



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 06:55 PM EDT

PDB ID : 5VAF
Title : Crystal structure of accessory secretion protein 1
Authors : Chen, Y.; Rapoport, T.A.; Jeffrey, P.D.
Deposited on : 2017-03-25
Resolution : 2.77 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
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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

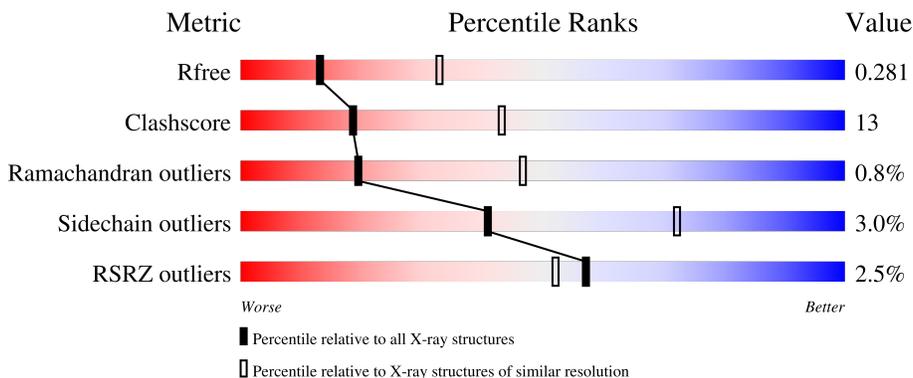
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	533	 68% 26% . .
1	B	533	 4% 68% 26% . .
1	C	533	 5% 63% 31% . .
1	D	533	 % 64% 31% . .

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 17260 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 Accessory Sec system protein Asp1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	510	4292	2776	705	802	9	0	0	0
1	B	515	4329	2802	710	808	9	0	0	0
1	C	516	4338	2807	712	810	9	0	0	0
1	D	511	4298	2779	706	804	9	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	527	VAL	-	expression tag	UNP Q9AET9
A	528	ASP	-	expression tag	UNP Q9AET9
A	529	LYS	-	expression tag	UNP Q9AET9
A	530	LEU	-	expression tag	UNP Q9AET9
A	531	VAL	-	expression tag	UNP Q9AET9
A	532	PRO	-	expression tag	UNP Q9AET9
A	533	ARG	-	expression tag	UNP Q9AET9
B	527	VAL	-	expression tag	UNP Q9AET9
B	528	ASP	-	expression tag	UNP Q9AET9
B	529	LYS	-	expression tag	UNP Q9AET9
B	530	LEU	-	expression tag	UNP Q9AET9
B	531	VAL	-	expression tag	UNP Q9AET9
B	532	PRO	-	expression tag	UNP Q9AET9
B	533	ARG	-	expression tag	UNP Q9AET9
C	527	VAL	-	expression tag	UNP Q9AET9
C	528	ASP	-	expression tag	UNP Q9AET9
C	529	LYS	-	expression tag	UNP Q9AET9
C	530	LEU	-	expression tag	UNP Q9AET9
C	531	VAL	-	expression tag	UNP Q9AET9
C	532	PRO	-	expression tag	UNP Q9AET9
C	533	ARG	-	expression tag	UNP Q9AET9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	527	VAL	-	expression tag	UNP Q9AET9
D	528	ASP	-	expression tag	UNP Q9AET9
D	529	LYS	-	expression tag	UNP Q9AET9
D	530	LEU	-	expression tag	UNP Q9AET9
D	531	VAL	-	expression tag	UNP Q9AET9
D	532	PRO	-	expression tag	UNP Q9AET9
D	533	ARG	-	expression tag	UNP Q9AET9

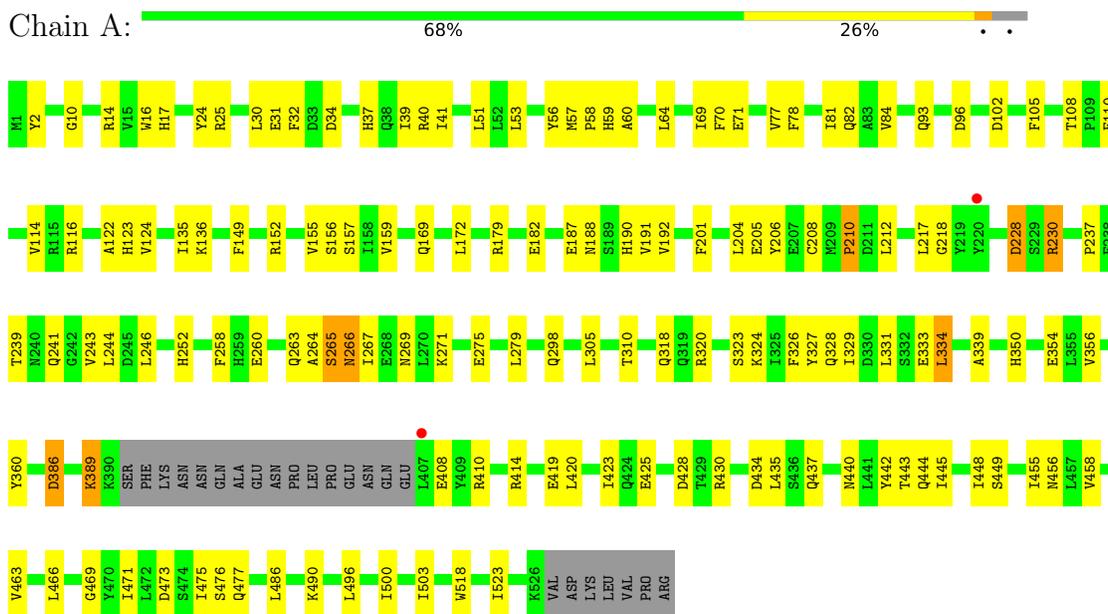
- Molecule 2 is water.

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

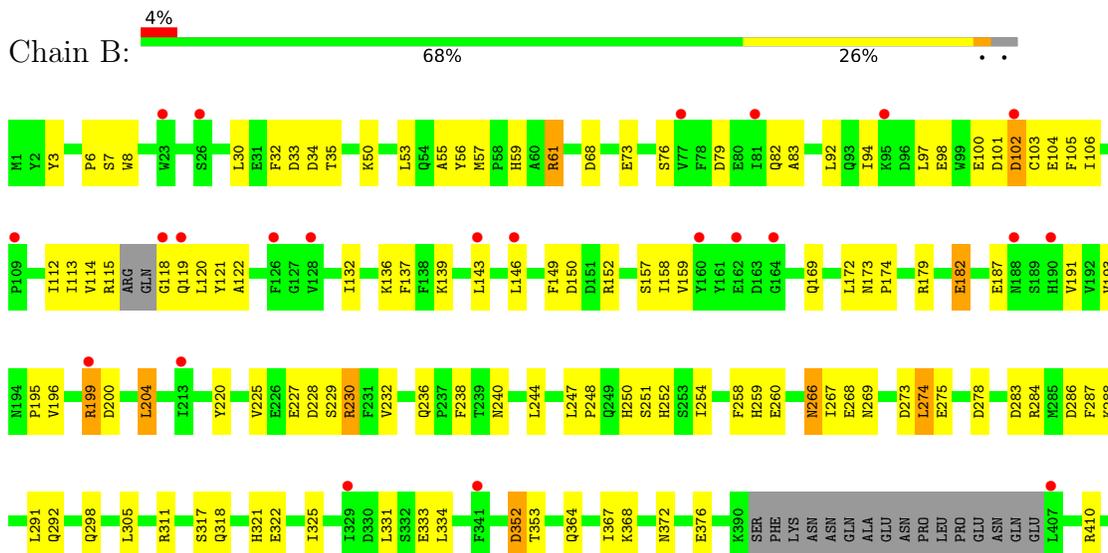
3 Residue-property plots [i](#)

