



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:52 PM UTC

PDB ID : 1DVM / pdb_00001dvm
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 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:

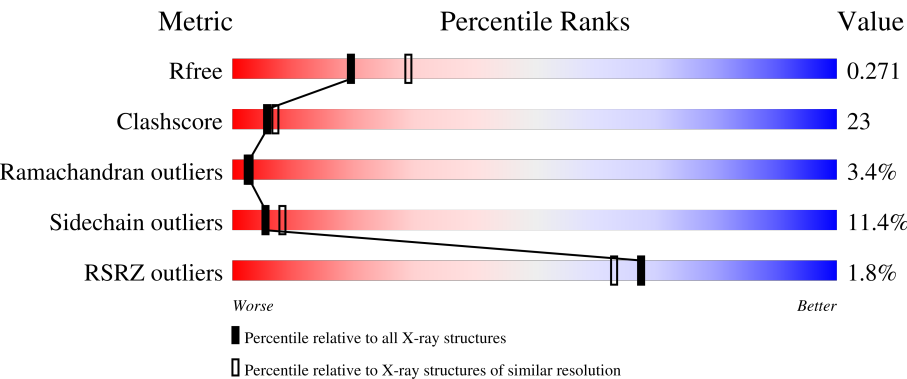
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	379	2% 52%41%6% ..
1	B	379	2% 51%37%8% . .
1	C	379	% 49%37%8% . .
1	D	379	% 51%38%9% .

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 (CCD ID: 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

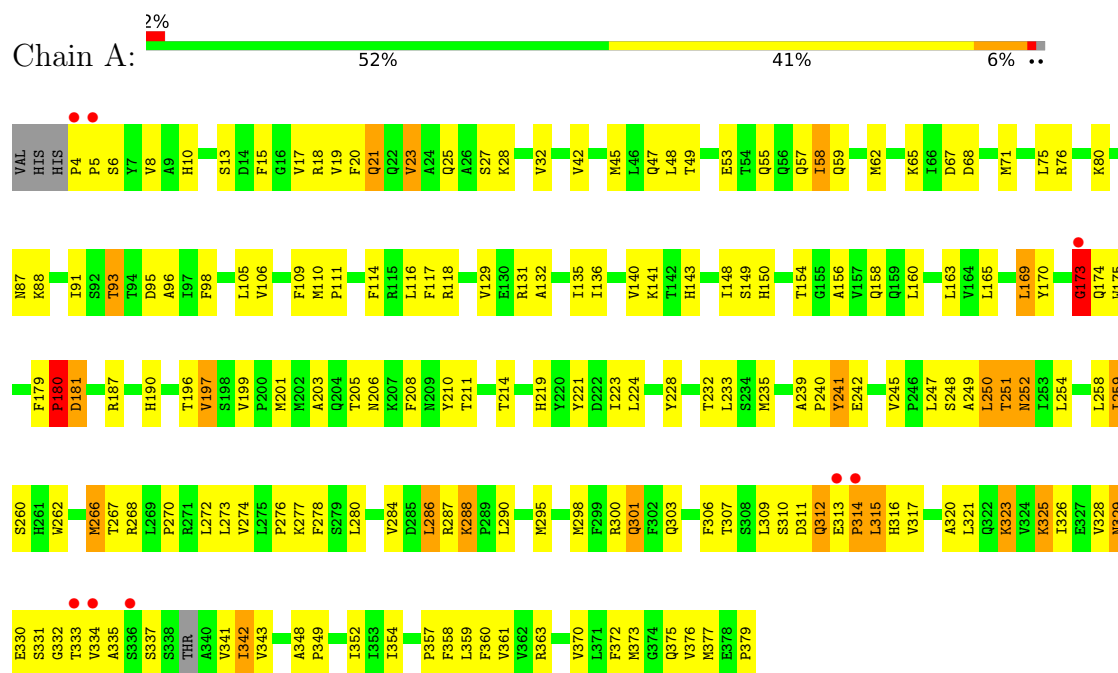
- Molecule 3 is water.

