



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:33 PM UTC

PDB ID : 4FB8 / pdb_00004fb8
Title : Crystal Structure of apo Acyl-CoA Carboxylase
Authors : Reddy, M.C.M.; Bruning, J.B.; Sherekar, M.; Valluru, S.; Ehrenfeld, H.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2012-05-22
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

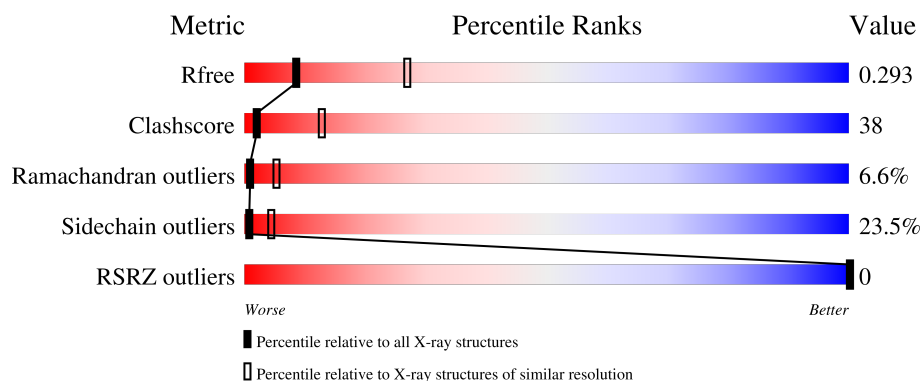
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

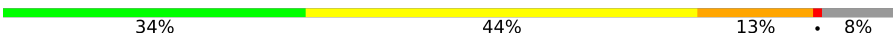
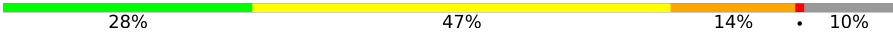
The reported resolution of this entry is 3.00 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	473	
1	B	473	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6220 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 Probable propionyl-CoA carboxylase beta chain 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3135	1959	577	585	14			
1	B	427	Total	C	N	O	S	0	0	0
			3080	1933	561	572	14			

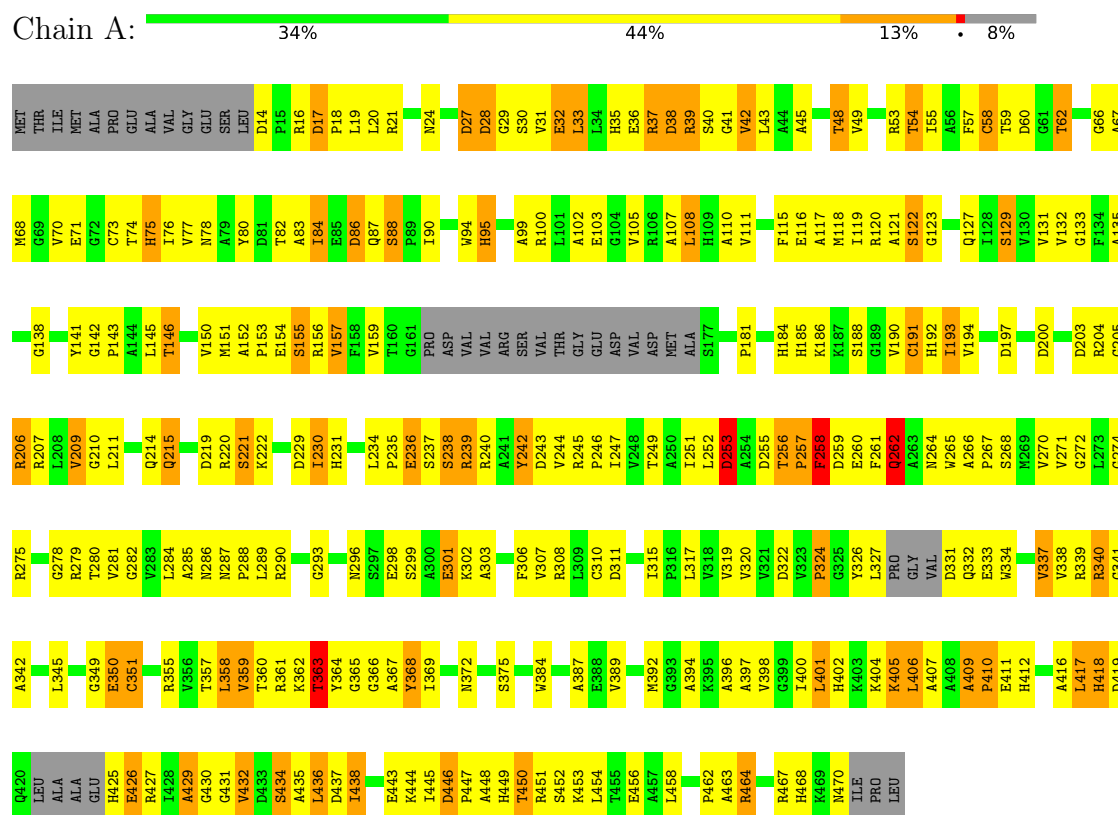
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	3	Total	O	0	0
			3	3		

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: Probable propionyl-CoA carboxylase beta chain 6



- Molecule 1: Probable propionyl-CoA carboxylase beta chain 6



D197	E260	G325	A387	K453
F261	F261	Y326	E388	L454
Q262	Q262	L327	V389	
A263	A263	P328	A390	A459
Y202	N264	G329	V391	Q460
D203		VAL	M392	A461
R204	P267	ASP	G393	
G205	S268	G332	A394	R464
R206	M269	E333	K395	R465
R207	V270	W334	A396	GLY
L208	V271	G335	A397	ARG
V209	G272	G336	V398	HIS
G210	L273	V337	G399	LYS
L211	G274	V338	I400	ASN
F212	R275	R339	L401	ILE
C213	L276	R340	H402	PRO
Q214	S277	G341	K403	LEU
Q215	G278	A342	K404	
G216	R279	K343	K405	
R217	T280	L344	L406	
F218	V281	L345	A407	
D219	G282	H346		
R220	V283	A347	E411	
S221	L284	F348	H412	
K222	A285	G349	E413	
A223	N286	E350		
E224	N287	C351	L417	
A225	P288	T352	H418	
G226	L289	V353	D419	
D227	R290	P354	Q420	
T228	L291	R355	L421	
D229			A422	
I230	C294	L388	A423	
L233	L295	V359	E424	
LEU	N296	T360	E425	
PRO	S297	R361	E426	
GLU	E298	K362		
SER	S299	T363	A429	
ARG	A300	Y364	G430	
ARG	E301	G365	G431	
A241	K302	G366	V432	