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

- Molecule 1: Accessory Sec system protein Asp1

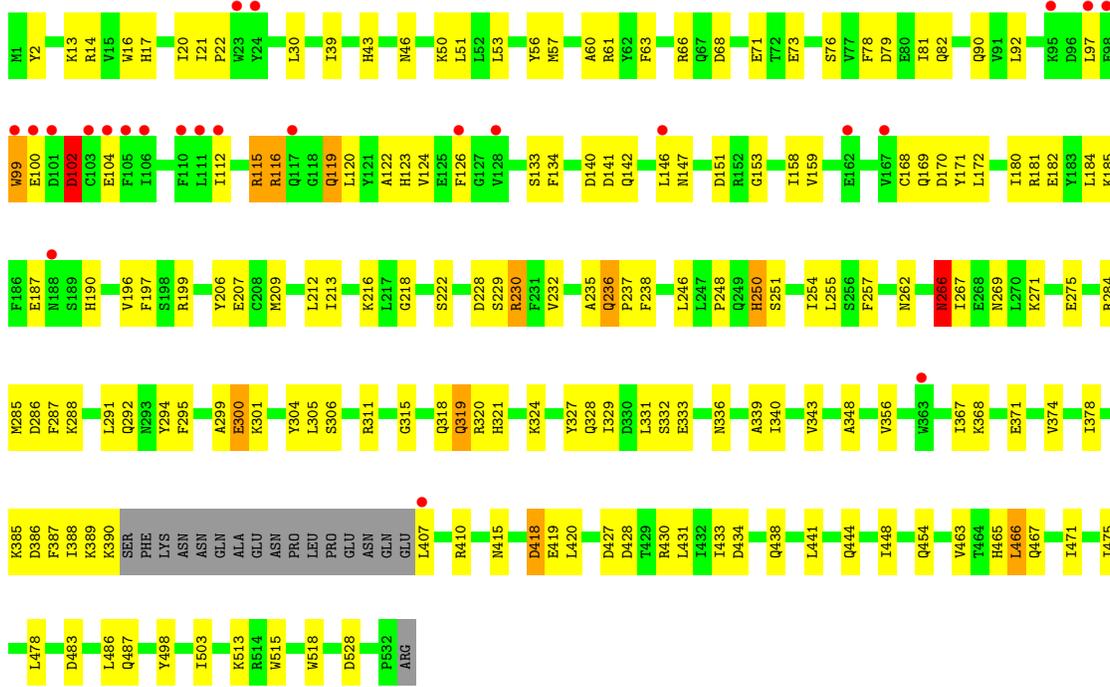


- Molecule 1: Accessory Sec system protein Asp1

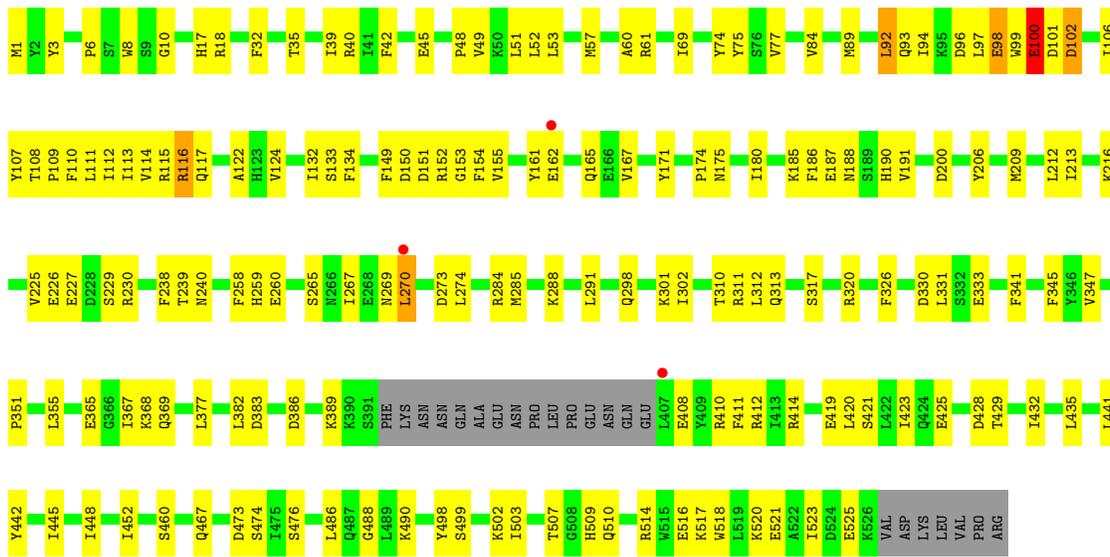




● Molecule 1: Accessory Sec system protein Asp1



● Molecule 1: Accessory Sec system protein Asp1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.50Å 99.90Å 179.07Å 100.66° 90.07° 95.78°	Depositor
Resolution (Å)	97.65 – 2.77 97.65 – 2.77	Depositor EDS
% Data completeness (in resolution range)	92.7 (97.65-2.77) 92.7 (97.65-2.77)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.208 , 0.282 0.208 , 0.281	Depositor DCC
R_{free} test set	3344 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtrriage
Anisotropy	0.613	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17260	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7622e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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	0.48	0/4400	0.62	0/5962
1	B	0.48	0/4437	0.61	1/6012 (0.0%)
1	C	0.51	0/4447	0.64	2/6027 (0.0%)
1	D	0.51	0/4406	0.64	3/5970 (0.1%)
All	All	0.49	0/17690	0.63	6/23971 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	ASP	CB-CG-OD1	6.77	124.39	118.30
1	D	107	TYR	C-N-CA	6.70	138.44	121.70
1	D	97	LEU	N-CA-C	6.45	128.41	111.00
1	D	312	LEU	CA-CB-CG	5.47	127.88	115.30
1	C	528	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	530	LEU	CA-CB-CG	5.32	127.53	115.30

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	4292	0	4164	101	0
1	B	4329	0	4208	110	1
1	C	4338	0	4217	126	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4298	0	4169	116	0
2	A	2	0	0	1	0
2	B	1	0	0	0	0
All	All	17260	0	16758	448	1

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 13.