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

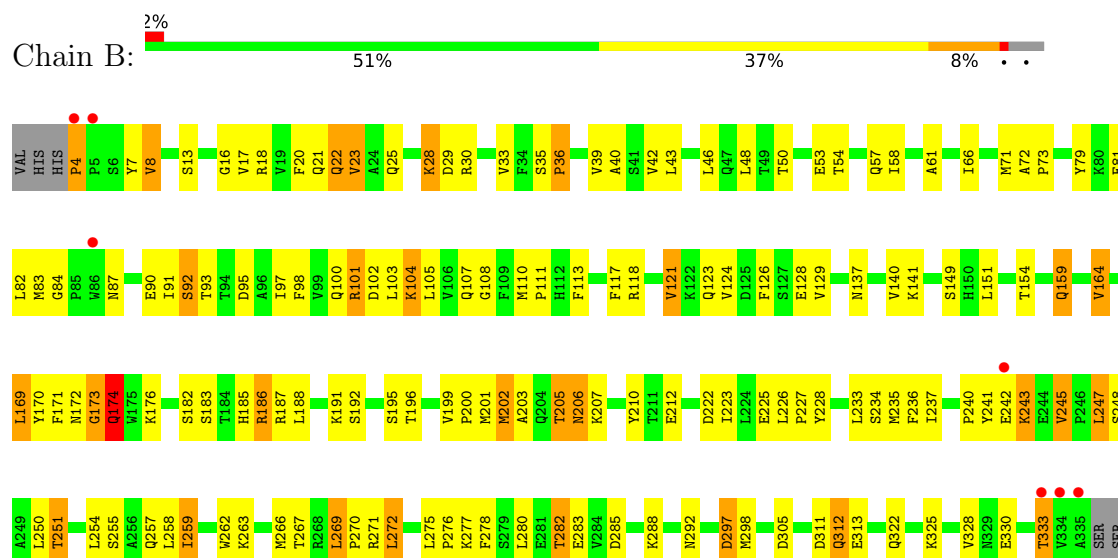
3 Residue-property plots

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

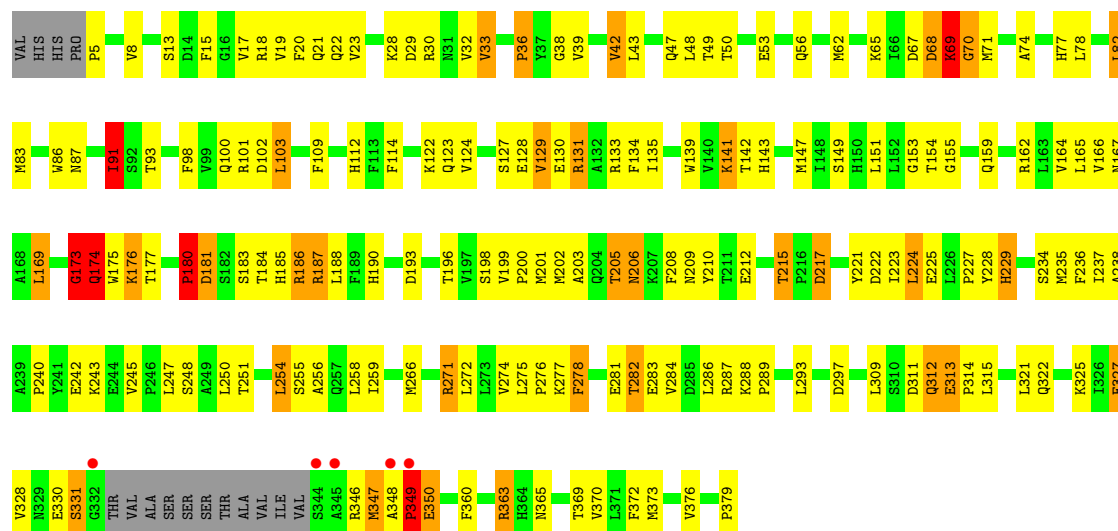


• Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1

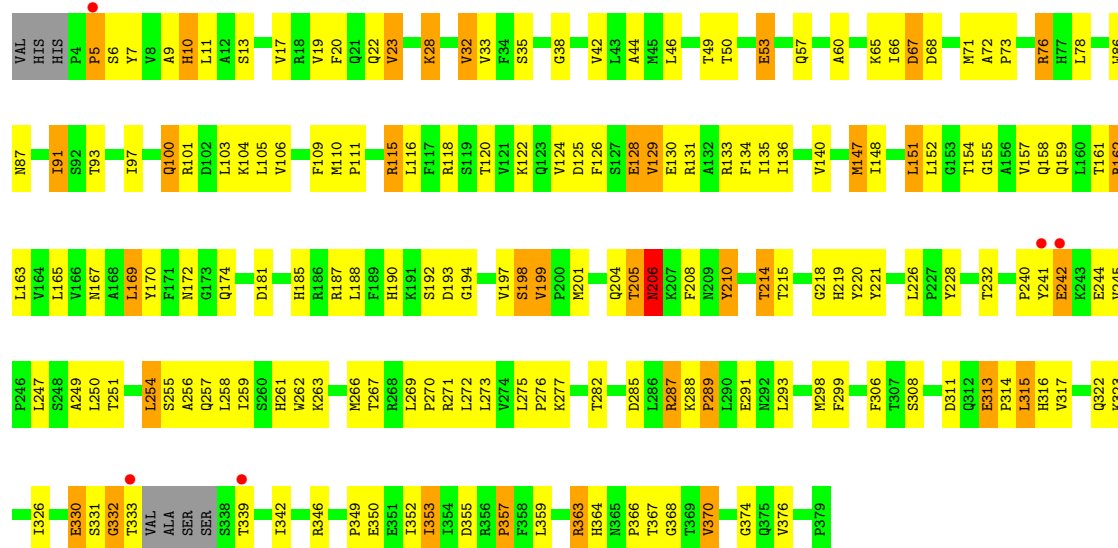




• Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1



• Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1



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 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	80.5 (30.00-2.40) 80.5 (30.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (Å ²)	18.6	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 102.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.53	0/3045	1.05	15/4129 (0.4%)
1	B	0.50	0/2984	1.02	15/4045 (0.4%)
1	C	0.51	0/2973	1.07	17/4028 (0.4%)
1	D	0.54	0/3028	1.05	15/4106 (0.4%)
All	All	0.52	0/12030	1.05	62/16308 (0.4%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	VAL	N-CA-C	8.37	119.15	110.36
1	C	91	ILE	N-CA-C	7.71	118.45	110.05
1	C	70	GLY	N-CA-C	-7.25	105.71	115.36
1	A	173	GLY	N-CA-C	6.99	129.74	113.18
1	D	155	GLY	N-CA-C	-6.97	104.78	115.66
1	A	315	LEU	N-CA-C	6.83	119.55	110.53
