



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 5HY7 / pdb_00005hy7
Title : SF3B10-SF3B130 from Chaetomium thermophilum
Authors : Ponce-Salvatierra, A.; Schmitzova, J.; Pena, V.
Deposited on : 2016-02-01
Resolution : 2.90 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
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

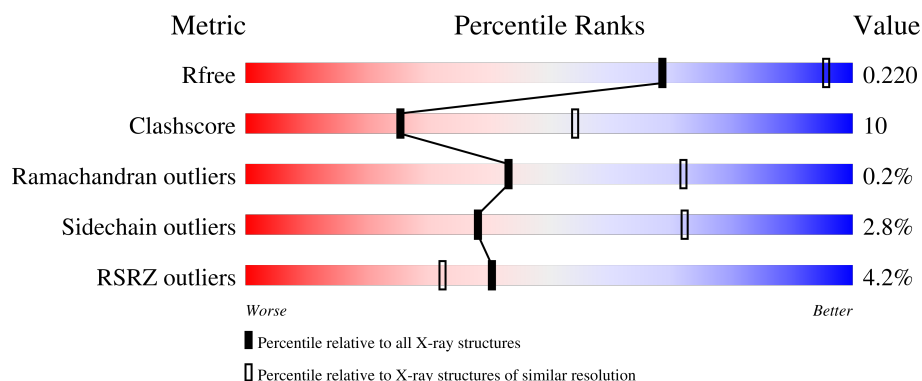
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	1213	3% 73% 22% ..
1	B	1213	5% 75% 20% ..
2	C	95	% 47% 9% 42%
2	D	95	% 45% 13% 42%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19210 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 Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1173	Total	C	N	O	S	0	0	0
			9164	5827	1556	1742	39			
1	B	1170	Total	C	N	O	S	0	0	0
			9149	5815	1555	1741	38			

- Molecule 2 is a protein called YSF3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	55	Total	C	N	O	S	0	0	0
			444	288	78	75	3			
2	C	55	Total	C	N	O	S	0	0	0
			444	288	78	75	3			

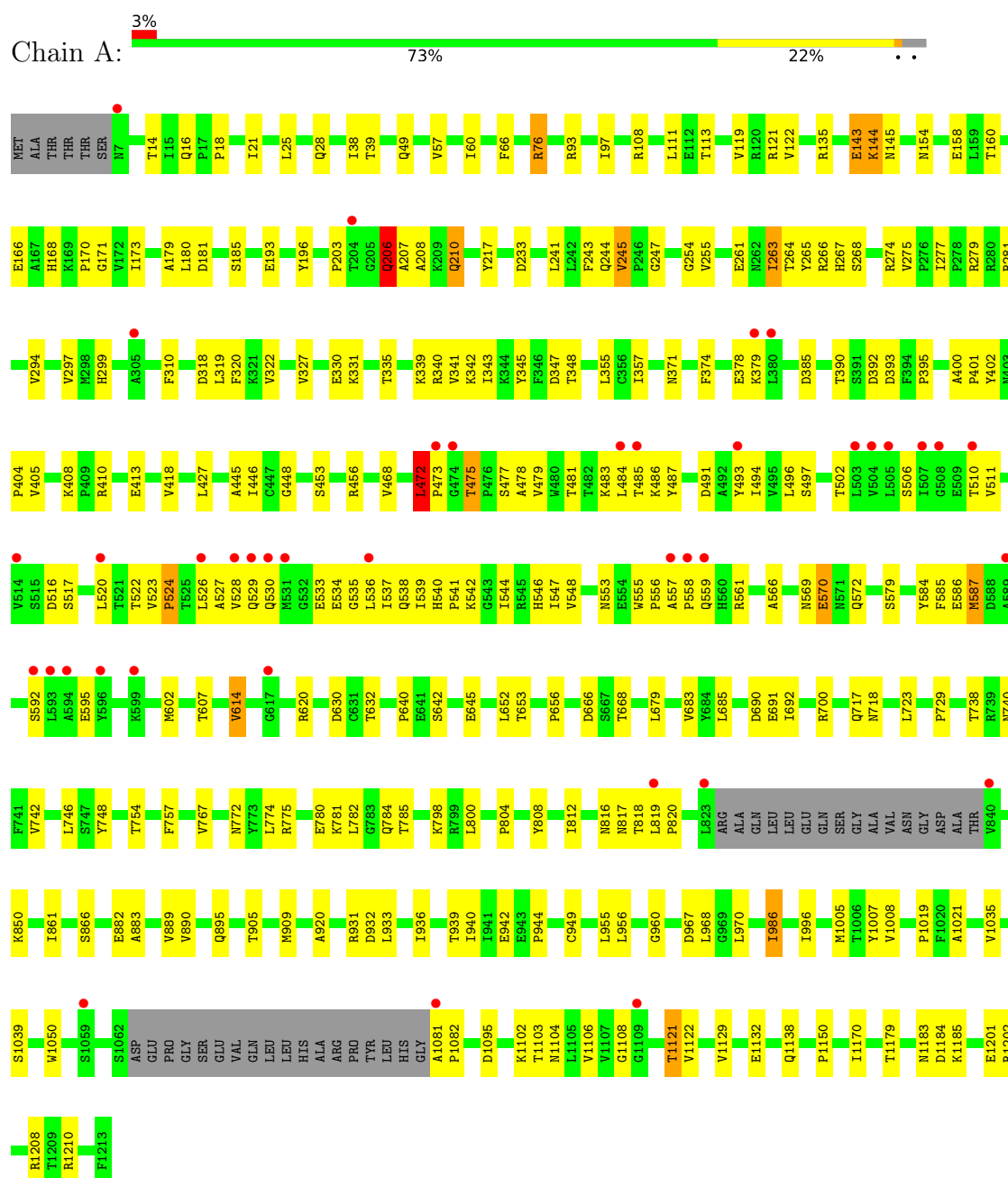
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		
3	B	5	Total	Ca	0	0
			5	5		

