:A:534:GLY:HA2	1:A:543:ALA:H	1.84	0.41
1:B:344:ARG:O	1:B:347:ILE:HG22	2.20	0.41
1:A:217:LYS:HG2	1:A:221:TRP:CZ3	2.55	0.41
1:A:333:VAL:O	1:A:337:VAL:HB	2.20	0.41
1:B:321:PRO:HD2	1:B:439:ARG:NH2	2.34	0.41
1:B:346:TYR:O	1:B:376:ASN:HB3	2.20	0.41
1:B:544:ARG:HH12	1:B:546:GLU:CG	2.34	0.41
1:B:587:PRO:HA	1:B:618:LYS:O	2.20	0.41
1:A:29:ARG:HH11	1:A:29:ARG:HG3	1.86	0.41
1:A:279:SER:HB2	1:A:312:ILE:O	2.21	0.41
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.95	0.41
1:A:1:MET:HE2	1:A:202:SER:CA	2.43	0.41
1:A:39:GLU:HG2	1:A:39:GLU:O	2.20	0.41
1:A:269:ILE:HD11	1:B:128:PRO:HG3	2.02	0.41
1:A:494:LYS:CG	1:A:510:LEU:HD11	2.51	0.41
1:A:576:ILE:HD12	1:A:642:MET:HE1	2.02	0.41
1:B:292:VAL:HG13	1:B:301:PHE:CE1	2.56	0.41
1:B:431:ASN:ND2	1:B:431:ASN:C	2.75	0.41
1:B:544:ARG:NH1	1:B:546:GLU:CG	2.83	0.41
1:A:322:GLU:H	1:A:322:GLU:CD	2.28	0.41
1:B:118:GLY:HA3	1:B:141:TYR:CE1	2.56	0.41
1:B:303:LYS:HE3	1:B:304:TYR:CE1	2.56	0.40
1:B:362:GLY:HA2	1:B:366:LEU:HG	2.03	0.40
1:B:515:ASN:HD22	1:B:515:ASN:C	2.29	0.40
1:B:567:PRO:HA	1:B:647:GLU:O	2.21	0.40
1:B:29:ARG:HG3	1:B:29:ARG:NH1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PRO:HB3	1:A:354:ASP:OD2	2.22	0.40
1:A:250:MET:HE2	1:A:255:TYR:N	2.35	0.40
1:B:206:SER:HB3	1:B:259:PHE:CD2	2.56	0.40
1:A:278:TRP:CG	1:A:359:GLY:HA2	2.56	0.40
1:A:314:LYS:HG2	1:B:266:TYR:CD2	2.55	0.40
1:A:585:GLU:CD	1:A:618:LYS:HD2	2.47	0.40
1:B:15:PRO:HB3	1:B:354:ASP:OD2	2.21	0.40
1:B:520:TYR:CD1	1:B:520:TYR:C	2.99	0.40
1:A:62:LYS:N	1:A:63:PRO:HD3	2.36	0.40
1:A:135:ARG:HG2	4:A:1879:HOH:O	2.21	0.40
1:A:281:PRO:HD3	4:A:1809:HOH:O	2.22	0.40
1:A:435:VAL:CG1	1:A:436:LEU:N	2.84	0.40
1:B:574:VAL:HG21	1:B:652:PHE:CZ	2.56	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	632/659 (96%)	599 (95%)	30 (5%)	3 (0%)	24	37
1	B	632/659 (96%)	599 (95%)	27 (4%)	6 (1%)	14	22
All	All	1264/1318 (96%)	1198 (95%)	57 (4%)	9 (1%)	18	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	TYR
1	A	584	MET
1	B	507	TYR
1	B	524	GLU
1	A	488	LEU

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Mol	Chain	Res	Type
1	B	488	LEU
1	B	588	GLU
1	B	83	ALA
1	B	471	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	567/586 (97%)	549 (97%)	18 (3%)	34	56
1	B	567/586 (97%)	547 (96%)	20 (4%)	32	53
All	All	1134/1172 (97%)	1096 (97%)	38 (3%)	32	54