1	C	103	LEU	N-CA-C	6.80	119.60	110.35
1	D	241	TYR	N-CA-C	6.73	121.40	112.25
1	B	102	ASP	N-CA-C	6.72	121.64	113.38
1	C	350	GLU	N-CA-C	6.64	124.95	110.80
1	B	129	VAL	N-CA-C	6.44	117.12	110.36
1	A	332	GLY	N-CA-C	-6.20	98.48	113.18
1	D	10	HIS	N-CA-C	-6.17	104.48	111.14
1	A	259	ILE	N-CA-C	-6.10	104.80	110.53
1	A	4	PRO	CA-C-N	6.05	127.41	119.84
1	A	4	PRO	C-N-CA	6.05	127.41	119.84
1	B	351	GLU	N-CA-C	6.05	118.27	109.07
1	D	308	SER	N-CA-C	-5.99	106.10	113.41
1	A	348	ALA	CA-C-N	5.92	125.40	119.24
1	A	348	ALA	C-N-CA	5.92	125.40	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	LEU	N-CA-C	-5.88	104.94	111.71
1	C	147	MET	N-CA-C	5.82	117.63	111.28
1	C	297	ASP	N-CA-C	5.81	117.29	111.07
1	B	121	VAL	N-CA-C	-5.79	102.10	109.80
1	C	278	PHE	N-CA-C	5.73	117.56	108.79
1	B	84	GLY	CA-C-N	5.71	126.10	119.47
1	B	84	GLY	C-N-CA	5.71	126.10	119.47
1	D	35	SER	CA-C-N	5.69	124.89	118.97
1	D	35	SER	C-N-CA	5.69	124.89	118.97
1	B	4	PRO	CA-C-N	5.66	126.04	119.47
1	B	4	PRO	C-N-CA	5.66	126.04	119.47
1	A	287	ARG	N-CA-C	5.64	117.91	111.02
1	A	334	VAL	N-CA-C	-5.64	105.23	110.53
1	C	284	VAL	N-CA-C	5.62	116.84	108.46
1	D	134	PHE	N-CA-C	-5.52	105.18	111.14
1	C	127	SER	N-CA-C	-5.49	105.21	111.14
1	B	285	ASP	N-CA-C	-5.47	99.60	108.41
