Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 02:33 PM EDT

PDB ID	:	1DVM
Title	:	ACTIVE FORM OF HUMAN PAI-1
Authors	:	Stout, T.J.; Graham, H.; Buckley, D.I.; Matthews, D.J.
Deposited on	:	2000-01-21
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 following versions of software and data (see references ⓘ) were used in the production of this report:

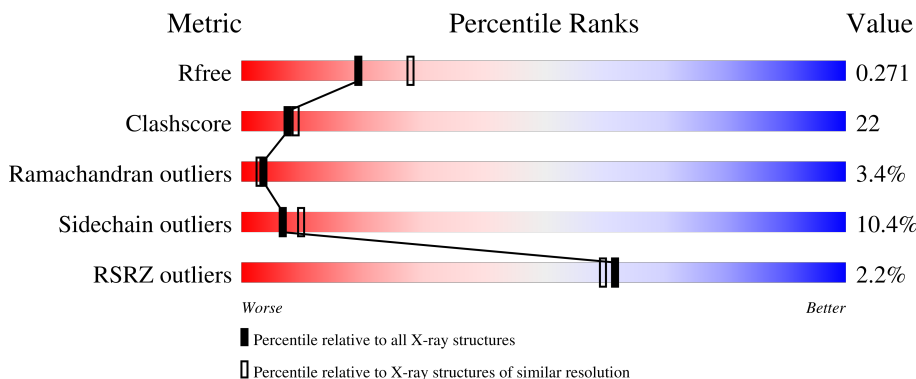|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	Percentile Ranks	Value
Rfree		0.271
Clashscore		22
Ramachandran outliers		3.4%
Sidechain outliers		10.4%
RSRZ outliers		2.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	379	2% / 56% / 39% / • ••
1	B	379	2% / 54% / 36% / 6% • •
1	C	379	2% / 51% / 36% / 7% • •
1	D	379	2% / 54% / 36% / 7% •

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
2	CL	A	1001	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 13383 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 PLASMINOGEN ACTIVATOR INHIBITOR-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2973	1909	505	544	15			
1	B	365	Total	C	N	O	S	0	0	0
			2912	1872	495	530	15			
1	C	364	Total	C	N	O	S	11	0	0
			2902	1864	494	529	15			
1	D	372	Total	C	N	O	S	0	0	0
			2956	1899	502	540	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	HIS	ASN	engineered mutation	UNP P05121
A	154	THR	LYS	engineered mutation	UNP P05121
A	319	LEU	GLN	engineered mutation	UNP P05121
A	354	ILE	MET	engineered mutation	UNP P05121
B	150	HIS	ASN	engineered mutation	UNP P05121
B	154	THR	LYS	engineered mutation	UNP P05121
B	319	LEU	GLN	engineered mutation	UNP P05121
B	354	ILE	MET	engineered mutation	UNP P05121
C	150	HIS	ASN	engineered mutation	UNP P05121
C	154	THR	LYS	engineered mutation	UNP P05121
C	319	LEU	GLN	engineered mutation	UNP P05121
C	354	ILE	MET	engineered mutation	UNP P05121
D	150	HIS	ASN	engineered mutation	UNP P05121
D	154	THR	LYS	engineered mutation	UNP P05121
D	319	LEU	GLN	engineered mutation	UNP P05121
D	354	ILE	MET	engineered mutation	UNP P05121

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0
2	B	1	Total 1	Cl 1	0	0
2	C	1	Total 1	Cl 1	0	0
2	D	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	434	Total 434	O 434	0	0
3	B	398	Total 398	O 398	0	0
3	C	352	Total 352	O 352	0	0
3	D	452	Total 452	O 452	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: PLASMINOGEN ACTIVATOR INHIBITOR-1

- Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1

E350 E351 I354 D355 R356 P357 F358 L359 F360 R363 H364 V370 L371 F372 M373 V376 P379

• Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1

Chain C:

• Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.76Å 74.67Å 103.44Å 85.19° 86.17° 64.34°	Depositor
Resolution (Å)	30.00 – 2.40 25.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	80.5 (30.00-2.40) 80.5 (25.76-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 98.0	Depositor
R, R_{free}	0.218 , 0.292 0.188 , 0.271	Depositor DCC
R_{free} test set	2433 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å²)	18.6	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.32 , 101.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13383	wwPDB-VP
Average B, all atoms (Å²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.45	2/3045 (0.1%)	0.74	3/4129 (0.1%)
1	B	0.41	0/2984	0.70	1/4045 (0.0%)
1	C	0.41	0/2973	0.71	1/4028 (0.0%)
1	D	0.44	0/3028	0.73	0/4106
All	All	0.43	2/12030 (0.0%)	0.72	5/16308 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	TYR	CD2-CE2	-6.08	1.30	1.39
1	A	241	TYR	CE2-CZ	-5.53	1.31	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	GLY	N-CA-C	6.66	129.74	113.10
1	A	169	LEU	CA-CB-CG	5.90	128.87	115.30
1	A	332	GLY	N-CA-C	-5.85	98.48	113.10
1	B	233	LEU	CA-CB-CG	5.33	127.57	115.30
1	C	350	GLU	N-CA-C	5.17	124.95	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2973	0	2967	116	0
1	B	2912	0	2906	136	0
1	C	2902	0	2890	131	0
1	D	2956	0	2950	142	0
2	A	1	0	0	2	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	434	0	0	7	0
3	B	398	0	0	6	0
3	C	352	0	0	8	0
3	D	452	0	0	10	0
All	All	13383	0	11713	516	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (516) 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:271:ARG:HH11	1:C:271:ARG:HG2	1.14	1.08
1:B:243:LYS:H	1:B:243:LYS:HD3	1.17	1.06
1:B:104:LYS:H	1:B:104:LYS:HD2	1.19	1.05
1:D:162:ARG:HG2	1:D:162:ARG:HH11	1.24	0.98
1:A:254:LEU:HD23	1:A:373:MET:HE3	1.43	0.97
1:D:33:VAL:HG22	1:D:282:THR:HG23	1.47	0.93
1:C:33:VAL:HG12	1:C:282:THR:HG23	1.52	0.92
1:A:251:THR:HG21	1:A:375:GLN:HE21	1.35	0.90
1:C:176:LYS:HG2	1:C:227:PRO:HB2	1.54	0.88
1:B:98:PHE:HB2	1:B:164:VAL:HG13	1.56	0.87
1:B:205:THR:HG22	1:B:272:LEU:HD23	1.56	0.87
1:B:54:THR:HG22	1:B:297:ASP:HB3	1.57	0.86
1:B:275:LEU:HD13	1:B:354:ILE:HD12	1.61	0.82
1:B:104:LYS:HD2	1:B:104:LYS:N	1.96	0.81
1:C:176:LYS:HE2	1:C:177:THR:HB	1.64	0.80
1:D:313:GLU:HG3	1:D:314:PRO:HA	1.63	0.79
1:D:364:HIS:CE1	1:D:366:PRO:HG2	2.18	0.78
1:D:13:SER:HB3	1:D:370:VAL:HG13	1.66	0.77
1:D:87:ASN:HD21	1:D:91:ILE:HG23	1.51	0.76
1:B:275:LEU:HD12	1:B:276:PRO:HD2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:HH11	1:D:115:ARG:HG3	1.48	0.76
1:B:250:LEU:HD22	1:B:359:LEU:HD21	1.65	0.76
1:D:205:THR:HG22	1:D:272:LEU:HD13	1.68	0.76
1:D:42:VAL:HB	1:D:165:LEU:HD21	1.68	0.76
1:D:128:GLU:HG2	1:D:131:ARG:HD2	1.67	0.74
1:A:300:ARG:HD3	1:A:303:GLN:OE1	1.87	0.74
1:A:290:LEU:HD13	1:A:298:MET:HE3	1.70	0.73
1:C:254:LEU:HD23	1:C:373:MET:HE3	1.70	0.73
1:B:33:VAL:H	1:B:282:THR:HG21	1.51	0.73
1:D:100:GLN:NE2	1:D:125:ASP:HA	2.03	0.73
1:D:353:ILE:HD11	1:D:355:ASP:HB3	1.71	0.73
1:B:90:GLU:HA	1:B:333:THR:HG21	1.69	0.72
1:B:172:ASN:HB3	1:B:333:THR:HG22	1.70	0.72
1:A:313:GLU:HG2	1:A:315:LEU:H	1.52	0.72
1:C:271:ARG:HG2	1:C:271:ARG:NH1	1.92	0.72
1:B:4:PRO:HG2	1:B:7:TYR:HB3	1.72	0.72
1:C:242:GLU:HB2	1:C:245:VAL:HG23	1.73	0.71
1:A:254:LEU:HA	1:A:258:LEU:HD23	1.73	0.71
1:A:288:LYS:HB2	3:A:1392:HOH:O	1.89	0.71
1:D:190:HIS:O	1:D:357:PRO:HD3	1.90	0.71
1:D:67:ASP:HB2	3:D:1132:HOH:O	1.91	0.70
1:A:42:VAL:HB	1:A:165:LEU:HD21	1.73	0.70
1:B:97:ILE:HB	1:B:121:VAL:HG23	1.72	0.70
1:C:240:PRO:HG3	1:C:250:LEU:HD13	1.72	0.70
1:D:199:VAL:HG13	3:D:1303:HOH:O	1.91	0.70
1:C:327:GLU:HG3	3:C:1249:HOH:O	1.92	0.70
1:C:206:ASN:HD22	1:C:206:ASN:N	1.89	0.70
1:D:5:PRO:HG2	1:D:6:SER:H	1.56	0.69
1:D:287:ARG:HA	1:D:299:PHE:CZ	2.27	0.69
1:B:98:PHE:HB2	1:B:164:VAL:CG1	2.22	0.69
1:A:251:THR:HG21	1:A:375:GLN:NE2	2.06	0.69
1:A:313:GLU:HG3	1:A:315:LEU:HD12	1.75	0.69
1:C:174:GLN:NE2	1:C:229:HIS:HB3	2.07	0.69
1:A:270:PRO:O	1:A:349:PRO:HD2	1.93	0.68
1:B:243:LYS:H	1:B:243:LYS:CD	1.97	0.68
1:B:54:THR:HG22	1:B:297:ASP:CB	2.23	0.68
1:D:100:GLN:HB3	1:D:103:LEU:HG	1.76	0.68
1:A:17:VAL:O	1:A:21:GLN:HG2	1.93	0.67
1:B:4:PRO:O	1:B:8:VAL:HG23	1.94	0.67
1:D:263:LYS:HE3	1:D:363:ARG:NH1	2.09	0.67
1:A:106:VAL:HG23	1:A:310:SER:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLN:HG2	1:D:126:PHE:HD2	1.59	0.67
1:C:210:TYR:HD1	1:C:224:LEU:HD23	1.58	0.67
1:C:275:LEU:HD12	1:C:276:PRO:HD2	1.76	0.67
1:B:272:LEU:HB3	1:B:351:GLU:HB3	1.76	0.66
1:A:248:SER:HA	1:A:251:THR:HG23	1.76	0.66
1:A:221:TYR:OH	1:A:249:ALA:HB3	1.96	0.66
1:A:8:VAL:HG22	1:A:71:MET:SD	2.37	0.65
1:A:247:LEU:HD11	1:A:358:PHE:HA	1.77	0.65
1:A:42:VAL:HG12	1:A:95:ASP:HB3	1.77	0.65
1:D:214:THR:HB	1:D:220:TYR:CD1	2.31	0.65
1:A:45:MET:HG2	1:A:117:PHE:CE2	2.31	0.65