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	54	LEU
1	A	99	LEU
1	A	121	LEU
1	A	127	GLN
1	A	144	VAL
1	A	154	LEU
1	A	186	PRO
1	A	234	LEU
1	A	249	LEU
1	A	330	MET
1	A	337	VAL
1	A	431	ASN
1	A	496	GLU
1	A	515	ASN
1	A	524	GLU
1	A	623	THR
1	A	641	THR
1	B	16	LEU

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Mol	Chain	Res	Type
1	B	54	LEU
1	B	79	GLU
1	B	90	LEU
1	B	99	LEU
1	B	124	ARG
1	B	186	PRO
1	B	191	LYS
1	B	234	LEU
1	B	241	ILE
1	B	330	MET
1	B	427	ARG
1	B	431	ASN
1	B	475	ARG
1	B	515	ASN
1	B	527	VAL
1	B	532	GLU
1	B	590	PHE
1	B	596	GLU
1	B	623	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	18	ASN
1	A	127	GLN
1	A	148	HIS
1	A	248	ASN
1	A	358	HIS
1	A	376	ASN
1	A	431	ASN
1	A	501	ASN
1	A	515	ASN
1	A	581	HIS
1	B	5	ASN
1	B	14	GLN
1	B	28	ASN
1	B	248	ASN
1	B	315	ASN
1	B	376	ASN
1	B	431	ASN
1	B	501	ASN

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Mol	Chain	Res	Type
1	B	515	ASN
1	B	598	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
3	TRS	B	1604	-	7,7,7	1.45	0	9,9,9	2.50	4 (44%)

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
3	TRS	B	1604	-	-	6/9/9/9	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1604	TRS	C2-C-C1	-3.63	101.00	110.66
3	B	1604	TRS	O1-C1-C	-3.38	101.46	110.88
3	B	1604	TRS	C2-C-N	3.32	116.64	108.17
3	B	1604	TRS	C3-C-N	2.76	115.22	108.17

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1604	TRS	C3-C-C2-O2
3	B	1604	TRS	N-C-C2-O2
3	B	1604	TRS	C1-C-C3-O3
3	B	1604	TRS	C2-C-C3-O3
3	B	1604	TRS	N-C-C3-O3
3	B	1604	TRS	C1-C-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	636/659 (96%)	-0.05	24 (3%)	44 40	6, 25, 75, 125	0
1	B	636/659 (96%)	0.15	21 (3%)	49 45	11, 32, 80, 115	0
All	All	1272/1318 (96%)	0.05	45 (3%)	47 43	6, 29, 78, 125	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	VAL	5.0
1	A	1	MET	3.6
1	B	345	LYS	3.3
1	B	3	ARG	3.1
1	A	586	LYS	3.0
1	B	631	TRP	3.0
1	B	524	GLU	2.9
1	B	528	LYS	2.9
1	B	183	TYR	2.9
1	A	584	MET	2.8
1	B	626	GLN	2.8
1	B	446	VAL	2.8
1	B	302	GLU	2.8
1	A	503	ARG	2.7
1	B	473	GLU	2.7
1	A	494	LYS	2.6
1	A	398	ARG	2.6
1	B	477	GLU	2.6
1	B	561	ARG	2.6
1	A	293	GLU	2.6
1	B	476	ARG	2.6
1	A	644	PHE	2.5
1	A	649	GLU	2.5
1	A	591	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	564	LEU	2.4
1	A	563	LEU	2.4
1	B	305	ARG	2.4
1	B	569	LYS	2.4
1	A	303	LYS	2.3
1	A	566	LYS	2.2
1	B	624	LEU	2.2
1	A	561	ARG	2.2
1	A	469	GLN	2.2
1	A	499	LEU	2.2
1	A	594	GLU	2.2
1	B	445	GLU	2.2
1	B	537	ALA	2.1
1	B	523	ILE	2.1
1	B	532	GLU	2.1
1	A	528	LYS	2.1
1	A	170	GLU	2.1
1	B	293	GLU	2.1
1	A	569	LYS	2.1
1	A	203	ASP	2.1
1	A	300	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TRS	B	1604	8/8	0.85	0.11	34,34,34,34	0
2	CA	A	1601	1/1	0.88	0.08	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	1603	1/1	0.96	0.10	34,34,34,34	0
2	CA	B	1602	1/1	0.97	0.06	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.