Y242	A303	A367	D433	
D243	R304	Y368	S434	
V244	R305	I369	A435	
R245	F306	A370	L436	
P246	V307	P371	D437	
L247	R308	N372	I438	
V248	L309	S373		
	G310	R374	V441	
	D311	S375	D442	
	A312	L376	E443	
	F313	R377	R444	
		A378	I445	
	P316	T379	D446	
		K380	P447	
	V320	V381	A448	
	V321		H449	
	D322		T450	
	V323	W384	R451	
	P324	D386	S452	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.28Å 82.36Å 157.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.85 – 3.00 46.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (46.85-3.00) 93.3 (46.85-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.233 , 0.304 0.233 , 0.293	Depositor DCC
R_{free} test set	1041 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.429 for k,h,-l	Xtriage
Reported twinning fraction	0.479 for K,H,-L	Depositor
Outliers	0 of 20652 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6220	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.14 % 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 9.8635e-04. 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

5.1 Standard geometry

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	0.54	1/3191 (0.0%)	1.00	12/4337 (0.3%)
1	B	0.49	0/3137	1.02	14/4267 (0.3%)
All	All	0.52	1/6328 (0.0%)	1.01	26/8604 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	467	ARG	CA-C	7.66	1.56	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	ASP	CA-C-N	8.17	128.63	119.32
1	B	446	ASP	C-N-CA	8.17	128.63	119.32
1	A	446	ASP	CA-C-N	7.57	127.28	119.56
1	A	446	ASP	C-N-CA	7.57	127.28	119.56
1	B	103	GLU	N-CA-C	-6.95	105.08	113.97
1	A	334	TRP	N-CA-C	-6.87	104.89	113.28
1	B	334	TRP	N-CA-C	-6.75	105.02	113.18
1	B	17	ASP	CA-C-N	6.75	126.25	119.24
1	B	17	ASP	C-N-CA	6.75	126.25	119.24
1	A	17	ASP	CA-C-N	6.35	125.85	119.24
1	A	17	ASP	C-N-CA	6.35	125.85	119.24
1	A	368	TYR	N-CA-C	-6.21	104.43	111.07
1	A	274	GLY	N-CA-C	6.16	119.32	111.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	TRP	CA-C-N	6.12	127.49	119.84
1	B	384	TRP	C-N-CA	6.12	127.49	119.84
1	B	70	VAL	N-CA-C	5.82	116.28	110.23
1	B	157	VAL	CB-CA-C	5.80	120.80	111.29
1	A	467	ARG	N-CA-C	5.71	117.19	108.12