1:B:100:GLN:HE22	1:B:126:PHE:HB2	1.62	0.65
1:C:251:THR:HA	1:C:254:LEU:HD22	1.78	0.65
1:A:49:THR:HG22	1:A:109:PHE:CZ	2.32	0.64
1:B:227:PRO:HA	1:B:234:SER:HB3	1.79	0.64
1:C:13:SER:O	1:C:17:VAL:HG23	1.97	0.64
1:A:58:ILE:HD11	1:A:62:MET:SD	2.38	0.64
1:A:180:PRO:O	1:A:181:ASP:HB2	1.96	0.64
1:C:128:GLU:HG3	3:C:1020:HOH:O	1.98	0.64
1:C:167:ASN:HB3	1:C:322:GLN:HG3	1.80	0.64
1:C:201:MET:HG2	1:C:276:PRO:HA	1.79	0.64
1:D:187:ARG:HD3	1:D:353:ILE:HD13	1.79	0.64
1:B:104:LYS:H	1:B:104:LYS:CD	1.95	0.64
1:B:243:LYS:HD3	1:B:243:LYS:N	2.02	0.64
1:B:141:LYS:HB2	1:B:149:SER:HA	1.79	0.63
1:D:270:PRO:O	1:D:349:PRO:HD2	1.99	0.63
1:D:46:LEU:O	1:D:50:THR:HG23	1.98	0.63
1:D:330:GLU:HG3	1:D:333:THR:O	1.97	0.63
1:B:35:SER:OG	1:B:169:LEU:HD11	1.98	0.63
1:D:162:ARG:HH11	1:D:162:ARG:CG	2.07	0.63
1:C:331:SER:HA	3:C:1253:HOH:O	1.98	0.62
1:A:58:ILE:CD1	1:A:62:MET:SD	2.88	0.62
1:A:55:GLN:O	1:A:59:GLN:HG3	2.00	0.62
1:B:20:PHE:O	1:B:23:VAL:HG13	1.99	0.62
1:A:323:LYS:NZ	2:A:1001:CL:CL	2.69	0.61
1:B:237:ILE:HG21	1:B:354:ILE:HD13	1.81	0.61
1:B:4:PRO:HG2	1:B:7:TYR:CB	2.31	0.61
1:C:240:PRO:HG3	1:C:250:LEU:CD1	2.30	0.61
1:D:7:TYR:O	1:D:10:HIS:HB3	2.00	0.61
1:B:207:LYS:NZ	1:B:270:PRO:HD3	2.16	0.61
1:C:139:TRP:O	1:C:143:HIS:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:HIS:HE1	1:D:185:HIS:CD2	2.19	0.60
1:A:190:HIS:O	1:A:357:PRO:HD3	2.00	0.60
1:D:76:ARG:HD2	1:D:118:ARG:HG2	1.84	0.60
1:C:48:LEU:HD11	1:C:112:HIS:CE1	2.35	0.60
1:C:348:ALA:HB1	1:C:349:PRO:HD2	1.84	0.60
1:B:21:GLN:O	1:B:25:GLN:HB2	2.01	0.60
1:B:205:THR:CG2	1:B:272:LEU:HD23	2.31	0.60
1:C:87:ASN:HB3	1:C:91:ILE:HB	1.84	0.59
1:D:65:LYS:O	1:D:71:MET:HG3	2.01	0.59
1:B:110:MET:HB2	1:B:111:PRO:HD3	1.83	0.59
1:B:278:PHE:CE2	1:B:328:VAL:HG11	2.38	0.59
1:D:50:THR:HG22	1:D:306:PHE:CE1	2.38	0.59
1:D:6:SER:HB2	3:D:1465:HOH:O	2.01	0.59
1:B:57:GLN:HE22	1:B:297:ASP:H	1.50	0.59
1:D:33:VAL:HB	1:D:326:ILE:HD12	1.83	0.59
1:B:242:GLU:O	1:B:245:VAL:HG22	2.03	0.59
1:D:187:ARG:O	1:D:198:SER:O	2.21	0.59
1:D:313:GLU:HB2	1:D:314:PRO:C	2.23	0.59
1:D:323:LYS:HE2	3:D:1099:HOH:O	2.03	0.59
1:D:221:TYR:OH	1:D:249:ALA:HB3	2.02	0.58
1:D:313:GLU:CG	1:D:314:PRO:HA	2.32	0.58
1:B:137:ASN:HD21	1:B:154:THR:HG21	1.68	0.58
1:B:104:LYS:HD3	1:B:312:GLN:HB2	1.84	0.58
1:D:205:THR:HG22	1:D:272:LEU:CD1	2.32	0.58
1:A:341:VAL:HG12	3:A:1408:HOH:O	2.03	0.58
1:D:275:LEU:HD12	1:D:276:PRO:HD2	1.86	0.58
1:B:188:LEU:HB3	1:B:196:THR:CG2	2.33	0.58
1:B:254:LEU:HD13	1:B:373:MET:CE	2.34	0.58
1:D:53:GLU:O	1:D:57:GLN:HG3	2.04	0.58
1:D:162:ARG:HG2	1:D:162:ARG:NH1	2.02	0.58
1:A:53:GLU:O	1:A:57:GLN:HG3	2.03	0.58
1:B:201:MET:HG2	1:B:276:PRO:HA	1.84	0.57
1:A:19:VAL:O	1:A:23:VAL:HG13	2.04	0.57
1:A:210:TYR:CG	1:A:211:THR:N	2.73	0.57
1:A:13:SER:O	1:A:17:VAL:HG23	2.05	0.57
1:C:236:PHE:O	1:C:360:PHE:HA	2.04	0.57
1:C:65:LYS:O	1:C:71:MET:HG2	2.05	0.57
1:C:188:LEU:HB2	1:C:196:THR:CG2	2.35	0.57
1:C:49:THR:HG22	1:C:109:PHE:CZ	2.40	0.56
1:B:288:LYS:HD2	3:B:1166:HOH:O	2.04	0.56
1:D:33:VAL:H	1:D:282:THR:HG21	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:THR:HB	1:C:272:LEU:HA	1.88	0.56
1:B:137:ASN:ND2	1:B:154:THR:HG21	2.21	0.56
1:D:87:ASN:ND2	1:D:91:ILE:HG23	2.19	0.56
1:D:120:THR:O	1:D:122:LYS:HE2	2.04	0.56
1:B:328:VAL:O	1:B:328:VAL:HG13	2.06	0.56
1:D:78:LEU:HD13	1:D:367:THR:HG21	1.87	0.56
1:A:313:GLU:CG	1:A:315:LEU:HB2	2.36	0.56
1:C:151:LEU:HD11	1:C:166:VAL:HG11	1.87	0.56
1:D:313:GLU:HB2	1:D:315:LEU:N	2.21	0.56
1:A:76:ARG:O	1:A:80:LYS:HG2	2.06	0.55
1:D:13:SER:CB	1:D:370:VAL:HG13	2.35	0.55
1:D:10:HIS:CD2	1:D:256:ALA:HB3	2.41	0.55
1:D:19:VAL:O	1:D:23:VAL:HG12	2.06	0.55
1:B:226:LEU:HD12	1:B:237:ILE:HD11	1.88	0.55
1:C:130:GLU:HG2	1:D:11:LEU:HD22	1.88	0.55
1:A:110:MET:HB2	1:A:111:PRO:HD3	1.89	0.55
1:D:163:LEU:HB2	1:D:315:LEU:HD12	1.88	0.55
1:A:199:VAL:HG22	3:A:1389:HOH:O	2.06	0.55
1:A:205:THR:HG22	1:A:272:LEU:HB2	1.89	0.55
1:D:32:VAL:HA	1:D:282:THR:HG21	1.88	0.55
1:D:72:ALA:O	1:D:76:ARG:HB2	2.07	0.55
1:D:93:THR:HB	1:D:169:LEU:HD13	1.89	0.55
1:A:306:PHE:CE2	1:A:316:HIS:HA	2.42	0.55
1:A:312:GLN:O	1:A:313:GLU:HB3	2.07	0.55
1:B:269:LEU:HD22	1:B:271:ARG:NH2	2.23	0.54
1:A:8:VAL:CG2	1:A:71:MET:SD	2.95	0.54
1:D:228:TYR:HB2	3:D:1380:HOH:O	2.06	0.54
1:D:313:GLU:HB2	1:D:314:PRO:CA	2.37	0.54
1:A:148:ILE:CG2	1:A:323:LYS:HD2	2.38	0.54
1:A:326:ILE:HD11	1:A:372:PHE:CD1	2.42	0.54
1:C:53:GLU:HA	1:C:56:GLN:HG2	1.89	0.54
1:A:87:ASN:ND2	1:A:91:ILE:HG23	2.23	0.54
1:B:205:THR:O	1:B:206:ASN:HB3	2.07	0.54
1:C:70:GLY:O	1:C:74:ALA:HB2	2.07	0.54
1:D:42:VAL:HG11	1:D:167:ASN:HB2	1.90	0.54
1:C:256:ALA:HB1	3:C:1306:HOH:O	2.08	0.54
1:D:100:GLN:HE22	1:D:125:ASP:HA	1.70	0.54
1:A:278:PHE:HB2	1:A:280:LEU:HD23	1.89	0.53
1:B:210:TYR:CE2	1:B:222:ASP:HB3	2.43	0.53
1:C:49:THR:HB	1:C:309:LEU:HB2	1.90	0.53