All (448) 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:C:236:GLN:HG3	1:C:237:PRO:HD2	1.49	0.94
1:D:414:ARG:NH1	1:D:425:GLU:OE1	2.09	0.85
1:A:108:THR:HG22	1:A:110:PHE:H	1.43	0.83
1:C:257:PHE:HD1	1:C:262:ASN:HD22	1.27	0.82
1:B:100:GLU:HB2	1:B:103:CYS:SG	2.19	0.82
1:C:385:LYS:O	1:C:388:ILE:HD12	1.78	0.82
1:B:532:PRO:HB2	1:B:533:ARG:HG2	1.61	0.81
1:D:45:GLU:OE2	1:D:509:HIS:HA	1.84	0.78
1:A:389:LYS:HE3	1:A:408:GLU:HB3	1.65	0.77
1:D:108:THR:HG22	1:D:110:PHE:H	1.50	0.76
1:A:51:LEU:HG	1:A:53:LEU:HD21	1.67	0.76
1:A:500:ILE:O	1:A:503:ILE:HG22	1.86	0.75
1:D:185:LYS:HE2	1:D:187:GLU:HB3	1.69	0.75
1:D:389:LYS:HD2	1:D:408:GLU:OE1	1.86	0.75
1:D:100:GLU:CB	1:D:116:ARG:HH12	2.00	0.74
1:C:14:ARG:HH12	1:C:169:GLN:HE22	1.30	0.74
1:D:265:SER:O	1:D:267:ILE:CD1	2.35	0.74
1:D:112:ILE:HB	1:D:124:VAL:HB	1.70	0.73
1:C:17:HIS:HE1	1:C:20:ILE:HD11	1.53	0.72
1:B:50:LYS:NZ	1:B:220:TYR:OH	2.19	0.72
1:B:56:TYR:HH	1:B:157:SER:HG	1.37	0.72
1:C:14:ARG:HH12	1:C:169:GLN:NE2	1.86	0.72
1:A:159:VAL:HG22	1:A:169:GLN:HG3	1.72	0.71
1:B:92:LEU:HD21	1:B:132:ILE:HB	1.73	0.71
1:B:244:LEU:HA	1:B:247:LEU:HD12	1.72	0.71
1:A:190:HIS:HB2	1:A:206:TYR:O	1.91	0.71
1:D:288:LYS:HG3	1:D:302:ILE:HG22	1.73	0.70
1:D:412:ARG:NH2	1:D:425:GLU:OE2	2.25	0.70
1:D:100:GLU:HB3	1:D:116:ARG:HH12	1.58	0.69
1:D:6:PRO:HB3	1:D:35:THR:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ARG:NH2	1:D:175:ASN:HB3	2.07	0.68
1:D:150:ASP:OD1	1:D:152:ARG:HD2	1.93	0.68
1:A:57:MET:HB2	1:A:60:ALA:HB2	1.75	0.68
1:C:168:CYS:SG	1:C:181:ARG:NH1	2.65	0.68
1:C:235:ALA:HB2	1:C:255:LEU:HG	1.76	0.68
1:D:448:ILE:HD13	1:D:502:LYS:HB3	1.75	0.68
1:C:159:VAL:HG22	1:C:169:GLN:HG3	1.75	0.68
1:B:114:VAL:CG1	1:B:122:ALA:HB3	2.24	0.68
1:B:120:LEU:HD12	1:B:121:TYR:N	2.09	0.68
1:C:199:ARG:HH21	1:D:175:ASN:HB3	1.59	0.68
1:A:40:ARG:NH2	1:A:419:GLU:OE1	2.27	0.66
1:D:100:GLU:HA	1:D:100:GLU:OE1	1.93	0.66
1:C:134:PHE:HB2	1:C:146:LEU:HD11	1.76	0.66
1:D:102:ASP:OD2	1:D:102:ASP:N	2.14	0.65
1:B:53:LEU:HB3	1:B:57:MET:HE3	1.77	0.65
1:A:78:PHE:HA	1:A:81:ILE:HD12	1.77	0.65
1:D:330:ASP:CG	1:D:333:GLU:HG3	2.17	0.65
1:C:248:PRO:O	1:C:251:SER:OG	2.14	0.65
1:D:84:VAL:HG23	1:D:174:PRO:HG3	1.78	0.65
1:B:317:SER:OG	1:B:430:ARG:NH1	2.26	0.64
1:B:434:ASP:OD1	1:B:439:PRO:HA	1.97	0.64
1:D:419:GLU:OE1	1:D:442:TYR:OH	2.14	0.64
1:A:208:CYS:HB2	1:A:210:PRO:HD2	1.79	0.64
1:D:507:THR:HG22	1:D:510:GLN:HG2	1.79	0.64
1:A:51:LEU:HG	1:A:53:LEU:CD2	2.28	0.63
1:C:232:VAL:HG22	1:C:254:ILE:HD12	1.81	0.63
1:A:56:TYR:HH	1:A:157:SER:HG	1.47	0.62
1:C:57:MET:HB2	1:C:60:ALA:HB2	1.80	0.62
1:C:16:TRP:HH2	1:C:182:GLU:OE2	1.82	0.62
1:C:271:LYS:O	1:C:275:GLU:HG3	1.99	0.62
1:A:449:SER:HA	1:A:503:ILE:HD11	1.80	0.62
1:B:187:GLU:OE1	1:B:187:GLU:N	2.32	0.62
1:B:325:ILE:HG23	1:B:431:LEU:HD23	1.82	0.62
1:C:299:ALA:O	1:C:300:GLU:HB2	1.99	0.62
1:D:265:SER:O	1:D:267:ILE:HD13	1.99	0.61
1:D:93:GLN:N	1:D:96:ASP:OD1	2.33	0.61
1:D:162:GLU:HG2	1:D:167:VAL:HG21	1.82	0.61
1:A:14:ARG:HD2	1:A:16:TRP:CH2	2.36	0.61
1:A:419:GLU:OE2	1:A:442:TYR:OH	2.17	0.61
1:B:318:GLN:HG3	1:B:430:ARG:HH12	1.66	0.61
1:B:115:ARG:HH12	1:B:118:GLY:N	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:MET:HE3	1:C:212:LEU:HB3	1.81	0.60
1:A:182:GLU:HB2	1:A:191:VAL:HG22	1.82	0.60
1:D:133:SER:HG	1:D:134:PHE:HD1	1.48	0.60
1:D:100:GLU:CB	1:D:116:ARG:NH1	2.63	0.60
1:C:78:PHE:HE1	1:C:213:ILE:HD11	1.65	0.60
1:B:6:PRO:HB3	1:B:35:THR:HG21	1.83	0.60
1:A:102:ASP:OD1	1:A:102:ASP:N	2.35	0.60
1:B:115:ARG:NH1	1:B:119:GLN:H	2.00	0.60
1:A:327:TYR:CE2	1:A:329:ILE:HD11	2.37	0.60
1:B:115:ARG:HD3	1:B:119:GLN:HG2	1.84	0.60
1:B:159:VAL:HB	1:B:169:GLN:HG3	1.82	0.60
1:A:328:GLN:NE2	1:A:443:THR:HG21	2.17	0.59
1:A:333:GLU:HG3	1:A:334:LEU:O	2.02	0.59
1:B:7:SER:OG	1:B:236:GLN:NE2	2.36	0.59
1:A:16:TRP:HH2	1:A:182:GLU:OE2	1.86	0.59
1:A:449:SER:HA	1:A:503:ILE:CD1	2.32	0.59
1:B:248:PRO:O	1:B:251:SER:OG	2.19	0.59
1:A:237:PRO:HA	1:A:265:SER:HB2	1.85	0.58