1	A	417	LEU	CA-C-N	5.48	131.56	121.70
1	A	417	LEU	C-N-CA	5.48	131.56	121.70
1	B	320	VAL	N-CA-C	5.47	114.49	106.55
1	A	409	ALA	CA-C-N	-5.42	113.07	119.84
1	A	409	ALA	C-N-CA	-5.42	113.07	119.84
1	B	79	ALA	N-CA-C	-5.09	105.38	111.03
1	B	256	THR	CA-C-N	5.09	126.21	119.84
1	B	256	THR	C-N-CA	5.09	126.21	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	THR	Peptide

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	3135	0	3012	240	1
1	B	3080	0	2982	245	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
All	All	6220	0	5994	465	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 38.

All (465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PHE:N	1:A:259:ASP:HB2	1.58	1.19
1:A:258:PHE:CD1	1:A:260:GLU:HB3	1.89	1.07
1:A:258:PHE:CA	1:A:259:ASP:HB2	1.85	1.04
1:A:257:PRO:O	1:A:258:PHE:HB2	1.60	0.98
1:A:258:PHE:CE1	1:A:260:GLU:HB3	2.02	0.95
1:B:339:ARG:HE	1:B:340:ARG:HG2	1.31	0.95
1:A:256:THR:N	1:A:257:PRO:HD3	1.82	0.94
1:B:344:LEU:HD23	1:B:370:ALA:HB1	1.55	0.88
1:B:402:HIS:O	1:B:404:LYS:N	2.10	0.84
1:A:184:HIS:HB3	1:A:191:CYS:H	1.43	0.83
1:B:355:ARG:HG3	1:B:355:ARG:HH11	1.41	0.83
1:A:258:PHE:H	1:A:259:ASP:HB2	1.39	0.81
1:A:181:PRO:HB2	1:A:194:VAL:HG22	1.61	0.81
1:A:258:PHE:HA	1:A:259:ASP:HB2	1.62	0.80
1:A:108:LEU:HD12	1:B:369:ILE:HD11	1.63	0.79
1:B:358:LEU:HD22	1:B:454:LEU:HD11	1.64	0.79
1:B:296:ASN:H	1:B:299:SER:HB2	1.47	0.78
1:B:151:MET:HE3	1:B:157:VAL:H	1.49	0.78
1:B:227:ASP:HB3	1:B:451:ARG:H	1.47	0.78
1:B:215:GLN:NE2	1:B:313:PHE:O	2.17	0.77
1:A:234:LEU:HD22	1:A:235:PRO:HD2	1.67	0.76
1:B:305:ARG:H	1:B:305:ARG:HD3	1.51	0.76
1:B:435:ALA:HA	1:B:438:ILE:HG13	1.68	0.76
1:A:188:SER:HB2	1:A:190:VAL:HG23	1.69	0.75
1:A:214:GLN:O	1:A:275:ARG:NH2	2.18	0.74
1:A:42:VAL:HG11	1:A:76:ILE:HD11	1.67	0.74
1:A:446:ASP:HB3	1:A:449:HIS:CE1	2.22	0.73
1:A:58:CYS:SG	1:A:59:THR:N	2.62	0.73
1:B:305:ARG:HH11	1:B:305:ARG:HB2	1.54	0.73
1:A:296:ASN:N	1:A:299:SER:OG	2.20	0.72
1:B:96:SER:OG	1:B:97:GLY:N	2.22	0.72
1:A:49:VAL:HG13	1:A:206:ARG:HG2	1.71	0.72
1:A:257:PRO:O	1:A:258:PHE:CB	2.34	0.72
1:B:355:ARG:NH2	1:B:376:LEU:O	2.22	0.72
1:B:185:HIS:HD2	1:B:264:ASN:HB2	1.53	0.71
1:A:243:ASP:HB2	1:A:289:LEU:HD13	1.72	0.71