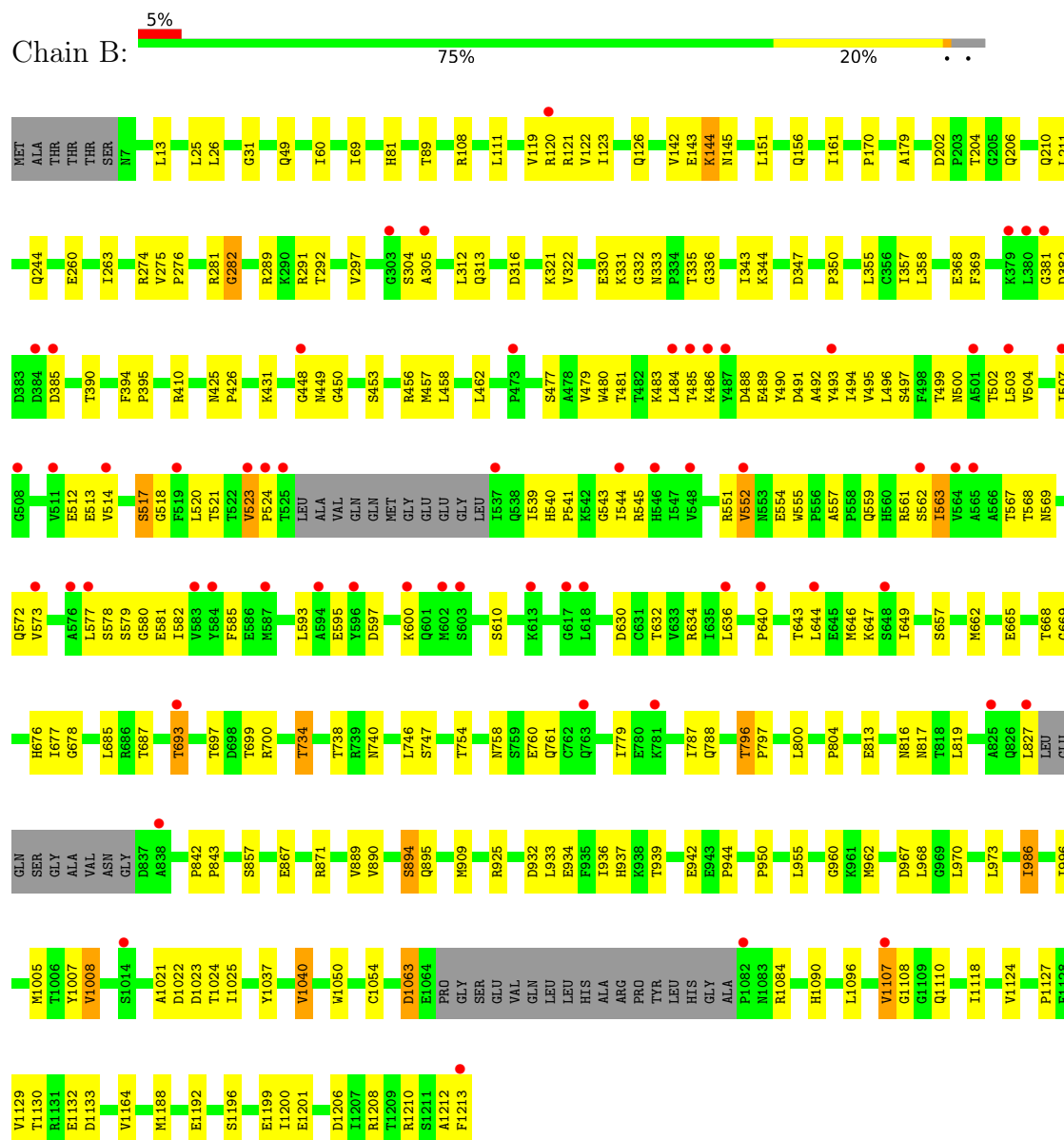
3 Residue-property plots

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

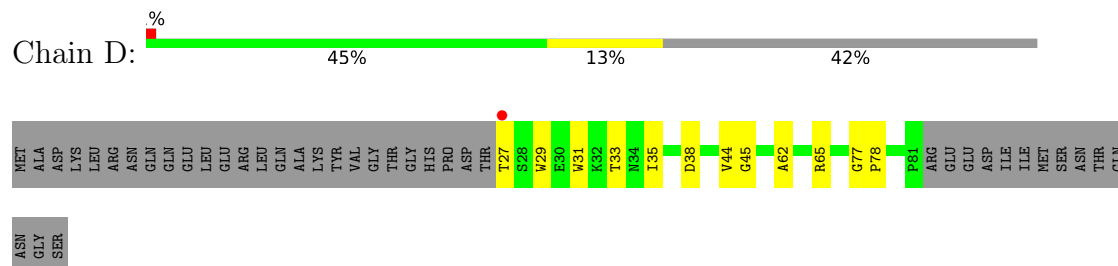
• Molecule 1: Putative pre-mRNA splicing protein



- Molecule 1: Putative pre-mRNA splicing protein

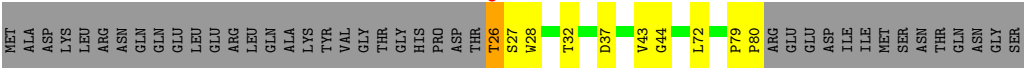


- Molecule 2: YSF3



- Molecule 2: YSF3





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	197.08Å 197.08Å 446.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.27 – 2.90 49.27 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-2.90) 100.0 (49.27-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.214 , 0.253 (Not available) , 0.220	Depositor DCC
R_{free} test set	7005 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	97.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19210	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0.24	0/9363	0.43	2/12721 (0.0%)
1	B	0.26	0/9347	0.44	0/12698
2	C	0.26	0/460	0.37	0/629
2	D	0.21	0/460	0.34	0/629
All	All	0.25	0/19630	0.43	2/26677 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	GLN	CA-C-N	5.33	131.29	121.70
1	A	206	GLN	C-N-CA	5.33	131.29	121.70

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	9164	0	9131	189	0
1	B	9149	0	9110	175	0
2	C	444	0	448	7	0
2	D	444	0	448	8	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
All	All	19210	0	19137	367	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 10.