1:B:259:HIS:HB3	1:B:284:ARG:HD2	1.85	0.58
1:D:51:LEU:HB3	1:D:53:LEU:HD21	1.86	0.58
1:B:467:GLN:HA	1:B:498:TYR:CD2	2.38	0.58
1:B:94:ILE:HD12	1:B:94:ILE:H	1.69	0.58
1:C:182:GLU:HG2	1:C:184:LEU:HD23	1.85	0.58
1:B:322:GLU:OE1	1:B:322:GLU:N	2.33	0.58
1:D:517:LYS:O	1:D:521:GLU:HG2	2.04	0.58
1:A:56:TYR:CZ	1:A:58:PRO:HG3	2.39	0.57
1:B:288:LYS:O	1:B:292:GLN:HG3	2.04	0.57
1:A:263:GLN:HG3	1:A:264:ALA:N	2.20	0.57
1:C:218:GLY:HA3	1:C:246:LEU:HD22	1.85	0.57
1:B:120:LEU:HD12	1:B:121:TYR:H	1.69	0.57
1:C:483:ASP:O	1:C:487:GLN:HB3	2.04	0.57
1:A:275:GLU:HG2	1:A:298:GLN:NE2	2.20	0.57
1:B:372:ASN:O	1:B:376:GLU:HG3	2.05	0.57
1:C:327:TYR:CE2	1:C:329:ILE:HD11	2.39	0.57
1:A:51:LEU:CG	1:A:53:LEU:HD21	2.34	0.57
1:A:204:LEU:HD13	1:B:196:VAL:HG11	1.87	0.57
1:A:339:ALA:HB2	1:A:475:ILE:HD13	1.87	0.57
1:B:3:TYR:CZ	1:B:225:VAL:HG22	2.41	0.56
1:C:112:ILE:HG12	1:C:126:PHE:HZ	1.70	0.56
1:B:83:ALA:HB2	1:B:179:ARG:CZ	2.35	0.56
1:A:30:LEU:HD21	1:A:419:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:GLU:O	1:D:525:GLU:HG2	2.06	0.56
1:D:61:ARG:NH1	1:D:74:TYR:OH	2.39	0.56
1:C:78:PHE:HA	1:C:81:ILE:HB	1.87	0.56
1:D:226:GLU:OE2	1:D:226:GLU:N	2.37	0.56
1:D:355:LEU:O	1:D:411:PHE:HA	2.05	0.56
1:D:117:GLN:HA	1:D:117:GLN:OE1	2.06	0.55
1:D:265:SER:O	1:D:267:ILE:HD12	2.05	0.55
1:B:275:GLU:HA	1:B:298:GLN:OE1	2.06	0.55
1:C:78:PHE:O	1:C:82:GLN:HG3	2.06	0.55
1:C:185:LYS:HD2	1:C:187:GLU:HB2	1.87	0.55
1:B:158:ILE:HD11	1:B:172:LEU:HD11	1.88	0.55
1:C:51:LEU:HD13	1:C:53:LEU:HD21	1.89	0.55
1:C:315:GLY:HA2	1:C:427:ASP:OD1	2.07	0.55
1:C:324:LYS:HE3	1:C:356:VAL:HG21	1.89	0.55
1:C:294:TYR:O	1:C:295:PHE:HB2	2.06	0.55
1:B:286:ASP:OD1	1:B:286:ASP:N	2.39	0.55
1:C:444:GLN:HA	1:C:454:GLN:OE1	2.07	0.55
1:B:528:ASP:OD2	1:B:528:ASP:N	2.36	0.54
1:D:326:PHE:HB2	1:D:429:THR:HG21	1.88	0.54
1:C:112:ILE:HB	1:C:124:VAL:HB	1.89	0.54
1:A:239:THR:N	1:A:269:ASN:OD1	2.41	0.54
1:A:37:HIS:O	1:A:41:ILE:HG13	2.08	0.54
1:B:252:HIS:CE1	1:B:532:PRO:HG3	2.42	0.54
1:B:115:ARG:C	1:B:115:ARG:HD2	2.29	0.54
1:A:310:THR:HG22	1:A:445:ILE:HG23	1.89	0.54
1:B:305:LEU:HD13	1:B:518:TRP:CH2	2.43	0.54
1:B:463:VAL:HG12	1:B:471:ILE:HD11	1.90	0.54
1:C:61:ARG:NE	1:C:151:ASP:OD1	2.33	0.54
1:C:190:HIS:HB2	1:C:206:TYR:O	2.08	0.54
1:C:367:ILE:HD11	1:C:415:ASN:HB2	1.90	0.54
1:C:306:SER:HA	1:C:441:LEU:HD21	1.90	0.53
1:A:82:GLN:HA	1:A:179:ARG:HG3	1.89	0.53
1:B:228:ASP:HB3	1:B:533:ARG:HD2	1.89	0.53
1:B:278:ASP:HA	1:B:526:LYS:NZ	2.23	0.53
1:D:285:MET:HE3	1:D:460:SER:HA	1.90	0.53
1:C:331:LEU:C	1:C:333:GLU:H	2.12	0.53
1:A:93:GLN:HB2	1:A:96:ASP:OD2	2.09	0.53
1:B:473:ASP:H	1:B:477:GLN:NE2	2.07	0.53
1:A:455:ILE:O	1:A:456:ASN:ND2	2.42	0.53
1:B:448:ILE:HG23	1:B:502:LYS:HB3	1.91	0.53
1:A:305:LEU:HD13	1:A:518:TRP:HH2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ILE:O	1:B:113:ILE:HD12	2.10	0.52
1:C:112:ILE:HG12	1:C:126:PHE:CZ	2.44	0.52
1:D:108:THR:HB	1:D:111:LEU:H	1.73	0.52
1:C:2:TYR:CE1	1:C:230:ARG:HD2	2.44	0.52
1:C:266:ASN:HB2	1:C:269:ASN:HB3	1.91	0.52
1:D:106:ILE:HG13	1:D:115:ARG:HH21	1.75	0.52
1:B:34:ASP:HB3	1:B:258:PHE:HB2	1.92	0.52
1:C:236:GLN:CG	1:C:237:PRO:HD2	2.32	0.52
1:D:341:PHE:HB2	1:D:377:LEU:HD22	1.91	0.52
1:C:305:LEU:HD13	1:C:518:TRP:CZ3	2.45	0.52
1:D:285:MET:CE	1:D:460:SER:HA	2.39	0.52
1:D:92:LEU:HD13	1:D:153:GLY:O	2.09	0.52
1:D:259:HIS:ND1	1:D:284:ARG:HG3	2.24	0.52
1:A:463:VAL:HG12	1:A:471:ILE:HD11	1.92	0.51
1:C:431:LEU:HD22	1:C:486:LEU:HD13	1.91	0.51
1:A:122:ALA:HA	1:A:136:LYS:O	2.10	0.51
1:C:63:PHE:HA	1:C:66:ARG:NH2	2.26	0.51
1:B:106:ILE:HD13	1:B:113:ILE:HD11	1.92	0.51
1:B:115:ARG:NH1	1:B:119:GLN:N	2.59	0.51
1:D:200:ASP:O	1:D:216:LYS:NZ	2.44	0.51
1:B:101:ASP:OD1	1:B:102:ASP:OD2	2.28	0.51
1:A:123:HIS:HB2	1:A:136:LYS:HB2	1.93	0.51
1:A:473:ASP:HB2	1:A:477:GLN:OE1	2.10	0.51
1:C:17:HIS:CE1	1:C:20:ILE:HD11	2.39	0.51
1:C:53:LEU:HB3	1:C:57:MET:HE3	1.92	0.51
1:A:324:LYS:HE3	1:A:356:VAL:HG21	1.94	0.50