1:A:93:THR:CG2	1:A:169:LEU:HD13	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:VAL:HG23	1:C:370:VAL:O	2.09	0.53
1:B:18:ARG:NH2	1:B:61:ALA:O	2.42	0.53
1:B:202:MET:HG2	1:B:277:LYS:HB3	1.90	0.53
1:D:167:ASN:O	1:D:322:GLN:HA	2.08	0.53
1:B:39:VAL:O	1:B:43:LEU:HD23	2.09	0.53
1:C:243:LYS:HG3	3:C:1194:HOH:O	2.08	0.53
1:A:49:THR:HG22	1:A:109:PHE:HZ	1.73	0.53
1:B:278:PHE:O	1:B:328:VAL:HG12	2.09	0.52
1:C:98:PHE:CD1	1:C:122:LYS:HB2	2.44	0.52
1:D:49:THR:HG22	1:D:109:PHE:CZ	2.44	0.52
1:A:179:PHE:O	1:A:330:GLU:HB3	2.10	0.52
1:C:36:PRO:HB2	1:C:370:VAL:HG23	1.92	0.52
1:B:278:PHE:CD1	1:B:280:LEU:HD13	2.45	0.52
1:C:174:GLN:HE22	1:C:229:HIS:HB3	1.72	0.52
1:C:180:PRO:HD2	1:C:203:ALA:O	2.09	0.52
1:D:76:ARG:NH1	1:D:116:LEU:HA	2.24	0.52
1:B:91:ILE:HD12	1:B:170:TYR:O	2.10	0.52
1:A:224:LEU:HD11	1:A:352:ILE:HG21	1.91	0.52
1:B:87:ASN:OD1	1:B:91:ILE:HG22	2.10	0.52
1:B:105:LEU:HD23	1:B:110:MET:SD	2.50	0.52
1:C:78:LEU:O	1:C:82:LEU:HG	2.10	0.52
1:C:312:GLN:CA	1:C:312:GLN:HE21	2.23	0.52
1:B:173:GLY:HA2	3:B:1347:HOH:O	2.10	0.51
1:B:13:SER:HB3	1:B:370:VAL:HG23	1.92	0.51
1:C:153:GLY:HA3	1:C:321:LEU:HD11	1.92	0.51
1:A:205:THR:O	1:A:206:ASN:HB3	2.11	0.51
1:B:54:THR:HG21	1:B:305:ASP:N	2.25	0.51
1:A:150:HIS:CE1	1:D:185:HIS:CD2	2.99	0.51
1:B:191:LYS:HB2	1:B:195:SER:HB2	1.92	0.51
1:C:139:TRP:O	1:C:143:HIS:CD2	2.63	0.51
1:D:129:VAL:O	1:D:133:ARG:HG2	2.10	0.51
1:D:254:LEU:HA	1:D:258:LEU:HD23	1.93	0.51
1:A:140:VAL:HG12	1:A:148:ILE:O	2.11	0.51
1:D:76:ARG:HD3	1:D:116:LEU:O	2.11	0.51
1:A:21:GLN:NE2	1:A:251:THR:O	2.44	0.51
1:B:54:THR:CG2	1:B:297:ASP:HB3	2.35	0.51
1:B:126:PHE:O	1:B:159:GLN:HA	2.11	0.51
1:B:250:LEU:O	1:B:254:LEU:HG	2.10	0.51
1:C:183:SER:HB3	1:C:203:ALA:HB3	1.93	0.51
1:C:186:ARG:NH1	1:C:200:PRO:HD3	2.26	0.51
1:A:148:ILE:HG12	1:A:325:LYS:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HD21	1:A:262:TRP:HZ2	1.76	0.51
1:B:72:ALA:HB3	1:B:73:PRO:HD3	1.93	0.51
1:B:87:ASN:CG	1:B:91:ILE:HG22	2.31	0.51
1:C:180:PRO:O	1:C:181:ASP:HB2	2.11	0.51
1:D:97:ILE:HG12	1:D:165:LEU:HD23	1.92	0.51
1:D:359:LEU:HD12	1:D:374:GLY:O	2.10	0.51
1:B:49:THR:HG1	1:B:306:PHE:HD2	1.58	0.51
1:D:20:PHE:HA	1:D:23:VAL:HG13	1.92	0.51
1:B:104:LYS:HD3	1:B:312:GLN:HG3	1.92	0.50
1:B:110:MET:HB3	1:C:114:PHE:CE2	2.45	0.50
1:B:243:LYS:HA	1:B:356:ARG:HE	1.76	0.50
1:A:329:ASN:HD22	1:A:331:SER:H	1.58	0.50
1:B:33:VAL:H	1:B:282:THR:CG2	2.19	0.50
1:C:8:VAL:HG21	1:C:74:ALA:HB3	1.91	0.50
1:C:217:ASP:HB2	3:C:1135:HOH:O	2.11	0.50
1:C:348:ALA:HB1	1:C:349:PRO:CD	2.41	0.50
1:D:28:LYS:H	1:D:28:LYS:HD2	1.75	0.50
1:C:33:VAL:H	1:C:282:THR:HG21	1.76	0.50
1:D:115:ARG:HG3	1:D:115:ARG:NH1	2.19	0.50
1:B:278:PHE:CD2	1:B:328:VAL:HG11	2.47	0.50
1:D:288:LYS:HB2	1:D:289:PRO:HD3	1.93	0.50
1:C:19:VAL:O	1:C:22:GLN:HB2	2.12	0.50
1:D:205:THR:O	1:D:206:ASN:HB3	2.12	0.50
1:A:55:GLN:O	1:A:58:ILE:HG22	2.13	0.49
1:C:8:VAL:HG21	1:C:74:ALA:CB	2.42	0.49
1:C:248:SER:HA	1:C:251:THR:CG2	2.41	0.49
1:A:87:ASN:HD21	1:A:91:ILE:HG23	1.76	0.49
1:A:276:PRO:HD3	1:A:354:ILE:HB	1.94	0.49
1:C:174:GLN:HE22	1:C:229:HIS:CB	2.24	0.49
1:D:205:THR:CG2	1:D:272:LEU:HD13	2.41	0.49
1:B:104:LYS:HD3	1:B:312:GLN:CB	2.43	0.49
1:C:254:LEU:HA	1:C:258:LEU:HD23	1.93	0.49
1:A:306:PHE:CZ	1:A:317:VAL:HG23	2.48	0.49
1:B:79:TYR:CE1	1:B:83:MET:HG3	2.47	0.49
1:B:92:SER:O	1:B:169:LEU:HA	2.13	0.49
1:B:223:ILE:HD13	1:B:262:TRP:CG	2.48	0.49
1:B:236:PHE:O	1:B:360:PHE:HA	2.13	0.49
1:A:175:TRP:HZ2	1:A:328:VAL:HG13	1.78	0.48
1:C:185:HIS:NE2	1:C:187:ARG:HD2	2.28	0.48
1:A:8:VAL:CG1	1:A:75:LEU:HD13	2.43	0.48
1:A:106:VAL:HG23	1:A:310:SER:CA	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:PRO:HD2	1:B:356:ARG:NH1	2.28	0.48
1:C:131:ARG:O	1:C:135:ILE:HG13	2.12	0.48
1:D:255:SER:O	1:D:259:ILE:HD12	2.12	0.48
1:A:181:ASP:HB3	3:A:1015:HOH:O	2.14	0.48
1:A:252:ASN:N	1:A:252:ASN:HD22	2.12	0.48
1:C:100:GLN:HE21	1:C:102:ASP:HB2	1.78	0.48
1:D:251:THR:HG22	1:D:359:LEU:HD22	1.94	0.48
1:A:15:PHE:O	1:A:19:VAL:HG23	2.13	0.48
1:A:342:ILE:HG13	1:A:343:VAL:N	2.25	0.48
1:B:48:LEU:CD2	1:B:113:PHE:HA	2.44	0.48
1:D:306:PHE:CE2	1:D:316:HIS:HA	2.49	0.48
1:D:100:GLN:HE21	1:D:101:ARG:H	1.60	0.48
1:A:254:LEU:HD11	1:A:259:ILE:HD11	1.96	0.48
1:B:267:THR:HB	3:B:1296:HOH:O	2.13	0.48
1:B:278:PHE:H	1:B:328:VAL:CG1	2.25	0.48
1:A:208:PHE:O	1:A:268:ARG:HA	2.13	0.48
1:A:240:PRO:HB3	1:A:245:VAL:HB	1.96	0.48
1:C:86:TRP:O	1:C:229:HIS:HE1	1.97	0.48
1:C:248:SER:HA	1:C:251:THR:HG22	1.94	0.48
1:A:173:GLY:HA2	1:A:228:TYR:CE1	2.49	0.48
1:A:190:HIS:HD2	1:A:196:THR:HG22	1.78	0.48
1:B:269:LEU:HD13	1:B:271:ARG:CZ	2.43	0.48
1:A:295:MET:HB3	1:A:298:MET:HE2	1.96	0.47
1:C:129:VAL:O	1:C:133:ARG:HG2	2.14	0.47
1:C:167:ASN:O	1:C:322:GLN:HA	2.13	0.47
1:A:58:ILE:HD13	1:A:58:ILE:O	2.14	0.47
1:B:278:PHE:H	1:B:328:VAL:HG13	1.79	0.47
1:C:225:GLU:HG2	1:C:234:SER:OG	2.14	0.47