All (367) 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:A:535:GLY:HA2	1:A:547:ILE:O	1.67	0.93
1:A:319:LEU:HB2	1:A:347:ASP:O	1.69	0.92
1:A:527:ALA:HB2	1:A:536:LEU:HD23	1.53	0.90
1:A:506:SER:H	1:A:511:VAL:HG21	1.38	0.87
1:B:1007:TYR:HB2	1:B:1021:ALA:HB3	1.61	0.81
1:B:122:VAL:O	1:B:145:ASN:ND2	2.14	0.80
1:B:939:THR:HG21	1:B:973:LEU:H	1.48	0.78
1:B:108:ARG:HD2	1:B:111:LEU:HB2	1.66	0.78
1:A:1007:TYR:HB2	1:A:1021:ALA:HB3	1.65	0.77
1:B:448:GLY:HA3	1:B:453:SER:HA	1.66	0.76
1:A:233:ASP:OD2	1:A:266:ARG:NH2	2.13	0.75
1:A:717:GLN:NE2	1:A:780:GLU:O	2.20	0.75
1:B:554:GLU:HB3	1:B:555:TRP:HB2	1.67	0.74
1:B:551:ARG:HB3	1:B:552:VAL:HA	1.67	0.74
1:B:687:THR:HG22	1:B:699:THR:HG22	1.70	0.74
1:A:1106:VAL:HG12	1:A:1108:GLY:H	1.54	0.72
1:B:479:VAL:HG22	1:B:496:LEU:HG	1.71	0.71
1:B:1037:TYR:OH	1:B:1063:ASP:OD2	2.07	0.71
1:A:486:LYS:HG3	1:A:530:GLN:HA	1.73	0.71
1:B:368:GLU:O	1:B:425:ASN:ND2	2.24	0.70
1:A:206:GLN:HA	1:A:207:ALA:HB3	1.73	0.69
1:A:448:GLY:HA3	1:A:453:SER:HA	1.75	0.69
1:B:481:THR:HG22	1:B:494:ILE:HG13	1.74	0.69
1:B:291:ARG:NH1	1:B:316:ASP:OD2	2.23	0.69
1:A:206:GLN:HB2	1:A:208:ALA:N	2.08	0.68
1:A:572:GLN:NE2	1:A:584:TYR:OH	2.25	0.68
1:A:530:GLN:NE2	1:A:570:GLU:OE1	2.26	0.68
1:A:1129:VAL:HG21	1:A:1210:ARG:HH22	1.57	0.67
1:B:563:ILE:HA	1:B:577:LEU:HA	1.77	0.67
1:A:729:PRO:HG2	1:A:746:LEU:HB2	1.78	0.66
1:A:808:TYR:OH	1:A:931:ARG:NH1	2.27	0.66
1:A:524:PRO:HD2	1:A:539:ILE:HB	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ASN:OD1	1:A:456:ARG:NH2	2.28	0.65
1:A:243:PHE:O	1:A:255:VAL:HA	1.96	0.65
1:A:1035:VAL:O	1:A:1102:LYS:NZ	2.28	0.65
1:B:761:GLN:N	1:B:761:GLN:OE1	2.29	0.65
1:B:490:TYR:HB2	1:B:758:ASN:HB3	1.79	0.64
1:A:49:GLN:HB2	1:A:60:ILE:HD11	1.79	0.64
1:B:554:GLU:OE1	1:B:554:GLU:N	2.30	0.64
1:B:322:VAL:HG22	1:B:343:ILE:HG12	1.79	0.64
1:B:636:LEU:HD13	1:B:646:MET:HA	1.78	0.64
1:B:544:ILE:O	1:B:555:TRP:N	2.31	0.63
1:A:122:VAL:O	1:A:145:ASN:ND2	2.31	0.63
1:A:586:GLU:OE2	1:A:620:ARG:NE	2.26	0.63
1:A:506:SER:N	1:A:511:VAL:HG21	2.12	0.63
1:B:119:VAL:HG11	2:C:44:GLY:HA3	1.81	0.63
1:A:18:PRO:HG3	1:A:1121:THR:HG23	1.81	0.63
1:A:385:ASP:OD2	1:A:410:ARG:NH1	2.29	0.63
1:B:513:GLU:HG3	1:B:514:VAL:H	1.64	0.63
1:B:996:ILE:HB	1:B:1008:VAL:HG22	1.79	0.62
1:B:1110:GLN:HG2	1:B:1127:PRO:HG2	1.81	0.62
1:A:378:GLU:HB2	1:A:379:LYS:HA	1.81	0.62
1:B:942:GLU:OE1	1:B:942:GLU:N	2.31	0.62
1:B:517:SER:OG	1:B:545:ARG:NE	2.31	0.62
1:A:717:GLN:HE21	1:A:781:LYS:HA	1.64	0.62
1:B:804:PRO:HD3	1:B:889:VAL:HG11	1.81	0.62
1:A:909:MET:HE3	1:A:944:PRO:HG2	1.80	0.62
1:B:49:GLN:HB2	1:B:60:ILE:HD11	1.82	0.62
1:A:410:ARG:NH1	1:A:413:GLU:OE2	2.28	0.62
1:B:1206:ASP:OD2	1:B:1210:ARG:NH1	2.33	0.61
1:B:456:ARG:NH1	1:B:788:GLN:OE1	2.33	0.61
1:A:890:VAL:HG21	1:A:955:LEU:HD13	1.82	0.61
1:A:97:ILE:HA	1:A:108:ARG:HA	1.82	0.61
1:B:1096:LEU:HB3	1:B:1118:ILE:HG13	1.82	0.61
1:B:344:LYS:NZ	1:B:382:ASP:O	2.31	0.61
1:A:942:GLU:OE1	1:A:942:GLU:N	2.30	0.61
1:B:523:VAL:HG12	1:B:524:PRO:HD3	1.83	0.61
1:B:263:ILE:HD12	1:B:343:ILE:HD11	1.82	0.61
1:A:556:PRO:HB2	1:A:558:PRO:HB3	1.83	0.60
1:B:202:ASP:OD1	1:B:204:THR:HG22	2.00	0.60
1:B:431:LYS:NZ	1:B:800:LEU:O	2.35	0.60
1:A:310:PHE:HB2	1:A:322:VAL:HB	1.84	0.60
1:B:450:GLY:H	1:B:796:THR:HG22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:PRO:CD	1:A:539:ILE:HB	2.32	0.60
1:B:121:ARG:NH1	2:C:37:ASP:OD1	2.31	0.60
1:A:569:ASN:HD21	1:A:614:VAL:HG22	1.67	0.59
1:B:1022:ASP:HB3	1:B:1084:ARG:HH11	1.67	0.59
1:B:204:THR:HG23	1:B:206:GLN:H	1.67	0.59
1:B:894:SER:HB2	1:B:895:GLN:HE21	1.67	0.59
1:B:1129:VAL:HG13	1:B:1130:THR:HG23	1.84	0.59
1:A:523:VAL:HB	1:A:524:PRO:HD3	1.85	0.59
1:B:211:LEU:HD23	2:C:72:LEU:HD22	1.85	0.59
1:B:1130:THR:OG1	1:B:1133:ASP:OD2	2.20	0.58
1:A:1005:MET:HE3	1:A:1050:TRP:HH2	1.67	0.58
1:A:485:THR:HG22	1:A:487:TYR:H	1.68	0.58
1:B:909:MET:HE3	1:B:944:PRO:HG2	1.86	0.58
1:A:331:LYS:H	1:A:331:LYS:HD2	1.68	0.57
1:B:313:GLN:NE2	1:B:350:PRO:O	2.36	0.57
1:B:665:GLU:HG3	1:B:734:THR:HG21	1.86	0.57
1:A:1095:ASP:OD2	1:A:1121:THR:OG1	2.18	0.57
1:B:274:ARG:HD3	1:B:395:PRO:O	2.05	0.57
1:A:804:PRO:HD3	1:A:889:VAL:HG11	1.86	0.57