1:B:92:LEU:HD23	1:B:92:LEU:H	1.76	0.50
1:D:419:GLU:O	1:D:423:ILE:HG13	2.12	0.50
1:A:84:VAL:HG11	1:A:152:ARG:NH1	2.26	0.50
1:A:155:VAL:HG23	1:A:172:LEU:HD12	1.94	0.50
1:C:339:ALA:HA	1:C:475:ILE:HD11	1.92	0.50
1:D:94:ILE:HD13	1:D:124:VAL:HG11	1.94	0.50
1:A:437:GLN:O	1:A:458:VAL:HG11	2.11	0.50
1:D:258:PHE:CZ	1:D:260:GLU:HB2	2.45	0.50
1:A:389:LYS:CE	1:A:408:GLU:HB3	2.39	0.50
1:B:364:GLN:HG3	1:B:368:LYS:HE2	1.93	0.50
1:D:310:THR:HG22	1:D:445:ILE:HG23	1.94	0.50
1:C:465:HIS:CD2	1:C:466:LEU:HD22	2.46	0.50
1:A:320:ARG:NH2	1:A:354:GLU:OE1	2.37	0.50
1:A:414:ARG:NH1	1:A:425:GLU:OE1	2.39	0.50
1:D:10:GLY:HA3	1:D:17:HIS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ARG:HB3	1:C:286:ASP:OD1	2.12	0.50
1:A:124:VAL:HG13	1:A:135:ILE:HG12	1.93	0.49
1:B:101:ASP:OD1	1:B:101:ASP:N	2.45	0.49
1:B:451:GLY:O	1:B:496:LEU:HD12	2.12	0.49
1:C:13:LYS:N	1:C:13:LYS:HE2	2.27	0.49
1:C:104:GLU:N	1:C:115:ARG:O	2.37	0.49
1:C:120:LEU:HD21	1:C:123:HIS:CD2	2.47	0.49
1:C:291:LEU:O	1:C:294:TYR:O	2.31	0.49
1:C:368:LYS:HE3	1:C:371:GLU:HB2	1.94	0.49
1:D:57:MET:HB2	1:D:60:ALA:HB2	1.95	0.49
1:D:520:LYS:O	1:D:523:ILE:HG12	2.13	0.49
1:C:386:ASP:OD1	1:C:386:ASP:N	2.47	0.48
1:D:412:ARG:HH22	1:D:425:GLU:CD	2.16	0.48
1:B:258:PHE:CZ	1:B:260:GLU:HB2	2.48	0.48
1:B:267:ILE:O	1:B:268:GLU:HB3	2.13	0.48
1:C:285:MET:H	1:C:438:GLN:HE22	1.61	0.48
1:B:61:ARG:NH2	1:B:150:ASP:OD1	2.45	0.48
1:B:227:GLU:HA	1:B:250:HIS:ND1	2.28	0.48
1:B:195:PRO:HG3	1:B:204:LEU:HD11	1.96	0.48
1:B:232:VAL:HG22	1:B:254:ILE:HB	1.94	0.48
1:B:333:GLU:HG3	1:B:334:LEU:H	1.78	0.48
1:C:57:MET:CB	1:C:60:ALA:HB2	2.44	0.48
1:C:14:ARG:HD2	1:C:16:TRP:CH2	2.49	0.48
1:D:311:ARG:NH1	1:D:313:GLN:HE22	2.12	0.48
1:B:79:ASP:OD1	1:B:152:ARG:NH2	2.34	0.48
1:C:327:TYR:CZ	1:C:329:ILE:HD11	2.48	0.48
1:D:227:GLU:O	1:D:229:SER:N	2.43	0.48
1:A:30:LEU:HD22	1:A:32:PHE:CE1	2.48	0.48
1:A:350:HIS:O	1:A:410:ARG:NH2	2.46	0.48
1:C:336:ASN:O	1:C:340:ILE:HG13	2.13	0.48
1:C:102:ASP:OD2	1:C:116:ARG:HB2	2.14	0.47
1:D:100:GLU:HB2	1:D:116:ARG:NH1	2.29	0.47
1:C:43:HIS:O	1:C:46:ASN:N	2.44	0.47
1:C:288:LYS:O	1:C:292:GLN:HG3	2.14	0.47
1:A:466:LEU:N	1:A:469:GLY:O	2.48	0.47
1:B:432:ILE:HG13	1:B:452:ILE:HG21	1.97	0.47
1:A:2:TYR:CE1	1:A:230:ARG:HD3	2.49	0.47
1:A:39:ILE:HD11	1:A:51:LEU:HD13	1.95	0.47
1:A:218:GLY:HA2	1:A:246:LEU:HD23	1.97	0.47
1:B:82:GLN:HA	1:B:179:ARG:HG3	1.96	0.47
1:B:105:PHE:CE2	1:B:114:VAL:HG23	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:PHE:CE2	1:B:291:LEU:HD11	2.50	0.47
1:D:171:TYR:HB2	1:D:180:ILE:HG12	1.96	0.47
1:A:10:GLY:HA3	1:A:17:HIS:O	2.15	0.46
1:D:32:PHE:HE1	1:D:442:TYR:CG	2.34	0.46
1:D:514:ARG:HG2	1:D:518:TRP:CH2	2.50	0.46
1:A:386:ASP:OD1	1:A:386:ASP:N	2.48	0.46
1:B:146:LEU:HB3	1:B:159:VAL:HG13	1.96	0.46
1:C:328:GLN:HB3	1:C:434:ASP:OD2	2.15	0.46
1:B:105:PHE:CE2	1:B:114:VAL:CG2	2.98	0.46
1:C:463:VAL:HG12	1:C:471:ILE:HD11	1.97	0.46
1:D:270:LEU:HD23	1:D:270:LEU:HA	1.80	0.46
1:A:228:ASP:OD1	1:A:252:HIS:HE1	1.99	0.46
1:B:244:LEU:HA	1:B:247:LEU:CD1	2.44	0.46
1:C:14:ARG:NH1	1:C:169:GLN:HE22	2.07	0.46
1:B:94:ILE:HG21	1:B:112:ILE:HD12	1.98	0.46
1:D:52:LEU:HD23	1:D:75:TYR:HB3	1.97	0.46
1:C:407:LEU:HD23	1:C:407:LEU:HA	1.77	0.46
1:D:112:ILE:HG22	1:D:114:VAL:HG23	1.98	0.46
1:B:274:LEU:HD21	1:B:291:LEU:HD22	1.97	0.46
1:C:122:ALA:O	1:C:123:HIS:HD2	1.98	0.46
1:C:266:ASN:HB2	1:C:269:ASN:CB	2.46	0.46
1:C:331:LEU:HD12	1:C:331:LEU:HA	1.77	0.46
1:C:171:TYR:HD2	1:C:180:ILE:HG13	1.81	0.45
1:C:285:MET:HG3	1:C:304:TYR:CD2	2.52	0.45
1:B:98:GLU:O	1:B:98:GLU:HG3	2.15	0.45
1:D:77:VAL:HG11	1:D:213:ILE:HG23	1.99	0.45
1:B:353:THR:O	1:B:410:ARG:NH1	2.49	0.45
1:C:305:LEU:HD21	1:C:515:TRP:HE1	1.82	0.45
1:D:108:THR:HB	1:D:111:LEU:O	2.16	0.45
1:A:241:GLN:C	1:A:243:VAL:H	2.18	0.45
1:B:94:ILE:HG13	1:B:132:ILE:HD11	1.98	0.45
1:B:228:ASP:CB	1:B:533:ARG:HD2	2.46	0.45
1:D:92:LEU:HD11	1:D:149:PHE:CD2	2.51	0.45
1:D:367:ILE:HD12	1:D:368:LYS:N	2.32	0.45