1	D	247	LEU	N-CA-C	-5.45	105.36	112.23
1	C	186	ARG	N-CA-C	-5.42	103.74	110.41
1	D	242	GLU	N-CA-C	-5.40	99.30	108.26
1	C	33	VAL	N-CA-C	-5.39	100.43	108.46
1	B	297	ASP	N-CA-C	5.38	117.57	111.11
1	B	81	GLU	N-CA-C	-5.37	106.57	113.23
1	C	266	MET	N-CA-C	5.37	117.80	110.55
1	D	210	TYR	N-CA-C	5.35	118.15	109.06
1	B	241	TYR	N-CA-C	-5.26	105.46	111.14
1	C	175	TRP	N-CA-C	5.25	117.46	110.53
1	B	101	ARG	N-CA-C	5.21	118.42	111.75
1	C	155	GLY	N-CA-C	-5.20	108.51	115.32
1	A	301	GLN	N-CA-C	5.19	116.94	111.28
1	A	239	ALA	CA-C-N	5.17	125.18	119.90
1	A	239	ALA	C-N-CA	5.17	125.18	119.90
1	D	9	ALA	N-CA-C	-5.15	105.74	112.23
1	C	77	HIS	N-CA-C	-5.08	105.66	111.14
1	B	176	LYS	N-CA-C	-5.07	105.22	111.40
1	D	218	GLY	N-CA-C	5.05	124.27	114.16
1	D	76	ARG	N-CA-C	-5.05	105.78	111.28
1	D	285	ASP	N-CA-C	-5.04	100.30	108.41
1	C	173	GLY	N-CA-C	5.03	125.11	113.18
1	D	293	LEU	N-CA-C	-5.03	106.83	113.17
1	A	96	ALA	N-CA-C	5.03	117.61	109.06
1	A	143	HIS	N-CA-C	5.02	119.09	112.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2973	0	2967	132	0
1	B	2912	0	2906	142	0
1	C	2902	0	2890	136	0
1	D	2956	0	2950	144	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	545	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 23.