1:B:53:ARG:NH2	1:B:86:ASP:OD2	2.19	0.71
1:A:94:TRP:NE1	1:A:129:SER:HG	1.88	0.71
1:A:310:CYS:HB3	1:A:315:ILE:HB	1.73	0.71
1:A:120:ARG:HG3	1:A:120:ARG:HH11	1.54	0.71
1:B:398:VAL:HG13	1:B:425:HIS:NE2	2.04	0.70
1:A:122:SER:HA	1:A:127:GLN:HE22	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HG3	1:A:264:ASN:HB3	1.74	0.70
1:A:266:ALA:HB3	1:A:302:LYS:HD2	1.72	0.70
1:A:153:PRO:HG3	1:A:197:ASP:HA	1.73	0.69
1:A:275:ARG:NH1	1:A:278:GLY:O	2.24	0.69
1:A:40:SER:O	1:A:100:ARG:NH2	2.26	0.69
1:A:67:ALA:O	1:A:100:ARG:NE	2.22	0.69
1:A:152:ALA:O	1:A:155:SER:OG	2.10	0.68
1:A:394:ALA:HB1	1:A:426:GLU:HA	1.74	0.68
1:A:416:ALA:HB3	1:A:417:LEU:HA	1.74	0.68
1:B:262:GLN:HB2	1:B:302:LYS:HE3	1.74	0.68
1:B:294:CYS:HA	1:B:323:VAL:HG23	1.76	0.68
1:A:331:ASP:O	1:A:333:GLU:N	2.27	0.67
1:A:366:GLY:HA2	1:A:369:ILE:HD12	1.76	0.67
1:A:150:VAL:HG13	1:A:193:ILE:HG22	1.76	0.67
1:B:321:VAL:O	1:B:360:THR:OG1	2.11	0.67
1:A:73:CYS:HA	1:A:76:ILE:HD12	1.75	0.67
1:A:94:TRP:CD1	1:A:129:SER:HG	2.13	0.67
1:B:127:GLN:HG3	1:B:147:ASP:H	1.60	0.67
1:B:180:GLY:N	1:B:183:THR:OG1	2.27	0.66
1:B:308:ARG:HH12	1:B:350:GLU:HB2	1.60	0.66
1:B:179:GLY:HA3	1:B:184:HIS:CE1	2.30	0.66
1:A:262:GLN:O	1:A:302:LYS:NZ	2.23	0.66
1:A:94:TRP:HB2	1:A:131:VAL:HG22	1.77	0.66
1:A:405:LYS:O	1:A:407:ALA:N	2.29	0.66
1:A:255:ASP:HA	1:A:256:THR:CB	2.26	0.65
1:B:58:CYS:HB2	1:B:93:ILE:HB	1.76	0.65
1:B:395:LYS:HE2	1:B:419:ASP:HA	1.78	0.65
1:A:351:CYS:SG	1:A:355:ARG:NH2	2.70	0.65
1:B:361:ARG:HA	1:B:387:ALA:HA	1.79	0.65
1:A:17:ASP:HB3	1:A:20:LEU:HB3	1.77	0.65
1:A:145:LEU:HD23	1:B:342:ALA:HB1	1.77	0.65
1:A:339:ARG:NH2	1:B:188:SER:O	2.30	0.64
1:B:361:ARG:O	1:B:388:GLU:N	2.30	0.64
1:A:94:TRP:NE1	1:A:129:SER:OG	2.31	0.64
1:A:320:VAL:HG13	1:A:358:LEU:HD21	1.79	0.64
1:A:253:ASP:OD2	1:A:253:ASP:N	2.30	0.64
1:A:253:ASP:N	1:A:451:ARG:HH12	1.95	0.64
1:A:326:TYR:O	1:B:162:PRO:HD3	1.99	0.63
1:A:36:GLU:C	1:A:38:ASP:H	2.07	0.63
1:A:41:GLY:O	1:A:60:ASP:N	2.29	0.63
1:A:409:ALA:HB3	1:A:410:PRO:HD3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PHE:HA	1:A:259:ASP:CB	2.24	0.62
1:B:97:GLY:HA2	1:B:136:ALA:H	1.64	0.62
1:A:155:SER:O	1:A:156:ARG:NH1	2.32	0.62