1:C:318:GLN:HG3	1:C:430:ARG:HH12	1.82	0.45
1:C:319:GLN:O	1:C:320:ARG:HG2	2.17	0.45
1:B:283:ASP:N	1:B:283:ASP:OD1	2.50	0.45
1:D:432:ILE:HG13	1:D:452:ILE:HG21	1.97	0.45
1:C:56:TYR:HB2	1:C:78:PHE:CD2	2.51	0.45
1:C:158:ILE:HG13	1:C:172:LEU:HD11	1.99	0.45
1:C:304:TYR:OH	1:C:441:LEU:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASN:N	1:B:273:ASP:OD2	2.42	0.45
1:D:188:ASN:HB3	1:D:190:HIS:CE1	2.52	0.45
1:C:30:LEU:HD21	1:C:419:GLU:HG2	1.97	0.44
1:C:196:VAL:HG23	1:C:197:PHE:CD2	2.52	0.44
1:C:286:ASP:OD1	1:C:286:ASP:N	2.47	0.44
1:D:61:ARG:NE	1:D:151:ASP:OD1	2.36	0.44
1:D:345:PHE:HD1	1:D:382:LEU:HD21	1.82	0.44
1:A:24:TYR:CD2	1:A:110:PHE:HD2	2.36	0.44
1:A:56:TYR:HB2	1:A:78:PHE:CD2	2.52	0.44
1:A:318:GLN:HG3	1:A:430:ARG:HH12	1.82	0.44
1:A:326:PHE:HE1	1:A:328:GLN:NE2	2.15	0.44
1:C:14:ARG:NH1	1:C:169:GLN:NE2	2.61	0.44
1:C:348:ALA:HB2	1:C:387:PHE:CZ	2.53	0.44
1:D:347:VAL:HG21	1:D:355:LEU:HB2	1.99	0.44
1:A:218:GLY:CA	1:A:246:LEU:HD23	2.48	0.44
1:D:45:GLU:OE2	1:D:509:HIS:ND1	2.47	0.44
1:D:154:PHE:HD1	1:D:155:VAL:O	1.99	0.44
1:D:331:LEU:HD12	1:D:331:LEU:HA	1.65	0.44
1:A:305:LEU:HD22	1:A:518:TRP:HZ3	1.82	0.44
1:B:30:LEU:HD22	1:B:32:PHE:CE1	2.53	0.44
1:C:92:LEU:HD12	1:C:92:LEU:HA	1.67	0.44
1:C:140:ASP:O	1:C:142:GLN:N	2.51	0.44
1:D:92:LEU:HG	1:D:132:ILE:HD12	1.99	0.44
1:A:204:LEU:HD13	1:B:196:VAL:CG1	2.48	0.44
1:B:3:TYR:CE2	1:B:225:VAL:HG22	2.52	0.44
1:C:428:ASP:OD1	1:C:428:ASP:N	2.34	0.44
1:C:14:ARG:HB3	1:C:16:TRP:CE2	2.53	0.44
1:C:140:ASP:C	1:C:142:GLN:H	2.20	0.44
1:C:389:LYS:HD2	1:C:390:LYS:H	1.82	0.44
1:B:55:ALA:O	1:B:57:MET:HG3	2.17	0.44
1:C:228:ASP:N	1:C:250:HIS:O	2.46	0.44
1:D:230:ARG:NH2	1:D:516:GLU:OE1	2.51	0.44
1:A:56:TYR:HB2	1:A:78:PHE:CE2	2.53	0.44
1:A:360:TYR:OH	1:A:443:THR:HG22	2.18	0.44
1:A:428:ASP:OD1	1:A:428:ASP:N	2.51	0.44
1:D:365:GLU:O	1:D:369:GLN:HG3	2.18	0.44
1:A:105:PHE:CD1	1:A:114:VAL:HG22	2.53	0.43
1:A:326:PHE:HE1	1:A:328:GLN:HE21	1.66	0.43
1:A:434:ASP:HB3	1:A:456:ASN:HD21	1.83	0.43
1:A:496:LEU:O	1:A:500:ILE:HG13	2.18	0.43
1:D:185:LYS:HE3	1:D:185:LYS:HB2	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:SER:OG	1:C:134:PHE:N	2.51	0.43
1:A:25:ARG:HA	1:A:25:ARG:HD2	1.80	0.43
1:A:279:LEU:HD21	1:A:518:TRP:HE3	1.84	0.43
1:B:448:ILE:CG2	1:B:502:LYS:HB3	2.48	0.43
1:C:14:ARG:HB3	1:C:16:TRP:CZ2	2.53	0.43
1:C:50:LYS:HG3	1:C:73:GLU:O	2.19	0.43
1:A:64:LEU:HB3	1:A:70:PHE:HA	2.01	0.43
1:D:161:TYR:HA	1:D:165:GLN:O	2.18	0.43
1:D:320:ARG:HD2	1:D:428:ASP:HB2	2.00	0.43
1:D:467:GLN:HB3	1:D:498:TYR:CG	2.53	0.43
1:A:252:HIS:NE2	1:A:523:ILE:HD11	2.33	0.43
1:C:288:LYS:HD3	1:C:304:TYR:HB2	2.00	0.43
1:D:267:ILE:CD1	1:D:267:ILE:N	2.82	0.43
1:D:383:ASP:HB3	1:D:386:ASP:OD2	2.19	0.43
1:B:179:ARG:NH1	1:B:200:ASP:OD1	2.51	0.43
1:C:115:ARG:HD3	1:C:119:GLN:C	2.38	0.43
1:D:298:GLN:O	1:D:301:LYS:HG2	2.18	0.43
1:B:274:LEU:HD12	1:B:274:LEU:HA	1.84	0.43
1:D:351:PRO:HA	1:D:410:ARG:CZ	2.49	0.43
1:A:56:TYR:HE1	1:A:156:SER:HG	1.66	0.43
1:B:92:LEU:HG	1:B:132:ILE:HD13	2.01	0.43
1:B:173:ASN:HB2	1:B:174:PRO:HD2	2.01	0.43
1:B:248:PRO:HB3	1:B:250:HIS:CE1	2.53	0.43
1:A:440:ASN:OD1	1:A:443:THR:HG23	2.19	0.43
1:B:230:ARG:HH12	1:B:533:ARG:HD3	1.84	0.43
1:C:285:MET:H	1:C:438:GLN:NE2	2.17	0.43
1:D:389:LYS:HG3	1:D:410:ARG:HG2	2.01	0.43
1:A:271:LYS:O	1:A:275:GLU:HG3	2.18	0.42
1:B:150:ASP:OD1	1:B:152:ARG:HG2	2.18	0.42
1:B:284:ARG:NH2	1:B:438:GLN:HG3	2.33	0.42
1:A:31:GLU:O	1:A:37:HIS:HE1	2.03	0.42
1:B:137:PHE:O	1:B:143:LEU:HD12	2.19	0.42
1:C:267:ILE:HA	1:C:267:ILE:HD13	1.77	0.42
1:C:448:ILE:HG22	1:C:503:ILE:HG13	2.01	0.42
1:A:59:HIS:HE1	1:A:149:PHE:O	2.02	0.42
1:A:192:VAL:HB	1:A:205:GLU:HG3	2.01	0.42
1:B:422:LEU:HD22	1:B:422:LEU:HA	1.86	0.42
1:C:199:ARG:HH21	1:D:175:ASN:CB	2.31	0.42
1:D:61:ARG:HB2	1:D:151:ASP:OD2	2.19	0.42
1:D:98:GLU:O	1:D:98:GLU:HG2	2.18	0.42
1:C:22:PRO:HG3	1:C:134:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:PHE:HA	1:C:147:ASN:O	2.19	0.42