All (545) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:375:GLN:HB3	1:A:377:MET:HE3	1.63	0.81
1:C:176:LYS:HE2	1:C:177:THR:HB	1.64	0.80
1:A:295:MET:HB3	1:A:298:MET:HE2	1.63	0.79
1:D:313:GLU:HG3	1:D:314:PRO:HA	1.63	0.79
1:A:20:PHE:CD2	1:A:373:MET:HE2	2.19	0.78
1:D:364:HIS:CE1	1:D:366:PRO:HG2	2.18	0.78
1:C:20:PHE:CD2	1:C:373:MET:HE2	2.19	0.77
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
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:17:VAL:HG13	1:A:373:MET:HE1	1.69	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:A:211:THR:HG22	1:A:266:MET:HE3	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:313:GLU:HB2	1:D:314:PRO:C	2.23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:HD23	1:A:373:MET:HE3	1.81	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
1:A:150:HIS:HE1	1:D:185:HIS:CD2	2.19	0.60
1:D:262:TRP:HB3	1:D:266:MET:HE2	1.83	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:A:254:LEU:HD23	1:A:373:MET:CE	2.32	0.60
1:B:187:ARG:HB3	1:B:201:MET:HE3	1.83	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:295:MET:CB	1:A:298:MET:HE2	2.36	0.56
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:B:87:ASN:CG	1:B:91:ILE:HG22	2.31	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:254:LEU:HD23	1:C:373:MET:HE3	1.88	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
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:D:53:GLU:CD	1:D:53:GLU:H	2.16	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:20:PHE:HA	1:D:23:VAL:HG13	1.92	0.51
1:A:42:VAL:HA	1:A:45:MET:HE2	1.93	0.50
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:110:MET:HE1	1:B:121:VAL:HG12	1.93	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:228:TYR:OH	1:B:235:MET:HE3	2.12	0.49
1:A:290:LEU:HD13	1:A:298:MET:HE1	1.95	0.49
1:B:104:LYS:HD3	1:B:312:GLN:CB	2.43	0.49
1:B:108:GLY:C	1:B:111:PRO:HD2	2.38	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:C:20:PHE:CE2	1:C:373:MET:HE2	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
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:C:8:VAL:HG22	1:C:71:MET:HE3	1.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:254:LEU:HD13	1:B:373:MET:HE3	1.95	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:206:ASN:ND2	1:C:208:PHE:CZ	2.84	0.46
1:C:286:LEU:C	1:C:289:PRO:HD2	2.40	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
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:126:PHE:C	1:D:128:GLU:H	2.24	0.45
1:D:49:THR:HG22	1:D:109:PHE:HZ	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:MET:HE1	1:A:95:ASP:CB	2.47	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:A:45:MET:HE1	1:A:95:ASP:HB2	1.99	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: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
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:65:LYS:HB2	1:A:68:ASP:CG	2.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:LYS:C	1:C:71:MET:H	2.25	0.43
1:A:321:LEU:C	1:A:321:LEU:HD12	2.44	0.43
1:B:46:LEU:HD23	1:B:298:MET:HE1	2.00	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:71:MET:HE2	1:B:71:MET:HA	2.01	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
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:67:ASP:O	1:C:68:ASP:C	2.61	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:MET:HE2	1:C:62:MET:HB3	1.87	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:A:290:LEU:HD13	1:A:298:MET:CE	2.49	0.42
1:C:254:LEU:HD23	1:C:373:MET:CE	2.49	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:D:298:MET:HE2	1:D:299:PHE:CZ	2.55	0.42
1:A:247:LEU:HD23	1:A:377:MET:HE1	2.02	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: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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:29:ASP:HA	1:B:377:MET:HE2	2.03	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:A:154:THR:C	1:A:156:ALA:H	2.29	0.40
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:A:235:MET:HE2	1:A:360:PHE:CD2	2.56	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:147:MET:HA	1:D:147:MET:HE3	2.03	0.40
1:C:68:ASP:O	1:C:69:LYS:HB2	2.20	0.40
1:D:214:THR:HA	1:D:219:HIS:O	2.21	0.40
1:A:254:LEU:CD2	1:A:373:MET:HE3	2.49	0.40
1:D:267:THR:HG22	1:D:269:LEU:HD22	2.03	0.40
1:A:165:LEU:C	1:A:165:LEU:HD13	2.47	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:PRO:O	1:D:271:ARG:NH1	2.50	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	371/379 (98%)	330 (89%)	28 (8%)	13 (4%)	3	2
1	B	361/379 (95%)	333 (92%)	20 (6%)	8 (2%)	5	6
1	C	360/379 (95%)	325 (90%)	22 (6%)	13 (4%)	2	2
1	D	368/379 (97%)	326 (89%)	27 (7%)	15 (4%)	2	2
All	All	1460/1516 (96%)	1314 (90%)	97 (7%)	49 (3%)	3	2