1:B:185:HIS:CD2	1:B:264:ASN:HB2	2.34	0.62
1:B:355:ARG:HG3	1:B:355:ARG:NH1	2.15	0.62
1:B:425:HIS:O	1:B:429:ALA:N	2.25	0.61
1:B:188:SER:OG	1:B:189:GLY:N	2.33	0.61
1:B:398:VAL:HG21	1:B:421:LEU:HB2	1.82	0.61
1:B:348:PHE:HB2	1:B:376:LEU:HD13	1.83	0.61
1:A:270:VAL:N	1:A:285:ALA:O	2.29	0.61
1:A:446:ASP:HB3	1:A:449:HIS:NE2	2.16	0.61
1:B:219:ASP:H	1:B:277:SER:HB2	1.65	0.61
1:A:16:ARG:NH2	1:A:62:THR:HG23	2.16	0.61
1:A:35:HIS:HE2	1:A:43:LEU:HD12	1.66	0.61
1:A:108:LEU:HD21	1:B:391:VAL:HB	1.83	0.61
1:A:234:LEU:HD11	1:A:361:ARG:HD3	1.82	0.60
1:B:373:SER:OG	1:B:375:SER:OG	2.19	0.60
1:B:134:PHE:HB3	1:B:158:PHE:CE2	2.36	0.60
1:A:117:ALA:HA	1:A:120:ARG:HH12	1.67	0.60
1:A:308:ARG:NH2	1:A:350:GLU:OE2	2.34	0.60
1:A:143:PRO:O	1:A:146:THR:OG1	2.13	0.60
1:A:94:TRP:HE1	1:A:129:SER:HG	1.42	0.60
1:B:381:VAL:HG12	1:B:441:VAL:HG13	1.84	0.60
1:A:138:GLY:O	1:A:142:GLY:N	2.25	0.60
1:A:145:LEU:HD21	1:B:345:LEU:HD12	1.84	0.60
1:B:112:GLY:HA2	1:B:115:PHE:CD2	2.37	0.60
1:A:392:MET:HE3	1:B:101:LEU:HD21	1.84	0.59
1:B:148:VAL:HG11	1:B:208:LEU:HD11	1.84	0.59
1:B:248:VAL:HG13	1:B:283:VAL:HG11	1.84	0.59
1:A:55:ILE:HB	1:A:83:ALA:HB2	1.84	0.59
1:B:151:MET:CE	1:B:157:VAL:H	2.16	0.59
1:A:210:GLY:O	1:A:214:GLN:N	2.33	0.59
1:A:229:ASP:HA	1:A:448:ALA:HA	1.84	0.59
1:B:244:VAL:HG11	1:B:286:ASN:O	2.02	0.59
1:A:35:HIS:HE2	1:A:43:LEU:HA	1.68	0.59
1:A:200:ASP:O	1:A:204:ARG:N	2.31	0.59
1:A:258:PHE:CA	1:A:259:ASP:CB	2.63	0.59
1:B:20:LEU:O	1:B:24:ASN:N	2.34	0.59
1:B:260:GLU:HA	1:B:272:GLY:HA3	1.84	0.59
1:A:266:ALA:HB1	1:A:299:SER:HA	1.85	0.58
1:A:115:PHE:O	1:A:119:ILE:HG13	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:CYS:SG	1:B:192:HIS:N	2.77	0.58
1:B:252:LEU:HD13	1:B:274:GLY:HA3	1.86	0.58
1:B:355:ARG:O	1:B:372:ASN:ND2	2.30	0.58
1:A:35:HIS:NE2	1:A:43:LEU:HA	2.18	0.58
1:A:342:ALA:HA	1:A:345:LEU:HD12	1.83	0.58
1:B:328:PRO:HA	1:B:337:VAL:HG11	1.86	0.58
1:B:397:ALA:C	1:B:425:HIS:HE2	2.12	0.57
1:A:184:HIS:CG	1:A:190:VAL:HB	2.39	0.57
1:A:127:GLN:O	1:A:146:THR:HB	2.04	0.57
1:A:359:VAL:HG22	1:A:387:ALA:HB1	1.86	0.57
1:B:151:MET:HG2	1:B:181:PRO:HB3	1.85	0.57
1:A:365:GLY:HA2	1:B:108:LEU:HD11	1.87	0.57
1:B:127:GLN:NE2	1:B:145:LEU:O	2.37	0.57