1:A:148:ILE:HG23	1:A:323:LYS:HD2	1.95	0.47
1:C:83:MET:SD	1:C:91:ILE:CG2	3.02	0.47
1:D:263:LYS:HA	1:D:266:MET:HG3	1.97	0.47
1:B:199:VAL:HG22	1:B:200:PRO:HD2	1.95	0.47
1:D:53:GLU:CD	1:D:53:GLU:H	2.16	0.47
1:C:93:THR:HG22	1:C:169:LEU:HD13	1.96	0.47
1:D:287:ARG:O	1:D:291:GLU:HG3	2.14	0.47
1:A:91:ILE:HA	1:A:170:TYR:O	2.15	0.47
1:C:128:GLU:OE2	1:D:60:ALA:HA	2.15	0.47
1:C:186:ARG:O	1:C:187:ARG:HB2	2.14	0.47
1:D:151:LEU:HB3	1:D:154:THR:HG23	1.97	0.47
1:B:90:GLU:O	1:B:171:PHE:HA	2.14	0.47
1:B:91:ILE:HD13	1:B:372:PHE:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:GLN:HA	1:C:124:VAL:O	2.14	0.47
1:C:206:ASN:N	1:C:206:ASN:ND2	2.61	0.47
1:B:170:TYR:HD1	1:B:325:LYS:HB3	1.80	0.47
1:C:199:VAL:HG11	1:C:379:PRO:HG2	1.97	0.47
1:D:110:MET:HB2	1:D:111:PRO:HD3	1.97	0.47
1:D:201:MET:HG2	1:D:276:PRO:HA	1.97	0.47
1:A:214:THR:HA	1:A:219:HIS:O	2.15	0.47
1:A:361:VAL:HG13	1:A:370:VAL:HG13	1.96	0.47
1:B:226:LEU:HD12	1:B:237:ILE:CD1	2.45	0.47
1:C:222:ASP:O	1:C:238:ALA:HA	2.14	0.47
1:A:160:LEU:N	1:A:160:LEU:HD22	2.29	0.46
1:C:49:THR:HG22	1:C:109:PHE:HZ	1.79	0.46
1:D:163:LEU:HB2	1:D:315:LEU:CD1	2.45	0.46
1:D:258:LEU:O	1:D:261:HIS:HB3	2.15	0.46
1:B:206:ASN:N	1:B:206:ASN:HD22	2.13	0.46
1:B:348:ALA:HA	1:B:349:PRO:HD2	1.69	0.46
1:D:185:HIS:HD1	1:D:185:HIS:H	1.64	0.46
1:B:66:ILE:HG12	1:B:117:PHE:CZ	2.50	0.46
1:B:223:ILE:HD13	1:B:262:TRP:CD1	2.51	0.46
1:B:228:TYR:CD2	1:B:233:LEU:HD12	2.51	0.46
1:C:103:LEU:CD1	1:C:315:LEU:HD21	2.45	0.46
1:C:288:LYS:HB2	1:C:289:PRO:HD3	1.97	0.46
1:A:325:LYS:NZ	2:A:1001:CL:CL	2.86	0.46
1:B:42:VAL:HG12	1:B:95:ASP:HB3	1.97	0.46
1:C:215:THR:CG2	1:C:217:ASP:H	2.29	0.46
1:D:161:THR:O	1:D:162:ARG:HG2	2.14	0.46
1:A:313:GLU:HA	1:A:314:PRO:HD3	1.71	0.46
1:C:103:LEU:HD11	1:C:315:LEU:HD21	1.98	0.46
1:A:313:GLU:HG2	1:A:315:LEU:HB2	1.96	0.46
1:C:347:MET:SD	1:C:347:MET:N	2.89	0.46
1:D:100:GLN:HG2	1:D:126:PHE:CD2	2.47	0.46
1:A:27:SER:CB	1:A:32:VAL:HG21	2.45	0.46
1:A:197:VAL:HG23	3:A:1104:HOH:O	2.16	0.46
1:C:20:PHE:CD2	1:C:373:MET:HE1	2.51	0.46
1:C:206:ASN:ND2	1:C:208:PHE:CZ	2.84	0.46
1:D:306:PHE:CZ	1:D:317:VAL:HG23	2.51	0.46
1:B:272:LEU:H	1:B:351:GLU:HA	1.80	0.45
1:C:131:ARG:HA	1:C:134:PHE:HB3	1.98	0.45
1:A:150:HIS:HE1	1:D:185:HIS:HD2	1.62	0.45
1:C:5:PRO:HB3	3:C:1276:HOH:O	2.16	0.45
1:C:32:VAL:HA	1:C:282:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ARG:HA	1:B:123:GLN:HB3	1.99	0.45
1:C:185:HIS:NE2	1:C:187:ARG:NH1	2.61	0.45
1:D:135:ILE:HG23	3:D:1365:HOH:O	2.15	0.45
1:A:49:THR:HB	1:A:309:LEU:HB2	1.97	0.45
1:B:48:LEU:HD23	1:B:113:PHE:HA	1.98	0.45
1:B:54:THR:OG1	1:B:305:ASP:HB3	2.15	0.45
1:B:199:VAL:HG21	1:B:379:PRO:HG2	1.99	0.45
1:B:225:GLU:OE2	1:B:263:LYS:HE2	2.15	0.45
1:D:215:THR:OG1	1:D:219:HIS:HB2	2.16	0.45
1:B:207:LYS:HZ2	1:B:270:PRO:HD3	1.79	0.45
1:B:237:ILE:HG23	1:B:358:PHE:CD2	2.51	0.45
1:B:250:LEU:O	1:B:250:LEU:HD23	2.15	0.45
1:C:38:GLY:O	1:C:42:VAL:HG22	2.17	0.45
1:A:114:PHE:O	1:A:118:ARG:N	2.44	0.45
1:A:313:GLU:HG3	1:A:315:LEU:HB2	1.98	0.45
1:D:49:THR:HG22	1:D:109:PHE:HZ	1.81	0.45
1:D:116:LEU:HD22	3:D:1411:HOH:O	2.14	0.45
1:D:201:MET:HG2	1:D:276:PRO:CA	2.47	0.45
1:A:247:LEU:HB3	1:A:359:LEU:HD23	1.98	0.45
1:B:13:SER:O	1:B:17:VAL:HG23	2.17	0.45
1:A:76:ARG:HB2	3:A:1409:HOH:O	2.16	0.44
1:C:174:GLN:HE21	1:C:174:GLN:HB3	1.58	0.44
1:D:332:GLY:O	1:D:333:THR:HB	2.17	0.44
1:B:107:GLN:NE2	1:C:123:GLN:OE1	2.51	0.44
1:D:33:VAL:H	1:D:282:THR:CG2	2.30	0.44
1:B:50:THR:HG21	1:B:58:ILE:HD11	1.98	0.44
1:D:262:TRP:HB3	1:D:266:MET:HE2	2.00	0.44
1:A:150:HIS:CE1	1:D:185:HIS:HD2	2.34	0.44
1:C:17:VAL:O	1:C:21:GLN:HG3	2.18	0.44
1:A:211:THR:CG2	1:A:223:ILE:HB	2.47	0.44
1:B:108:GLY:C	1:B:111:PRO:HD2	2.38	0.44
1:C:363:ARG:HH11	1:C:365:ASN:HA	1.83	0.44
1:A:199:VAL:HG21	1:A:379:PRO:HB2	2.00	0.44
1:B:82:LEU:HD21	1:B:364:HIS:HB2	2.00	0.44
1:B:312:GLN:H	1:B:312:GLN:HG2	1.59	0.44
1:C:101:ARG:HD3	1:C:123:GLN:O	2.17	0.44
1:C:141:LYS:HB2	1:C:149:SER:HA	1.99	0.44
1:C:224:LEU:O	1:C:236:PHE:HA	2.18	0.44
1:C:281:GLU:HG2	1:C:325:LYS:HG3	1.99	0.44
1:C:330:GLU:O	1:C:331:SER:HB3	2.17	0.44
1:B:140:VAL:HG11	1:B:151:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LYS:HG3	1:C:29:ASP:H	1.82	0.44
1:C:312:GLN:HE21	1:C:312:GLN:HA	1.82	0.44
1:D:206:ASN:ND2	1:D:208:PHE:CZ	2.85	0.44
1:D:313:GLU:CB	1:D:314:PRO:CA	2.96	0.44
1:A:141:LYS:HD2	1:A:149:SER:HB2	2.00	0.44
1:B:39:VAL:HG13	1:B:40:ALA:N	2.32	0.44
1:D:44:ALA:HB1	1:D:66:ILE:HD13	2.00	0.44
1:D:50:THR:HG22	1:D:306:PHE:CD1	2.52	0.44
1:D:187:ARG:HD3	1:D:353:ILE:CD1	2.46	0.44
1:A:201:MET:HG2	1:A:276:PRO:HA	1.99	0.44
1:A:307:THR:HA	1:A:310:SER:O	2.17	0.44
1:D:313:GLU:OE1	1:D:315:LEU:HD23	2.17	0.44
1:A:131:ARG:O	1:A:135:ILE:HG13	2.18	0.43
1:A:341:VAL:HG23	1:A:342:ILE:HG23	2.00	0.43
1:B:255:SER:O	1:B:259:ILE:HG23	2.17	0.43
1:B:66:ILE:HG12	1:B:117:PHE:HZ	1.83	0.43