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
1	C	181	ASP
1	C	193	ASP
1	C	331	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	296 (90%)	32 (10%)	7	12
1	B	321/333 (96%)	285 (89%)	36 (11%)	6	9
1	C	319/333 (96%)	281 (88%)	38 (12%)	5	7
1	D	326/333 (98%)	285 (87%)	41 (13%)	4	6
All	All	1294/1332 (97%)	1147 (89%)	147 (11%)	5	8

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	21	GLN
1	A	23	VAL
1	A	25	GLN
1	A	48	LEU
1	A	58	ILE
1	A	67	ASP
1	A	88	LYS
1	A	93	THR
1	A	105	LEU
1	A	116	LEU
1	A	158	GLN
1	A	169	LEU
1	A	180	PRO
1	A	197	VAL
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	288	LYS
1	A	301	GLN
1	A	311	ASP
1	A	312	GLN
1	A	323	LYS
1	A	325	LYS
1	A	329	ASN
1	A	342	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	363	ARG
1	B	8	VAL
1	B	22	GLN
1	B	23	VAL
1	B	28	LYS
1	B	30	ARG
1	B	36	PRO
1	B	92	SER
1	B	93	THR
1	B	103	LEU
1	B	104	LYS
1	B	118	ARG
1	B	124	VAL
1	B	128	GLU
1	B	159	GLN
1	B	164	VAL
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	245	VAL
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	330	GLU
1	B	349	PRO
1	B	376	VAL
1	C	23	VAL
1	C	30	ARG
1	C	36	PRO
1	C	42	VAL
1	C	69	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	82	LEU
1	C	91	ILE
1	C	131	ARG
1	C	141	LYS
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	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	22	GLN
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	130	GLU
1	D	147	MET
1	D	151	LEU
1	D	152	LEU
1	D	157	VAL
1	D	158	GLN
1	D	159	GLN
1	D	162	ARG
1	D	169	LEU
1	D	174	GLN
1	D	181	ASP
1	D	188	LEU
1	D	192	SER
1	D	197	VAL
1	D	198	SER
1	D	204	GLN
1	D	205	THR
1	D	206	ASN
1	D	214	THR
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	350	GLU
1	D	353	ILE
1	D	357	PRO
1	D	363	ARG
1	D	370	VAL
1	D	376	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	21	GLN
1	A	22	GLN
1	A	25	GLN
1	A	56	GLN
1	A	107	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	150	HIS
1	A	172	ASN
1	A	190	HIS
1	A	219	HIS
1	A	252	ASN
1	A	265	ASN
1	A	292	ASN
1	A	301	GLN
1	A	312	GLN
1	A	329	ASN
1	A	375	GLN
1	B	22	GLN
1	B	56	GLN
1	B	57	GLN
1	B	59	GLN
1	B	77	HIS
1	B	100	GLN
1	B	107	GLN
1	B	158	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	B	365	ASN
1	C	22	GLN
1	C	56	GLN
1	C	87	ASN
1	C	112	HIS
1	C	143	HIS
1	C	174	GLN
1	C	206	ASN
1	C	219	HIS
1	C	229	HIS
1	C	265	ASN
1	C	292	ASN
1	C	303	GLN
1	C	312	GLN
1	C	316	HIS
1	C	375	GLN
1	D	10	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	22	GLN
1	D	77	HIS
1	D	100	GLN
1	D	112	HIS
1	D	158	GLN
1	D	159	GLN
1	D	204	GLN
1	D	206	ASN
1	D	261	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 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 [i](#)

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%)	-0.38	8 (2%) 63 59	3, 16, 45, 80	2 (0%)
1	B	365/379 (96%)	-0.22	8 (2%) 62 58	5, 20, 51, 92	0
1	C	364/379 (96%)	-0.21	5 (1%) 73 69	4, 21, 49, 82	2 (0%)
1	D	372/379 (98%)	-0.40	5 (1%) 75 71	3, 17, 42, 82	0
All	All	1476/1516 (97%)	-0.30	26 (1%) 67 63	3, 18, 48, 92	4 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	333	THR	4.8
1	A	5	PRO	4.6
1	A	314	PRO	3.8
1	B	4	PRO	3.7
1	C	332	GLY	3.4
1	C	345	ALA	3.4
1	D	339	THR	3.3
1	B	333	THR	3.2
1	C	344	SER	3.1
1	A	4	PRO	3.0
1	A	334	VAL	2.8
1	B	334	VAL	2.7
1	B	242	GLU	2.7
1	C	349	PRO	2.7
1	A	336	SER	2.7
1	D	242	GLU	2.6
1	D	5	PRO	2.5
1	A	313	GLU	2.4
1	A	333	THR	2.4
1	D	241	TYR	2.4
1	C	348	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	86	TRP	2.2
1	B	335	ALA	2.2
1	B	348	ALA	2.1
1	B	5	PRO	2.1
1	A	173	GLY	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
2	CL	A	1001	1/1	0.98	0.06	24,24,24,24	0
2	CL	C	1003	1/1	0.98	0.04	26,26,26,26	0
2	CL	D	1002	1/1	0.98	0.03	21,21,21,21	0
2	CL	B	1004	1/1	0.99	0.10	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.