1:B:1096:LEU:HD22	1:B:1118:ILE:HD11	1.86	0.57
1:B:449:ASN:HA	1:B:796:THR:HB	1.86	0.57
1:A:540:HIS:ND1	1:A:541:PRO:O	2.38	0.57
1:B:126:GLN:HG2	1:B:142:VAL:HG22	1.86	0.57
1:A:738:THR:OG1	1:A:740:ASN:OD1	2.21	0.57
1:A:524:PRO:HG3	1:A:566:ALA:HB3	1.87	0.56
1:A:544:ILE:HB	1:A:555:TRP:HB3	1.86	0.56
1:A:816:ASN:OD1	1:A:817:ASN:ND2	2.37	0.56
1:B:483:LYS:HD2	1:B:490:TYR:C	2.29	0.56
1:B:179:ALA:O	1:B:244:GLN:NE2	2.29	0.56
1:B:569:ASN:OD1	1:B:572:GLN:N	2.37	0.56
1:A:119:VAL:HG11	2:D:45:GLY:HA3	1.87	0.56
1:A:281:ARG:HB3	1:A:408:LYS:HD2	1.87	0.55
1:B:491:ASP:OD1	1:B:758:ASN:HB2	2.06	0.55
1:B:562:SER:O	1:B:578:SER:N	2.38	0.55
1:B:925:ARG:HB3	1:B:936:ILE:HD11	1.87	0.55
1:A:143:GLU:HB2	1:A:173:ILE:HD13	1.87	0.55
1:B:867:GLU:OE2	1:B:871:ARG:NH1	2.39	0.55
1:B:512:GLU:N	1:B:512:GLU:OE1	2.39	0.55
1:B:561:ARG:HH11	1:B:579:SER:HB3	1.70	0.55
1:B:144:LYS:HG3	1:B:170:PRO:HA	1.88	0.55
1:A:493:TYR:HA	1:A:506:SER:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LYS:HE2	1:A:491:ASP:HB3	1.88	0.54
1:A:816:ASN:OD1	1:A:817:ASN:N	2.40	0.54
1:B:477:SER:OG	1:B:497:SER:O	2.25	0.54
1:A:528:VAL:HG13	1:A:570:GLU:O	2.08	0.54
1:B:297:VAL:HG11	1:B:357:ILE:HG13	1.90	0.54
1:B:289:ARG:NH2	1:B:316:ASP:OD1	2.39	0.54
1:B:483:LYS:HG3	1:B:492:ALA:HB2	1.90	0.54
1:A:502:THR:OG1	1:A:520:LEU:O	2.23	0.54
1:B:545:ARG:HG2	1:B:554:GLU:O	2.08	0.54
1:A:542:LYS:HA	1:A:557:ALA:HB2	1.90	0.54
1:B:321:LYS:HZ1	1:B:381:GLY:H	1.56	0.54
1:B:746:LEU:HD21	1:B:779:ILE:HD11	1.89	0.54
2:D:29:TRP:O	2:D:33:THR:OG1	2.26	0.53
1:A:486:LYS:NZ	1:A:527:ALA:HB3	2.22	0.53
1:A:534:GLU:HB3	1:A:548:VAL:HG13	1.89	0.53
1:A:122:VAL:HA	1:A:143:GLU:O	2.09	0.53
1:A:539:ILE:HG23	1:A:544:ILE:HG12	1.91	0.53
1:A:559:GLN:CD	1:A:559:GLN:H	2.15	0.53
1:A:208:ALA:C	1:A:210:GLN:H	2.16	0.52
1:B:457:MET:O	1:B:788:GLN:HA	2.09	0.52
1:A:522:THR:HB	1:A:538:GLN:HE21	1.74	0.52
1:B:816:ASN:OD1	1:B:817:ASN:N	2.43	0.52
1:B:643:THR:HG22	1:B:644:LEU:HD12	1.91	0.52
1:A:427:LEU:HD11	1:A:445:ALA:HB1	1.91	0.52
1:A:108:ARG:HD2	1:A:111:LEU:HB2	1.92	0.51
1:A:166:GLU:OE1	1:A:168:HIS:NE2	2.43	0.51
2:D:29:TRP:NE1	2:D:77:GLY:O	2.41	0.51
1:B:297:VAL:CG2	1:B:355:LEU:HB2	2.41	0.51
1:B:483:LYS:HB2	1:B:491:ASP:HA	1.92	0.51
1:B:1188:MET:HE3	1:B:1192:GLU:HG3	1.91	0.51
1:A:524:PRO:HG2	1:A:539:ILE:HD12	1.92	0.51
1:A:685:LEU:HA	1:A:700:ARG:O	2.10	0.51
1:A:294:VAL:HG13	2:D:62:ALA:HB3	1.92	0.51
1:B:481:THR:HA	1:B:493:TYR:O	2.11	0.51
1:B:523:VAL:N	1:B:539:ILE:O	2.42	0.51
1:B:573:VAL:HB	1:B:585:PHE:HB2	1.91	0.51
1:B:120:ARG:HD2	1:B:123:ILE:HD12	1.93	0.51
1:A:569:ASN:OD1	1:A:570:GLU:N	2.43	0.51
1:B:69:ILE:HA	1:B:89:THR:HG22	1.92	0.51
1:A:668:THR:HB	1:A:1183:ASN:HD21	1.75	0.50
1:A:1129:VAL:HG21	1:A:1210:ARG:NH2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:THR:OG1	1:B:1025:ILE:N	2.44	0.50
1:B:552:VAL:HB	1:B:554:GLU:OE1	2.12	0.50
1:B:581:GLU:HA	1:B:600:LYS:O	2.11	0.50
1:A:486:LYS:CG	1:A:530:GLN:HA	2.41	0.50
1:A:481:THR:HG22	1:A:494:ILE:HG13	1.94	0.50
1:A:754:THR:HA	1:A:767:VAL:O	2.11	0.50
1:A:254:GLY:HA2	1:A:267:HIS:HD2	1.77	0.50
1:A:516:ASP:OD1	1:A:517:SER:N	2.45	0.50
1:A:895:GLN:NE2	1:B:970:LEU:HB2	2.27	0.49
2:C:28:TRP:O	2:C:32:THR:OG1	2.27	0.49
1:B:156:GLN:OE1	1:B:156:GLN:N	2.45	0.49
1:B:121:ARG:NE	1:B:143:GLU:OE2	2.45	0.49
1:A:135:ARG:NH2	1:A:185:SER:O	2.38	0.49
1:B:932:ASP:OD1	1:B:933:LEU:N	2.41	0.49
1:A:932:ASP:OD1	1:A:933:LEU:N	2.41	0.49
1:B:369:PHE:HA	1:B:425:ASN:HD22	1.78	0.49
1:A:700:ARG:HG2	1:A:1202:ARG:HG3	1.94	0.49
1:A:483:LYS:HG2	1:A:491:ASP:HB3	1.93	0.49
1:A:154:ASN:OD1	1:A:158:GLU:N	2.41	0.49
1:B:144:LYS:HD3	1:B:145:ASN:OD1	2.12	0.49
1:B:543:GLY:HA2	1:B:557:ALA:HB2	1.95	0.49
1:B:738:THR:OG1	1:B:740:ASN:OD1	2.26	0.49
1:A:472:LEU:H	1:A:473:PRO:HA	1.77	0.48
1:A:819:LEU:HD12	1:A:820:PRO:HD2	1.94	0.48
1:A:956:LEU:HD11	1:A:996:ILE:HD13	1.95	0.48
1:B:544:ILE:H	1:B:555:TRP:HE3	1.59	0.48
1:B:925:ARG:HG2	1:B:934:GLU:HB3	1.94	0.48
1:A:14:THR:O	1:A:1208:ARG:NH2	2.46	0.48
1:A:261:GLU:OE1	1:A:402:TYR:OH	2.19	0.48
1:A:487:TYR:HE2	1:A:533:GLU:HG2	1.77	0.48
1:A:883:ALA:O	1:A:905:THR:HA	2.13	0.48
1:A:1008:VAL:HA	1:A:1019:PRO:HA	1.95	0.48
1:B:634:ARG:HG2	1:B:649:ILE:HG13	1.94	0.48