1:D:42:PHE:HB3	1:D:49:VAL:HG21	2.01	0.42
1:A:246:LEU:N	1:A:246:LEU:HD12	2.34	0.42
1:C:236:GLN:HG2	1:C:238:PHE:CZ	2.53	0.42
1:C:257:PHE:CD1	1:C:287:PHE:HE2	2.38	0.42
1:D:420:LEU:HD12	1:D:420:LEU:HA	1.84	0.42
1:A:34:ASP:OD1	1:A:34:ASP:N	2.53	0.42
1:A:71:GLU:H	1:A:71:GLU:HG2	1.46	0.42
1:B:104:GLU:N	1:B:115:ARG:O	2.44	0.42
1:B:305:LEU:HD13	1:B:518:TRP:CZ3	2.54	0.42
1:C:20:ILE:O	1:C:21:ILE:HD13	2.20	0.42
1:D:441:LEU:HA	1:D:441:LEU:HD12	1.57	0.42
1:D:499:SER:O	1:D:503:ILE:HG13	2.18	0.42
1:A:108:THR:HG22	1:A:110:PHE:N	2.22	0.42
1:A:267:ILE:HD13	1:A:267:ILE:HA	1.83	0.42
1:A:444:GLN:O	1:A:448:ILE:HG13	2.20	0.42
1:B:115:ARG:HH12	1:B:119:GLN:H	1.66	0.42
1:B:428:ASP:OD1	1:B:428:ASP:N	2.52	0.42
1:C:305:LEU:CD2	1:C:515:TRP:HE1	2.32	0.42
1:D:92:LEU:HD11	1:D:149:PHE:CE2	2.54	0.42
1:A:419:GLU:O	1:A:423:ILE:HG13	2.20	0.42
1:D:114:VAL:HB	1:D:122:ALA:HB3	2.01	0.42
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.84	0.42
1:C:331:LEU:C	1:C:333:GLU:N	2.73	0.42
1:D:93:GLN:HG3	1:D:94:ILE:H	1.85	0.42
1:C:76:SER:HB3	1:C:79:ASP:HB2	2.02	0.42
1:C:467:GLN:HB3	1:C:498:TYR:CD1	2.55	0.42
1:A:331:LEU:HD23	1:A:331:LEU:HA	1.67	0.41
1:B:136:LYS:HB3	1:B:143:LEU:HD13	2.02	0.41
1:B:532:PRO:HA	1:B:533:ARG:HA	1.63	0.41
1:C:53:LEU:HD22	1:C:57:MET:HE3	2.01	0.41
1:C:301:LYS:O	1:C:301:LYS:HG2	2.20	0.41
1:D:3:TYR:CZ	1:D:225:VAL:HG22	2.55	0.41
1:D:109:PRO:HG2	1:D:110:PHE:CE2	2.54	0.41
1:A:201:PHE:CD2	1:A:212:LEU:HD11	2.55	0.41
1:A:445:ILE:HA	1:A:445:ILE:HD13	1.78	0.41
1:C:43:HIS:CE1	1:C:71:GLU:HG3	2.55	0.41
1:D:1:MET:SD	1:D:48:PRO:HB2	2.60	0.41
1:D:89:MET:HE3	1:D:151:ASP:O	2.20	0.41
1:D:206:TYR:CZ	1:D:212:LEU:HD13	2.54	0.41
1:A:40:ARG:HG2	1:A:69:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ASP:HA	1:B:526:LYS:HZ2	1.85	0.41
1:C:39:ILE:HA	1:C:39:ILE:HD13	1.85	0.41
1:C:169:GLN:NE2	1:C:171:TYR:OH	2.54	0.41
1:D:53:LEU:HD13	1:D:57:MET:HE1	2.01	0.41
1:D:99:TRP:CH2	1:D:114:VAL:HG21	2.55	0.41
1:D:226:GLU:H	1:D:226:GLU:CD	2.23	0.41
1:A:329:ILE:HD13	1:A:329:ILE:HA	1.80	0.41
1:A:323:SER:HB3	1:A:486:LEU:HD22	2.03	0.41
1:B:50:LYS:HB2	1:B:73:GLU:O	2.21	0.41
1:B:259:HIS:HB3	1:B:284:ARG:CD	2.50	0.41
1:C:343:VAL:HG22	1:C:478:LEU:HD21	2.03	0.41
1:D:42:PHE:CB	1:D:49:VAL:HG21	2.50	0.41
1:D:191:VAL:HG21	1:D:209:MET:HG2	2.03	0.41
1:B:33:ASP:HA	1:B:258:PHE:CE2	2.55	0.41
1:C:374:VAL:O	1:C:378:ILE:HG13	2.21	0.41
1:C:465:HIS:NE2	1:C:466:LEU:HD22	2.36	0.41
1:D:39:ILE:HD11	1:D:51:LEU:HD21	2.03	0.41
1:A:258:PHE:CZ	1:A:260:GLU:HB2	2.56	0.41
1:B:367:ILE:HD11	1:B:415:ASN:HB2	2.03	0.41
1:C:90:GLN:O	1:C:153:GLY:HA3	2.20	0.41
1:C:97:LEU:HB2	1:C:99:TRP:CZ3	2.56	0.41
1:C:418:ASP:OD2	1:C:420:LEU:N	2.53	0.41
1:B:266:ASN:ND2	1:B:269:ASN:HB2	2.36	0.41
1:B:432:ILE:HB	1:B:454:GLN:HG2	2.01	0.41
1:C:82:GLN:HB3	1:C:172:LEU:O	2.21	0.41
1:C:327:TYR:HA	1:C:433:ILE:O	2.21	0.41
1:D:40:ARG:HG2	1:D:69:ILE:CG2	2.51	0.41
1:D:240:ASN:HB2	1:D:273:ASP:OD2	2.21	0.41
1:B:193:VAL:HB	1:B:204:LEU:HA	2.03	0.40
1:B:199:ARG:HD3	1:B:200:ASP:OD2	2.21	0.40
1:B:331:LEU:C	1:B:333:GLU:H	2.24	0.40
1:C:81:ILE:HG13	1:C:216:LYS:HD2	2.03	0.40
1:B:59:HIS:HE1	1:B:149:PHE:O	2.05	0.40
1:B:97:LEU:HD21	1:B:149:PHE:CZ	2.56	0.40
1:C:339:ALA:CA	1:C:475:ILE:HD11	2.50	0.40
1:C:389:LYS:HD3	1:C:410:ARG:HD3	2.03	0.40
1:D:8:TRP:O	1:D:18:ARG:HD3	2.21	0.40
1:A:77:VAL:HG21	1:A:217:LEU:HB2	2.02	0.40
1:A:435:LEU:N	2:A:601:HOH:O	2.54	0.40
1:B:182:GLU:HG3	1:B:191:VAL:HG22	2.04	0.40
1:D:239:THR:HB	1:D:269:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LEU:HD11	1:D:291:LEU:HD22	2.04	0.40
1:D:474:SER:C	1:D:476:SER:N	2.75	0.40
1:B:419:GLU:HG2	1:B:442:TYR:OH	2.21	0.40
1:D:106:ILE:HB	1:D:113:ILE:HB	2.02	0.40
1:D:435:LEU:HA	1:D:435:LEU:HD23	1.92	0.40
1:D:486:LEU:HD23	1:D:486:LEU:HA	1.73	0.40
1:A:266:ASN:CG	1:A:269:ASN:HB2	2.41	0.40
1:D:488:GLY:O	1:D:490:LYS:N	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ASP:OD2	1:C:390:LYS:NZ[1_445]	2.15	0.05