1:B:248:SER:HA	1:B:251:THR:OG1	2.18	0.43
1:C:39:VAL:O	1:C:43:LEU:HD23	2.18	0.43
1:D:106:VAL:HG23	1:D:311:ASP:H	1.82	0.43
1:D:269:LEU:HB3	1:D:271:ARG:CZ	2.48	0.43
1:A:203:ALA:HA	1:A:273:LEU:O	2.19	0.43
1:D:38:GLY:HA2	3:D:1327:HOH:O	2.17	0.43
1:D:148:ILE:HG23	1:D:323:LYS:HD3	1.99	0.43
1:B:254:LEU:HA	1:B:258:LEU:HD23	1.99	0.43
1:C:187:ARG:NH1	1:C:274:VAL:HG21	2.33	0.43
1:C:199:VAL:HG13	1:C:200:PRO:HD2	2.01	0.43
1:D:162:ARG:CG	1:D:162:ARG:NH1	2.71	0.43
1:A:278:PHE:CZ	1:A:328:VAL:HG21	2.53	0.43
1:B:171:PHE:HB2	1:B:372:PHE:CE2	2.53	0.43
1:C:151:LEU:HD11	1:C:166:VAL:CG1	2.49	0.43
1:C:184:THR:HA	1:C:202:MET:HA	1.99	0.43
1:C:346:ARG:HG2	1:C:346:ARG:HH11	1.83	0.43
1:D:86:TRP:CE3	1:D:232:THR:HG21	2.54	0.43
1:D:254:LEU:CD1	1:D:359:LEU:HD21	2.48	0.43
1:B:227:PRO:HA	1:B:234:SER:CB	2.44	0.43
1:D:17:VAL:HG11	1:D:254:LEU:O	2.18	0.43
1:A:132:ALA:O	1:A:136:ILE:HG13	2.19	0.43
1:B:53:GLU:O	1:B:57:GLN:HG3	2.19	0.43
1:B:272:LEU:HB3	1:B:351:GLU:CB	2.46	0.43
1:C:5:PRO:HD2	1:C:78:LEU:HB2	2.00	0.43
1:C:278:PHE:CZ	1:C:328:VAL:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLU:HA	1:B:322:GLN:O	2.18	0.43
1:C:255:SER:O	1:C:259:ILE:HG12	2.18	0.43
1:D:68:ASP:O	1:D:71:MET:HG2	2.19	0.43
1:D:210:TYR:HB3	1:D:269:LEU:HD23	2.01	0.43
1:A:6:SER:O	1:A:10:HIS:CD2	2.72	0.43
1:B:28:LYS:O	1:B:29:ASP:HB2	2.19	0.43
1:B:33:VAL:CG2	1:B:280:LEU:HB3	2.49	0.43
1:C:47:GLN:HA	1:C:50:THR:HG22	2.00	0.43
1:C:101:ARG:HA	1:C:123:GLN:HB3	2.00	0.43
1:B:54:THR:HG21	1:B:305:ASP:H	1.84	0.42
1:C:78:LEU:HD11	1:C:369:THR:OG1	2.20	0.42
1:D:201:MET:HA	1:D:276:PRO:HA	2.00	0.42
1:D:352:ILE:HG12	3:D:1169:HOH:O	2.18	0.42
1:A:165:LEU:HB3	1:A:320:ALA:HA	2.00	0.42
1:C:173:GLY:HA2	1:C:228:TYR:CE1	2.54	0.42
1:C:283:GLU:HA	1:C:322:GLN:O	2.19	0.42
1:D:100:GLN:HA	1:D:124:VAL:O	2.19	0.42
1:A:8:VAL:HG11	1:A:75:LEU:HD13	2.01	0.42
1:A:284:VAL:HG13	1:D:342:ILE:HG22	2.01	0.42
1:D:76:ARG:HH11	1:D:116:LEU:HA	1.82	0.42
1:D:136:ILE:O	1:D:140:VAL:HG23	2.20	0.42
1:D:10:HIS:CD2	3:D:1466:HOH:O	2.73	0.42
1:B:79:TYR:CZ	1:B:83:MET:HG3	2.55	0.42
1:B:201:MET:HG2	1:B:276:PRO:CA	2.49	0.42
1:D:364:HIS:O	1:D:368:GLY:N	2.44	0.42
1:B:22:GLN:HG3	1:B:292:ASN:HD22	1.84	0.42
1:A:329:ASN:HB2	1:A:333:THR:OG1	2.20	0.42
1:B:210:TYR:HE2	1:B:222:ASP:HB3	1.82	0.42
1:C:20:PHE:CD2	1:C:373:MET:CE	3.02	0.42
1:C:185:HIS:HD2	1:C:186:ARG:O	2.03	0.42
1:C:190:HIS:HE1	3:C:1336:HOH:O	2.02	0.42
1:D:6:SER:O	1:D:10:HIS:HB2	2.20	0.42
1:D:147:MET:HG3	1:D:170:TYR:CD2	2.55	0.42
1:A:211:THR:HG22	1:A:223:ILE:HB	2.00	0.42
1:C:91:ILE:HD11	1:C:372:PHE:CZ	2.55	0.42
1:D:100:GLN:NE2	1:D:101:ARG:H	2.18	0.41
1:A:175:TRP:NE1	1:A:329:ASN:O	2.44	0.41
1:A:267:THR:HG21	3:A:1058:HOH:O	2.19	0.41
1:C:235:MET:HG2	1:C:237:ILE:HD12	2.01	0.41
1:D:206:ASN:N	1:D:206:ASN:HD22	2.19	0.41
1:D:277:LYS:HE3	1:D:277:LYS:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:PHE:HA	1:D:23:VAL:CG1	2.50	0.41
1:D:254:LEU:HG	1:D:258:LEU:HD23	2.02	0.41
1:B:255:SER:HA	3:B:1277:HOH:O	2.20	0.41
1:C:68:ASP:O	1:C:69:LYS:HB2	2.20	0.41
1:C:313:GLU:HA	1:C:314:PRO:HD2	1.92	0.41
1:B:91:ILE:HD13	1:B:372:PHE:CE2	2.56	0.41
1:B:212:GLU:O	1:B:212:GLU:HG3	2.20	0.41
1:C:288:LYS:N	1:C:289:PRO:CD	2.83	0.41
1:D:104:LYS:HD3	1:D:104:LYS:HA	1.85	0.41
1:C:286:LEU:C	1:C:289:PRO:HD2	2.40	0.41
1:C:82:LEU:HG	1:C:82:LEU:H	1.48	0.41
1:C:151:LEU:HB2	1:C:154:THR:HG23	2.03	0.41
1:C:164:VAL:HG12	1:C:165:LEU:N	2.35	0.41
1:A:179:PHE:O	1:A:180:PRO:O	2.39	0.41
1:A:232:THR:O	1:A:233:LEU:HD23	2.21	0.41
1:A:376:VAL:CG1	1:A:379:PRO:HG3	2.51	0.41
1:B:174:GLN:HE21	1:B:174:GLN:HA	1.85	0.41
1:B:183:SER:HB3	1:B:203:ALA:HB3	2.03	0.41
1:B:257:GLN:NE2	3:B:1279:HOH:O	2.53	0.41
1:C:15:PHE:O	1:C:18:ARG:HB2	2.20	0.41
1:C:176:LYS:HE2	1:C:177:THR:CB	2.41	0.41
1:D:5:PRO:CG	1:D:6:SER:H	2.29	0.41
1:D:72:ALA:N	1:D:73:PRO:HD2	2.35	0.41
1:D:221:TYR:CE2	1:D:240:PRO:HB3	2.56	0.41
1:D:242:GLU:O	1:D:245:VAL:HG23	2.21	0.41
1:A:47:GLN:HG2	1:A:58:ILE:HD12	2.03	0.41
1:A:375:GLN:HB3	1:A:377:MET:CE	2.51	0.41
1:C:176:LYS:H	1:C:176:LYS:HG3	1.68	0.41
1:D:226:LEU:HD21	1:D:273:LEU:HD21	2.02	0.41
1:B:16:GLY:HA3	1:B:36:PRO:HB3	2.03	0.40
1:B:185:HIS:HA	1:B:186:ARG:HH21	1.87	0.40
1:B:236:PHE:CE1	1:B:363:ARG:HD3	2.56	0.40
1:C:215:THR:HG22	1:C:217:ASP:H	1.85	0.40
1:C:235:MET:HG2	1:C:237:ILE:CD1	2.51	0.40
1:A:98:PHE:O	1:A:163:LEU:HA	2.22	0.40
1:A:131:ARG:HD2	1:A:131:ARG:HA	1.89	0.40
1:B:243:LYS:CD	1:B:243:LYS:N	2.75	0.40
1:C:221:TYR:CE1	1:C:223:ILE:HD11	2.55	0.40
1:C:275:LEU:HA	1:C:276:PRO:HD3	1.95	0.40
1:D:126:PHE:C	1:D:128:GLU:H	2.24	0.40
1:D:214:THR:HA	1:D:219:HIS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:THR:HG22	1:D:269:LEU:HD22	2.03	0.40
1:A:187:ARG:NH1	1:A:274:VAL:HG11	2.36	0.40
1:B:259:ILE:HD11	3:B:1285:HOH:O	2.21	0.40
1:D:270:PRO:O	1:D:271:ARG:NH1	2.50	0.40