1:B:330:GLU:OE1	1:B:330:GLU:N	2.41	0.48
1:A:936:ILE:HG21	1:B:970:LEU:HD21	1.95	0.48
1:A:207:ALA:N	1:A:210:GLN:OE1	2.47	0.48
1:A:475:THR:HG22	1:A:772:ASN:OD1	2.14	0.48
1:B:630:ASP:OD1	1:B:632:THR:OG1	2.21	0.48
1:B:281:ARG:HA	1:B:282:GLY:HA2	1.71	0.47
1:B:967:ASP:OD1	1:B:968:LEU:N	2.47	0.47
1:B:502:THR:HB	1:B:518:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:THR:HA	1:B:500:ASN:HA	1.40	0.47
1:A:206:GLN:HB2	1:A:207:ALA:C	2.40	0.47
1:A:245:VAL:HG21	1:A:265:TYR:HE1	1.78	0.47
1:B:1063:ASP:N	1:B:1063:ASP:OD1	2.46	0.47
1:B:210:GLN:OE1	1:B:210:GLN:N	2.48	0.47
1:B:263:ILE:HD13	1:B:312:LEU:HD12	1.96	0.47
1:B:1005:MET:HE3	1:B:1050:TRP:HH2	1.80	0.47
1:A:267:HIS:CG	1:A:268:SER:H	2.33	0.47
1:B:520:LEU:HG	1:B:521:THR:H	1.79	0.47
1:A:318:ASP:OD1	1:A:348:THR:OG1	2.29	0.46
1:A:342:LYS:HG2	1:A:390:THR:HG22	1.96	0.46
1:A:478:ALA:HB3	1:A:497:SER:HB3	1.97	0.46
1:A:630:ASP:OD1	1:A:632:THR:OG1	2.24	0.46
1:A:28:GLN:NE2	1:A:76:ARG:HH12	2.13	0.46
1:A:494:ILE:HD11	1:A:757:PHE:HE2	1.80	0.46
2:D:31:TRP:O	2:D:35:ILE:HG12	2.15	0.46
1:A:66:PHE:HB2	1:A:1150:PRO:HB3	1.98	0.46
1:B:489:GLU:HA	1:B:490:TYR:HA	1.59	0.46
1:B:520:LEU:HG	1:B:521:THR:N	2.30	0.46
1:B:490:TYR:CB	1:B:758:ASN:HB3	2.45	0.46
1:A:180:LEU:HD11	1:A:217:TYR:CZ	2.50	0.46
1:A:477:SER:N	1:A:497:SER:O	2.35	0.46
1:A:496:LEU:HD21	1:A:774:LEU:HD12	1.98	0.46
1:A:339:LYS:HG3	1:A:340:ARG:HG3	1.98	0.46
1:B:331:LYS:O	1:B:333:ASN:N	2.44	0.46
1:B:685:LEU:HA	1:B:700:ARG:O	2.15	0.46
1:A:320:PHE:CD1	1:A:345:TYR:HA	2.51	0.46
1:A:666:ASP:OD2	1:A:668:THR:OG1	2.34	0.45
1:B:585:PHE:HD2	1:B:593:LEU:HB3	1.80	0.45
1:B:1212:ALA:O	1:B:1213:PHE:HB2	2.15	0.45
1:A:297:VAL:CG2	1:A:355:LEU:HB2	2.46	0.45
1:A:486:LYS:HZ1	1:A:527:ALA:HB3	1.79	0.45
1:A:607:THR:OG1	1:A:656:PRO:O	2.33	0.45
1:A:264:THR:HG22	1:A:266:ARG:HB2	1.97	0.45
1:B:567:THR:HG21	1:B:610:SER:HA	1.99	0.45
1:A:181:ASP:O	1:A:247:GLY:HA3	2.16	0.45
1:A:487:TYR:CE2	1:A:533:GLU:HG2	2.52	0.45
1:A:905:THR:OG1	1:A:920:ALA:HB3	2.16	0.45
1:B:1090:HIS:CD2	1:B:1164:VAL:HB	2.52	0.45
1:A:967:ASP:OD1	1:A:968:LEU:N	2.50	0.45
1:A:592:SER:O	1:A:592:SER:OG	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:GLY:O	1:B:986:ILE:HG12	2.17	0.45
1:A:723:LEU:HD23	1:A:754:THR:HG21	1.98	0.44
1:B:747:SER:HB2	1:B:787:ILE:HD12	1.98	0.44
1:B:962:MET:HE2	1:B:962:MET:HB2	1.85	0.44
1:B:890:VAL:HG22	1:B:950:PRO:HG3	1.99	0.44
1:A:527:ALA:HA	1:A:536:LEU:HA	1.99	0.44
1:A:748:TYR:OH	1:A:775:ARG:HD3	2.18	0.44
1:B:385:ASP:OD2	1:B:410:ARG:NH2	2.50	0.44
1:A:16:GLN:HB2	1:A:1122:VAL:HB	1.98	0.44
1:B:551:ARG:HA	1:B:551:ARG:HD2	1.89	0.44
1:B:1107:VAL:HG23	1:B:1108:GLY:H	1.83	0.44
2:C:26:THR:HG22	2:C:27:SER:H	1.82	0.44
1:A:1005:MET:HE3	1:A:1050:TRP:CH2	2.50	0.44
2:D:44:VAL:HG13	2:D:65:ARG:HG3	1.98	0.44
1:B:275:VAL:HG11	1:B:343:ILE:HG13	2.00	0.44
1:A:484:LEU:HD11	1:A:493:TYR:HE1	1.83	0.44
1:A:587:MET:HB3	1:A:587:MET:HE3	1.71	0.44
1:B:500:ASN:O	1:B:521:THR:N	2.51	0.44
1:B:1196:SER:OG	1:B:1199:GLU:HB2	2.18	0.44
1:B:541:PRO:HD2	1:B:543:GLY:O	2.18	0.43
1:A:25:LEU:HB3	1:A:38:ILE:HG22	2.00	0.43
1:A:483:LYS:HG2	1:A:491:ASP:CB	2.48	0.43
1:A:652:LEU:HD13	1:A:679:LEU:HD21	2.00	0.43
1:B:151:LEU:HD23	1:B:161:ILE:CD1	2.48	0.43
1:B:585:PHE:HB3	1:B:593:LEU:HG	2.00	0.43
1:B:936:ILE:HG22	1:B:937:HIS:ND1	2.33	0.43
1:A:690:ASP:O	1:A:691:GLU:HB2	2.18	0.43
1:A:327:VAL:O	1:A:335:THR:HG22	2.19	0.43
1:A:475:THR:O	1:A:475:THR:OG1	2.32	0.43
1:A:798:LYS:HB2	1:A:812:ILE:HG13	2.01	0.43
1:A:882:GLU:HG2	1:A:905:THR:HB	2.01	0.43
1:A:1103:THR:OG1	1:A:1104:ASN:N	2.52	0.43
1:B:577:LEU:HD11	1:B:581:GLU:N	2.34	0.43
1:A:546:HIS:HB3	1:A:553:ASN:O	2.19	0.43
1:A:558:PRO:HD2	1:A:559:GLN:NE2	2.33	0.43
1:A:572:GLN:NE2	1:A:620:ARG:HB2	2.33	0.43
1:B:540:HIS:ND1	1:B:543:GLY:O	2.51	0.43
1:A:1179:THR:HG22	1:A:1201:GLU:OE1	2.19	0.43
1:A:171:GLY:HA2	1:A:196:TYR:CE2	2.53	0.43
1:B:894:SER:OG	1:B:967:ASP:OD1	2.27	0.43
1:A:642:SER:HB2	1:A:645:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:GLY:O	1:A:986:ILE:HG12	2.19	0.43
1:B:304:SER:HA	1:B:305:ALA:HA	1.84	0.43
1:B:13:LEU:HD22	1:B:1208:ARG:NH1	2.33	0.43
1:B:26:LEU:HD11	1:B:358:LEU:HD12	2.00	0.43