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	506/533 (95%)	462 (91%)	40 (8%)	4 (1%)	19	47
1	B	509/533 (96%)	461 (91%)	44 (9%)	4 (1%)	19	47
1	C	512/533 (96%)	459 (90%)	47 (9%)	6 (1%)	13	36
1	D	507/533 (95%)	465 (92%)	39 (8%)	3 (1%)	25	54
All	All	2034/2132 (95%)	1847 (91%)	170 (8%)	17 (1%)	19	47

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLU
1	D	100	GLU

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Mol	Chain	Res	Type
1	A	266	ASN
1	B	352	ASP
1	C	319	GLN
1	C	300	GLU
1	D	270	LEU
1	A	490	LYS
1	B	8	TRP
1	C	207	GLU
1	C	418	ASP
1	C	102	ASP
1	C	266	ASN
1	D	98	GLU
1	B	266	ASN
1	B	459	ALA
1	A	210	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	471/493 (96%)	461 (98%)	10 (2%)	53	81
1	B	476/493 (97%)	458 (96%)	18 (4%)	33	64
1	C	477/493 (97%)	458 (96%)	19 (4%)	31	62
1	D	472/493 (96%)	462 (98%)	10 (2%)	53	81
All	All	1896/1972 (96%)	1839 (97%)	57 (3%)	41	72

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
1	A	188	ASN
1	A	228	ASP
1	A	230	ARG
1	A	265	SER
1	A	334	LEU

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Mol	Chain	Res	Type
1	A	386	ASP
1	A	389	LYS
1	A	420	LEU
1	A	476	SER
1	B	61	ARG
1	B	68	ASP
1	B	76	SER
1	B	102	ASP
1	B	139	LYS
1	B	182	GLU
1	B	199	ARG
1	B	204	LEU
1	B	229	SER
1	B	230	ARG
1	B	238	PHE
1	B	274	LEU
1	B	311	ARG
1	B	321	HIS
1	B	352	ASP
1	B	431	LEU
1	B	528	ASP
1	B	533	ARG
1	C	68	ASP
1	C	99	TRP
1	C	100	GLU
1	C	102	ASP
1	C	115	ARG
1	C	116	ARG
1	C	119	GLN
1	C	170	ASP
1	C	222	SER
1	C	229	SER
1	C	230	ARG
1	C	236	GLN
1	C	250	HIS
1	C	266	ASN
1	C	311	ARG
1	C	321	HIS
1	C	332	SER
1	C	466	LEU
1	C	513	LYS
1	D	92	LEU

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Mol	Chain	Res	Type
1	D	100	GLU
1	D	101	ASP
1	D	102	ASP
1	D	116	ARG
1	D	186	PHE
1	D	238	PHE
1	D	317	SER
1	D	421	SER
1	D	473	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	HIS
1	A	328	GLN
1	A	444	GLN
1	A	456	ASN
1	A	467	GLN
1	B	477	GLN
1	C	17	HIS
1	C	123	HIS
1	C	169	GLN
1	D	28	GLN
1	D	147	ASN
1	D	444	GLN

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](#)

There are no ligands in this entry.

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	510/533 (95%)	0.16	2 (0%) 92 92	25, 44, 71, 93	0
1	B	515/533 (96%)	0.33	23 (4%) 33 27	29, 49, 88, 118	0
1	C	516/533 (96%)	0.28	24 (4%) 31 25	32, 49, 89, 116	0
1	D	511/533 (95%)	0.19	3 (0%) 89 88	25, 45, 76, 105	0
All	All	2052/2132 (96%)	0.24	52 (2%) 57 52	25, 46, 84, 118	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	118	GLY	9.8
1	C	162	GLU	4.6
1	B	143	LEU	4.5
1	D	407	LEU	3.9
1	C	103	CYS	3.8
1	C	407	LEU	3.4
1	C	110	PHE	3.3
1	D	270	LEU	3.2
1	C	126	PHE	3.1
1	C	99	TRP	3.0
1	B	23	TRP	3.0
1	C	363	TRP	3.0
1	B	119	GLN	3.0
1	C	188	ASN	2.9
1	B	164	GLY	2.9
1	B	213	ILE	2.9
1	A	220	TYR	2.8
1	C	23	TRP	2.8
1	C	97	LEU	2.8
1	C	167	VAL	2.8
1	B	102	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	407	LEU	2.6
1	B	109	PRO	2.6
1	C	98	GLU	2.6
1	C	111	LEU	2.5
1	A	407	LEU	2.5
1	B	188	ASN	2.5
1	B	329	ILE	2.5
1	C	117	GLN	2.5
1	B	146	LEU	2.4
1	C	146	LEU	2.4
1	C	101	ASP	2.3
1	B	160	TYR	2.3
1	B	77	VAL	2.3
1	C	128	VAL	2.3
1	B	190	HIS	2.3
1	C	100	GLU	2.3
1	C	105	PHE	2.3
1	C	106	ILE	2.2
1	D	162	GLU	2.2
1	B	26	SER	2.2
1	B	126	PHE	2.2
1	B	128	VAL	2.2
1	B	162	GLU	2.1
1	B	81	ILE	2.1
1	C	104	GLU	2.1
1	B	199	ARG	2.1
1	C	112	ILE	2.1
1	C	24	TYR	2.1
1	B	95	LYS	2.0
1	C	95	LYS	2.0
1	B	341	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.