1:A:462:PRO:HG2	1:A:464:ARG:HE	1.69	0.57
1:A:35:HIS:NE2	1:A:43:LEU:HD12	2.20	0.57
1:A:230:ILE:HG13	1:A:450:THR:HB	1.86	0.57
1:A:243:ASP:O	1:A:246:PRO:HD2	2.04	0.57
1:B:358:LEU:HD11	1:B:445:ILE:HD11	1.86	0.57
1:B:227:ASP:OD2	1:B:227:ASP:N	2.37	0.56
1:B:252:LEU:HD21	1:B:283:VAL:HG21	1.86	0.56
1:B:210:GLY:O	1:B:275:ARG:NH2	2.38	0.56
1:B:224:GLU:O	1:B:226:GLY:N	2.37	0.56
1:A:258:PHE:H	1:A:259:ASP:CB	2.14	0.56
1:B:261:PHE:O	1:B:263:ALA:N	2.37	0.56
1:B:200:ASP:HA	1:B:203:ASP:OD2	2.05	0.56
1:A:73:CYS:O	1:A:76:ILE:HB	2.06	0.56
1:B:131:VAL:HG12	1:B:155:SER:HB2	1.87	0.56
1:B:321:VAL:N	1:B:358:LEU:O	2.39	0.56
1:B:328:PRO:O	1:B:337:VAL:HG11	2.05	0.56
1:A:74:THR:HG22	1:A:78:ASN:OD1	2.06	0.56
1:B:196:ASP:OD1	1:B:196:ASP:N	2.37	0.56
1:B:445:ILE:HG21	1:B:453:LYS:HG2	1.88	0.56
1:B:123:GLY:HA2	1:B:312:ALA:HB1	1.88	0.56
1:A:429:ALA:O	1:A:431:GLY:N	2.38	0.55
1:A:214:GLN:C	1:A:275:ARG:HH22	2.12	0.55
1:B:380:LYS:HG3	1:B:442:ASP:OD1	2.06	0.55
1:A:215:GLN:O	1:A:279:ARG:HA	2.05	0.55
1:B:339:ARG:NE	1:B:340:ARG:HG2	2.11	0.55
1:A:105:VAL:HG22	1:B:438:ILE:HD12	1.88	0.55
1:B:358:LEU:HD13	1:B:454:LEU:HD21	1.88	0.55
1:B:80:TYR:CZ	1:B:118:MET:HG2	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ALA:O	1:A:306:PHE:N	2.40	0.54
1:A:256:THR:N	1:A:257:PRO:CD	2.61	0.54
1:A:432:VAL:O	1:A:435:ALA:N	2.29	0.54
1:A:319:VAL:HG21	1:A:372:ASN:HB3	1.89	0.54
1:A:258:PHE:N	1:A:259:ASP:CB	2.52	0.54
1:A:151:MET:HB3	1:A:181:PRO:HB3	1.90	0.54
1:A:320:VAL:HA	1:A:358:LEU:HD23	1.89	0.53
1:A:49:VAL:HG11	1:A:209:VAL:HG13	1.90	0.53
1:A:37:ARG:O	1:A:39:ARG:N	2.42	0.53
1:A:454:LEU:O	1:A:458:LEU:N	2.36	0.53
1:B:394:ALA:HB1	1:B:422:ALA:HA	1.90	0.53
1:A:107:ALA:O	1:A:111:VAL:N	2.29	0.53
1:A:432:VAL:O	1:A:436:LEU:N	2.41	0.53
1:B:301:GLU:OE1	1:B:340:ARG:HD2	2.09	0.53
1:A:219:ASP:OD2	1:A:222:LYS:HE3	2.08	0.53
1:A:288:PRO:HA	1:A:293:GLY:N	2.24	0.53
1:B:364:TYR:HA	1:B:390:ALA:O	2.08	0.53
1:B:361:ARG:NH1	1:B:362:LYS:HE3	2.23	0.53
1:B:402:HIS:O	1:B:404:LYS:HG2	2.09	0.53
1:A:360:THR:HB	1:A:384:TRP:CE3	2.44	0.52
1:B:152:ALA:HB3	1:B:155:SER:HB3	1.90	0.52
1:B:259:ASP:OD1	1:B:259:ASP:N	2.39	0.52
1:B:335:GLY:O	1:B:338:VAL:HG23	2.09	0.52