1:B:485:THR:HG22	1:B:486:LYS:HG3	2.00	0.43
1:B:677:ILE:HB	1:B:685:LEU:HB2	2.00	0.43
1:A:203:PRO:O	2:D:78:PRO:HB2	2.19	0.42
1:A:208:ALA:C	1:A:210:GLN:N	2.77	0.42
1:A:949:CYS:O	1:A:956:LEU:HB2	2.19	0.42
1:A:491:ASP:N	1:A:491:ASP:OD1	2.51	0.42
1:A:263:ILE:HD11	1:A:277:ILE:HD11	2.02	0.42
1:B:369:PHE:HB3	1:B:426:PRO:HG3	2.02	0.42
1:B:595:GLU:HB3	1:B:597:ASP:OD1	2.20	0.42
1:B:1132:GLU:OE1	1:B:1132:GLU:N	2.39	0.42
1:A:144:LYS:HG2	1:A:170:PRO:HA	2.01	0.42
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.87	0.42
1:A:390:THR:C	1:A:392:ASP:H	2.27	0.42
1:A:1184:ASP:OD1	1:A:1185:LYS:N	2.52	0.42
1:B:480:TRP:HE3	1:B:495:VAL:HG23	1.85	0.42
1:A:93:ARG:HG2	1:A:113:THR:HA	2.01	0.42
1:A:322:VAL:HA	1:A:342:LYS:O	2.20	0.42
1:A:526:LEU:HD23	1:A:527:ALA:C	2.44	0.42
1:A:1132:GLU:OE1	1:A:1132:GLU:N	2.47	0.42
1:B:453:SER:HB3	1:B:797:PRO:HD3	2.02	0.42
1:B:462:LEU:N	1:B:787:ILE:HD11	2.35	0.42
1:B:480:TRP:HB2	1:B:495:VAL:HG22	2.01	0.42
1:B:335:THR:OG1	1:B:336:GLY:N	2.52	0.42
1:A:275:VAL:HG11	1:A:343:ILE:HG13	2.02	0.42
1:A:279:ARG:HE	1:A:404:PRO:HB3	1.84	0.42
1:A:341:VAL:O	1:A:390:THR:HA	2.18	0.42
1:A:970:LEU:HB2	1:B:895:GLN:OE1	2.19	0.42
1:B:126:GLN:NE2	2:C:43:VAL:HG12	2.34	0.42
1:B:260:GLU:HA	1:B:292:THR:HG22	2.02	0.42
1:A:861:ILE:HD11	1:A:933:LEU:HG	2.01	0.42
1:B:31:GLY:O	1:B:81:HIS:ND1	2.46	0.42
1:B:483:LYS:HG2	1:B:484:LEU:H	1.85	0.42
1:B:539:ILE:HG22	1:B:540:HIS:HB2	2.02	0.42
1:B:541:PRO:HG3	1:B:545:ARG:HG3	2.01	0.42
1:B:640:PRO:O	1:B:643:THR:OG1	2.38	0.42
1:A:179:ALA:O	1:A:244:GLN:NE2	2.49	0.41
1:B:662:MET:HE2	1:B:676:HIS:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:GLN:C	1:B:561:ARG:H	2.28	0.41
1:B:657:SER:N	1:B:678:GLY:O	2.49	0.41
1:B:813:GLU:O	1:B:857:SER:OG	2.36	0.41
1:B:842:PRO:HA	1:B:843:PRO:HD3	1.91	0.41
1:A:446:ILE:HD13	1:A:800:LEU:HB2	2.01	0.41
1:A:818:THR:HG22	1:A:850:LYS:HD3	2.02	0.41
1:A:330:GLU:CD	1:A:330:GLU:H	2.28	0.41
1:A:585:PHE:CE2	1:A:595:GLU:HB2	2.55	0.41
1:A:378:GLU:CB	1:A:379:LYS:HA	2.49	0.41
1:B:25:LEU:HD12	1:B:25:LEU:HA	1.91	0.41
1:A:254:GLY:HA2	1:A:267:HIS:CD2	2.54	0.41
1:A:297:VAL:HG11	1:A:357:ILE:HG13	2.03	0.41
1:A:374:PHE:O	1:A:418:VAL:HG22	2.20	0.41
1:B:577:LEU:HD12	1:B:580:GLY:H	1.86	0.41
1:B:668:THR:OG1	1:B:669:GLY:N	2.53	0.41
1:A:21:ILE:HG23	1:A:39:THR:HB	2.02	0.41
1:A:970:LEU:HD21	1:B:936:ILE:HG21	2.01	0.41
1:B:276:PRO:HG3	1:B:394:PHE:CE1	2.56	0.41
1:B:483:LYS:NZ	1:B:491:ASP:O	2.53	0.41
1:A:143:GLU:HA	1:A:144:LYS:HA	1.83	0.41
1:A:173:ILE:O	1:A:193:GLU:HA	2.21	0.41
1:A:486:LYS:HG3	1:A:529:GLN:O	2.21	0.41
1:A:526:LEU:HD23	1:A:527:ALA:N	2.36	0.41
1:A:1081:ALA:N	1:A:1082:PRO:HD3	2.35	0.41
1:B:492:ALA:HA	1:B:507:ILE:HG13	2.02	0.41
1:B:1022:ASP:OD1	1:B:1023:ASP:N	2.51	0.41
1:B:1196:SER:O	1:B:1200:ILE:HG12	2.20	0.41
1:A:154:ASN:HB3	1:A:160:THR:CG2	2.51	0.41
1:A:274:ARG:HG2	1:A:395:PRO:O	2.21	0.41
1:A:299:HIS:HB2	1:A:357:ILE:HD12	2.03	0.41
1:A:1138:GLN:HA	1:A:1170:ILE:HD12	2.03	0.41
1:B:540:HIS:CE1	1:B:563:ILE:HG12	2.55	0.41
1:B:939:THR:HG21	1:B:973:LEU:N	2.26	0.41
1:A:121:ARG:HD3	2:D:38:ASP:OD1	2.22	0.40
1:A:679:LEU:HD12	1:A:683:VAL:HB	2.04	0.40
1:A:816:ASN:CG	1:A:817:ASN:HD22	2.27	0.40
1:B:1007:TYR:CE2	1:B:1054:CYS:HB2	2.56	0.40
1:A:400:ALA:HA	1:A:401:PRO:HD3	1.98	0.40
1:A:620:ARG:NH1	1:A:640:PRO:HD3	2.37	0.40
1:B:647:LYS:HE3	1:B:693:THR:O	2.21	0.40
1:B:760:GLU:O	1:B:760:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:TYR:OH	1:B:1040:VAL:HG12	2.21	0.40
1:A:539:ILE:HG12	1:A:544:ILE:HG12	2.01	0.40
1:B:504:VAL:O	1:B:512:GLU:HB3	2.22	0.40
1:B:540:HIS:CG	1:B:563:ILE:HG12	2.56	0.40
1:A:561:ARG:HG2	1:A:579:SER:HB3	2.04	0.40
1:B:890:VAL:HG21	1:B:955:LEU:HD13	2.03	0.40
2:C:79:PRO:HA	2:C:80:PRO:HD3	1.93	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	1167/1213 (96%)	1101 (94%)	63 (5%)	3 (0%)	36	65
1	B	1162/1213 (96%)	1082 (93%)	77 (7%)	3 (0%)	36	65
2	C	53/95 (56%)	53 (100%)	0	0	100	100
2	D	53/95 (56%)	52 (98%)	1 (2%)	0	100	100
All	All	2435/2616 (93%)	2288 (94%)	141 (6%)	6 (0%)	43	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	PRO
1	A	570	GLU
1	B	332	GLY
1	B	144	LYS
1	A	472	LEU
1	B	282	GLY