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	371/379 (98%)	330 (89%)	28 (8%)	13 (4%)	3	3
1	B	361/379 (95%)	333 (92%)	20 (6%)	8 (2%)	6	7
1	C	360/379 (95%)	325 (90%)	22 (6%)	13 (4%)	3	3
1	D	368/379 (97%)	326 (89%)	27 (7%)	15 (4%)	3	2
All	All	1460/1516 (96%)	1314 (90%)	97 (7%)	49 (3%)	3	3

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	173	GLY
1	A	174	GLN
1	A	180	PRO
1	A	181	ASP
1	B	173	GLY
1	B	349	PRO
1	B	350	GLU
1	C	68	ASP
1	C	173	GLY
1	C	180	PRO

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Mol	Chain	Res	Type
1	C	181	ASP
1	C	193	ASP
1	C	331	SER
1	C	350	GLU
1	D	5	PRO
1	D	313	GLU
1	A	129	VAL
1	B	174	GLN
1	B	192	SER
1	B	333	THR
1	D	28	LYS
1	A	286	LEU
1	A	314	PRO
1	A	335	ALA
1	C	187	ARG
1	C	287	ARG
1	C	313	GLU
1	D	194	GLY
1	D	199	VAL
1	D	206	ASN
1	D	331	SER
1	A	242	GLU
1	B	313	GLU
1	C	174	GLN
1	D	172	ASN
1	D	287	ARG
1	A	28	LYS
1	A	241	TYR
1	A	337	SER
1	C	69	LYS
1	D	244	GLU
1	D	339	THR
1	B	348	ALA
1	D	129	VAL
1	D	193	ASP
1	C	349	PRO
1	D	332	GLY
1	D	32	VAL

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	328/333 (98%)	300 (92%)	28 (8%)	10	16
1	B	321/333 (96%)	290 (90%)	31 (10%)	8	12
1	C	319/333 (96%)	281 (88%)	38 (12%)	5	6
1	D	326/333 (98%)	289 (89%)	37 (11%)	6	8
All	All	1294/1332 (97%)	1160 (90%)	134 (10%)	7	10

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	23	VAL
1	A	25	GLN
1	A	30	ARG
1	A	58	ILE
1	A	67	ASP
1	A	88	LYS
1	A	92	SER
1	A	116	LEU
1	A	158	GLN
1	A	169	LEU
1	A	172	ASN
1	A	180	PRO
1	A	241	TYR
1	A	250	LEU
1	A	251	THR
1	A	252	ASN
1	A	260	SER
1	A	266	MET
1	A	277	LYS
1	A	286	LEU
1	A	301	GLN
1	A	311	ASP
1	A	312	GLN

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Mol	Chain	Res	Type
1	A	323	LYS
1	A	329	ASN
1	A	342	ILE
1	A	363	ARG
1	B	22	GLN
1	B	23	VAL
1	B	28	LYS
1	B	30	ARG
1	B	92	SER
1	B	103	LEU
1	B	104	LYS
1	B	118	ARG
1	B	124	VAL
1	B	128	GLU
1	B	158	GLN
1	B	159	GLN
1	B	169	LEU
1	B	174	GLN
1	B	182	SER
1	B	186	ARG
1	B	202	MET
1	B	205	THR
1	B	206	ASN
1	B	243	LYS
1	B	247	LEU
1	B	251	THR
1	B	259	ILE
1	B	266	MET
1	B	269	LEU
1	B	272	LEU
1	B	282	THR
1	B	311	ASP
1	B	312	GLN
1	B	349	PRO
1	B	376	VAL
1	C	30	ARG
1	C	42	VAL
1	C	69	LYS
1	C	82	LEU
1	C	91	ILE
1	C	131	ARG
1	C	141	LYS

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Mol	Chain	Res	Type
1	C	142	THR
1	C	159	GLN
1	C	162	ARG
1	C	169	LEU
1	C	174	GLN
1	C	176	LYS
1	C	180	PRO
1	C	181	ASP
1	C	186	ARG
1	C	198	SER
1	C	205	THR
1	C	206	ASN
1	C	209	ASN
1	C	212	GLU
1	C	215	THR
1	C	217	ASP
1	C	224	LEU
1	C	229	HIS
1	C	247	LEU
1	C	254	LEU
1	C	271	ARG
1	C	277	LYS
1	C	282	THR
1	C	293	LEU
1	C	311	ASP
1	C	312	GLN
1	C	327	GLU
1	C	347	MET
1	C	349	PRO
1	C	363	ARG
1	C	376	VAL
1	D	23	VAL
1	D	53	GLU
1	D	67	ASP
1	D	91	ILE
1	D	100	GLN
1	D	105	LEU
1	D	115	ARG
1	D	128	GLU
1	D	130	GLU
1	D	147	MET
1	D	152	LEU

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Mol	Chain	Res	Type
1	D	158	GLN
1	D	159	GLN
1	D	162	ARG
1	D	169	LEU
1	D	181	ASP
1	D	186	ARG
1	D	188	LEU
1	D	192	SER
1	D	193	ASP
1	D	197	VAL
1	D	198	SER
1	D	204	GLN
1	D	206	ASN
1	D	214	THR
1	D	241	TYR
1	D	250	LEU
1	D	254	LEU
1	D	257	GLN
1	D	289	PRO
1	D	315	LEU
1	D	330	GLU
1	D	346	ARG
1	D	353	ILE
1	D	357	PRO
1	D	363	ARG
1	D	376	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	107	GLN
1	A	150	HIS
1	A	172	ASN
1	A	190	HIS
1	A	219	HIS
1	A	252	ASN
1	A	301	GLN
1	A	329	ASN
1	A	375	GLN
1	B	22	GLN
1	B	57	GLN

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Mol	Chain	Res	Type
1	B	59	GLN
1	B	77	HIS
1	B	100	GLN
1	B	159	GLN
1	B	206	ASN
1	B	257	GLN
1	B	265	ASN
1	B	292	ASN
1	B	312	GLN
1	C	22	GLN
1	C	56	GLN
1	C	87	ASN
1	C	112	HIS
1	C	143	HIS
1	C	159	GLN
1	C	174	GLN
1	C	206	ASN
1	C	209	ASN
1	C	229	HIS
1	C	292	ASN
1	C	303	GLN
1	C	312	GLN
1	C	316	HIS
1	C	375	GLN
1	D	10	HIS
1	D	25	GLN
1	D	77	HIS
1	D	100	GLN
1	D	112	HIS
1	D	158	GLN
1	D	174	GLN
1	D	204	GLN
1	D	206	ASN
1	D	257	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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	375/379 (98%)	-0.51	9 (2%)	59	57	3, 16, 45, 80	2 (0%)
1	B	365/379 (96%)	-0.36	8 (2%)	62	60	5, 20, 51, 92	0
1	C	364/379 (96%)	-0.34	7 (1%)	66	64	4, 21, 49, 82	2 (0%)
1	D	372/379 (98%)	-0.51	8 (2%)	62	60	3, 17, 42, 82	0
All	All	1476/1516 (97%)	-0.43	32 (2%)	62	60	3, 18, 48, 92	4 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	SER	6.2
1	D	333	THR	6.2
1	A	5	PRO	6.1
1	B	333	THR	5.8
1	B	335	ALA	5.7
1	B	334	VAL	5.5
1	C	332	GLY	5.3
1	D	339	THR	4.8
1	D	338	SER	4.8
1	C	349	PRO	4.7
1	A	314	PRO	4.2
1	B	196	THR	3.8
1	A	334	VAL	3.7
1	C	346	ARG	3.5
1	B	85	PRO	3.4
1	D	5	PRO	3.4
1	A	333	THR	3.3
1	A	332	GLY	3.1
1	C	348	ALA	3.0
1	B	347	MET	3.0
1	C	312	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	4	PRO	2.8
1	D	332	GLY	2.8
1	A	335	ALA	2.8
1	B	312	GLN	2.6
1	C	85	PRO	2.6
1	A	337	SER	2.3
1	D	312	GLN	2.3
1	C	345	ALA	2.3
1	B	84	GLY	2.2
1	D	311	ASP	2.2
1	D	242	GLU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	C	1003	1/1	0.98	0.06	26,26,26,26	0
2	CL	D	1002	1/1	0.98	0.07	21,21,21,21	0
2	CL	A	1001	1/1	0.99	0.12	24,24,24,24	0
2	CL	B	1004	1/1	0.99	0.11	32,32,32,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.