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	1010/1041 (97%)	978 (97%)	32 (3%)	34	68
1	B	1009/1041 (97%)	983 (97%)	26 (3%)	40	73
2	C	50/85 (59%)	49 (98%)	1 (2%)	48	78
2	D	50/85 (59%)	49 (98%)	1 (2%)	48	78
All	All	2119/2252 (94%)	2059 (97%)	60 (3%)	38	72

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	76	ARG
1	A	143	GLU
1	A	144	LYS
1	A	206	GLN
1	A	210	GLN
1	A	245	VAL
1	A	263	ILE
1	A	393	ASP
1	A	405	VAL
1	A	468	VAL
1	A	472	LEU
1	A	475	THR
1	A	479	VAL
1	A	510	THR
1	A	537	ILE
1	A	587	MET
1	A	602	MET
1	A	614	VAL
1	A	653	THR
1	A	692	ILE
1	A	718	ASN
1	A	742	VAL
1	A	782	LEU

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Mol	Chain	Res	Type
1	A	784	GLN
1	A	785	THR
1	A	866	SER
1	A	939	THR
1	A	940	ILE
1	A	986	ILE
1	A	1039	SER
1	A	1121	THR
2	D	27	THR
1	B	347	ASP
1	B	390	THR
1	B	458	LEU
1	B	488	ASP
1	B	503	LEU
1	B	517	SER
1	B	523	VAL
1	B	552	VAL
1	B	563	ILE
1	B	568	THR
1	B	582	ILE
1	B	693	THR
1	B	697	THR
1	B	734	THR
1	B	754	THR
1	B	796	THR
1	B	819	LEU
1	B	827	LEU
1	B	894	SER
1	B	986	ILE
1	B	1008	VAL
1	B	1040	VAL
1	B	1063	ASP
1	B	1107	VAL
1	B	1124	VAL
1	B	1201	GLU
2	C	26	THR

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

Mol	Chain	Res	Type
1	A	226	HIS
1	A	299	HIS

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Mol	Chain	Res	Type
1	A	333	ASN
1	A	425	ASN
1	A	530	GLN
1	A	572	GLN
1	A	717	GLN
1	A	718	ASN
1	A	869	GLN
1	A	895	GLN
1	A	1003	HIS
1	A	1183	ASN
2	D	46	HIS
2	D	57	GLN
1	B	28	GLN
1	B	36	GLN
1	B	58	ASN
1	B	225	ASN
1	B	500	ASN
1	B	601	GLN
1	B	770	HIS
1	B	1083	ASN
2	C	45	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1173/1213 (96%)	0.14	40 (3%) 48 39	50, 88, 145, 190	0
1	B	1170/1213 (96%)	0.09	61 (5%) 33 26	48, 82, 154, 207	0
2	C	55/95 (57%)	-0.21	1 (1%) 67 59	53, 68, 99, 124	0
2	D	55/95 (57%)	-0.05	1 (1%) 67 59	63, 84, 111, 125	0
All	All	2453/2616 (93%)	0.11	103 (4%) 40 32	48, 84, 150, 207	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	840	VAL	6.1
1	B	380	LEU	5.7
1	B	537	ILE	5.7
1	A	593	LEU	5.5
1	B	485	THR	4.8
1	A	823	LEU	4.8
1	B	486	LYS	4.6
1	A	558	PRO	4.5
1	A	380	LEU	4.5
1	A	592	SER	4.3
1	A	528	VAL	4.3
1	A	493	TYR	3.9
1	B	573	VAL	3.7
1	A	819	LEU	3.6
1	B	827	LEU	3.6
1	B	594	ALA	3.4
1	B	484	LEU	3.4
1	B	525	THR	3.4
1	A	305	ALA	3.4
1	B	524	PRO	3.3
1	A	507	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	825	ALA	3.2
1	B	763	GLN	3.2
1	A	514	VAL	3.2
1	B	548	VAL	3.2
1	B	564	VAL	3.1
1	A	531	MET	3.1
1	A	589	ALA	3.0
1	A	557	ALA	3.0
1	B	1213	PHE	3.0
1	A	529	GLN	3.0
1	B	1082	PRO	2.9
1	B	584	TYR	2.9
1	A	1081	ALA	2.9
1	A	7	ASN	2.9
1	A	485	THR	2.9
1	B	303	GLY	2.8
1	B	385	ASP	2.8
1	B	600	LYS	2.7
2	C	26	THR	2.7
1	B	602	MET	2.7
1	B	511	VAL	2.7
1	B	552	VAL	2.7
1	A	536	LEU	2.7
1	A	204	THR	2.6
1	A	520	LEU	2.6
1	B	587	MET	2.6
1	B	781	LYS	2.6
1	B	644	LEU	2.6
1	B	508	GLY	2.5
1	B	603	SER	2.5
1	B	544	ILE	2.5
1	B	583	VAL	2.5
1	A	559	GLN	2.5
1	B	565	ALA	2.5
1	A	1059	SER	2.5
1	B	514	VAL	2.5
1	A	505	LEU	2.4
1	B	448	GLY	2.4
1	A	379	LYS	2.4
1	A	473	PRO	2.4
1	B	507	ILE	2.4
1	B	613	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1107	VAL	2.4
1	B	1014	SER	2.4
1	B	577	LEU	2.4
1	B	519	PHE	2.4
1	B	305	ALA	2.4
1	B	838	ALA	2.4
1	A	596	TYR	2.4
1	A	510	THR	2.3
1	B	618	LEU	2.3
1	B	473	PRO	2.3
1	B	523	VAL	2.3
1	A	508	GLY	2.3
1	B	381	GLY	2.3
1	A	530	GLN	2.3
1	B	562	SER	2.3
1	A	594	ALA	2.3
1	B	120	ARG	2.2
1	B	493	TYR	2.2
1	A	1109	GLY	2.2
1	B	617	GLY	2.2
1	B	384	ASP	2.2
1	B	546	HIS	2.2
1	A	526	LEU	2.2
1	B	501	ALA	2.2
1	B	379	LYS	2.1
2	D	27	THR	2.1
1	B	636	LEU	2.1
1	B	487	TYR	2.1
1	A	504	VAL	2.1
1	B	640	PRO	2.1
1	A	599	LYS	2.1
1	B	503	LEU	2.1
1	A	617	GLY	2.1
1	B	648	SER	2.0
1	A	484	LEU	2.0
1	B	693	THR	2.0
1	B	596	TYR	2.0
1	A	503	LEU	2.0
1	A	474	GLY	2.0
1	B	576	ALA	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	CA	B	1304	1/1	0.10	0.39	313,313,313,313	0
3	CA	A	1303	1/1	0.36	0.28	191,191,191,191	0
3	CA	B	1302	1/1	0.75	0.28	124,124,124,124	0
3	CA	A	1304	1/1	0.82	0.24	138,138,138,138	0
3	CA	A	1302	1/1	0.88	0.09	134,134,134,134	0
3	CA	B	1305	1/1	0.88	0.26	140,140,140,140	0
3	CA	B	1303	1/1	0.94	0.16	123,123,123,123	0
3	CA	A	1301	1/1	0.96	0.09	88,88,88,88	0
3	CA	B	1301	1/1	0.96	0.05	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.