1:A:394:ALA:HB3	1:A:426:GLU:OE2	2.09	0.52
1:A:417:LEU:CB	1:A:418:HIS:C	2.83	0.52
1:A:296:ASN:OD1	1:A:298:GLU:N	2.43	0.52
1:B:156:ARG:HB2	1:B:158:PHE:HB3	1.91	0.52
1:B:216:GLY:O	1:B:279:ARG:NH1	2.43	0.52
1:B:399:GLY:C	1:B:401:LEU:H	2.17	0.52
1:A:402:HIS:HB2	1:A:406:LEU:HD12	1.91	0.52
1:B:153:PRO:HA	1:B:181:PRO:HG3	1.92	0.52
1:A:151:MET:N	1:A:193:ILE:O	2.41	0.52
1:B:398:VAL:HG11	1:B:421:LEU:HB3	1.90	0.52
1:A:470:ASN:OD1	1:B:308:ARG:HD3	2.10	0.51
1:A:77:VAL:HG22	1:A:117:ALA:HB2	1.92	0.51
1:B:25:PHE:O	1:B:206:ARG:HD2	2.10	0.51
1:B:29:GLY:HA3	1:B:30:SER:HB2	1.91	0.51
1:B:255:ASP:OD2	1:B:255:ASP:N	2.36	0.51
1:A:121:ALA:O	1:A:123:GLY:N	2.43	0.51
1:B:111:VAL:O	1:B:114:VAL:N	2.42	0.51
1:B:127:GLN:HB2	1:B:146:THR:HG22	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:PRO:O	1:B:337:VAL:CG1	2.58	0.51
1:A:35:HIS:CE1	1:A:43:LEU:HA	2.46	0.51
1:B:16:ARG:HG2	1:B:95:HIS:CE1	2.45	0.51
1:B:219:ASP:H	1:B:277:SER:CB	2.23	0.51
1:A:205:GLY:O	1:A:209:VAL:HG12	2.11	0.51
1:A:219:ASP:OD2	1:A:222:LYS:HB2	2.11	0.51
1:B:154:GLU:O	1:B:156:ARG:HG2	2.10	0.51
1:A:200:ASP:O	1:A:204:ARG:HG2	2.10	0.50
1:A:237:SER:O	1:A:239:ARG:N	2.44	0.50
1:A:38:ASP:O	1:A:40:SER:N	2.41	0.50
1:A:122:SER:HA	1:A:127:GLN:NE2	2.25	0.50
1:A:215:GLN:HA	1:A:280:THR:OG1	2.12	0.50
1:A:443:GLU:HG2	1:A:444:LYS:N	2.26	0.50
1:B:366:GLY:HA2	1:B:369:ILE:HD12	1.93	0.50
1:B:210:GLY:O	1:B:214:GLN:HB2	2.12	0.50
1:A:14:ASP:N	1:A:16:ARG:HH21	2.10	0.50
1:B:301:GLU:O	1:B:305:ARG:HD3	2.12	0.50
1:A:200:ASP:HA	1:A:203:ASP:HB2	1.94	0.50
1:A:238:SER:HA	1:A:361:ARG:NH1	2.27	0.50
1:A:339:ARG:C	1:A:341:GLY:H	2.20	0.50
1:B:95:HIS:CD2	1:B:133:GLY:HA3	2.47	0.50
1:B:137:GLY:O	1:B:140:ALA:N	2.45	0.50
1:B:248:VAL:HA	1:B:251:ILE:HG13	1.93	0.50
1:B:368:TYR:CD2	1:B:369:ILE:HG13	2.46	0.49
1:A:154:GLU:HA	1:A:156:ARG:NH2	2.26	0.49
1:A:211:LEU:HB3	1:A:280:THR:HG21	1.94	0.49
1:B:32:GLU:N	1:B:46:ALA:O	2.40	0.49
1:B:431:GLY:O	1:B:434:SER:HB3	2.12	0.49
1:A:55:ILE:HG12	1:A:82:THR:HB	1.93	0.49
1:A:119:ILE:HD13	1:B:346:HIS:HA	1.93	0.49
1:B:221:SER:C	1:B:223:ALA:H	2.21	0.49
1:A:36:GLU:C	1:A:38:ASP:N	2.70	0.49
1:B:355:ARG:HB2	1:B:372:ASN:ND2	2.27	0.49
1:A:308:ARG:HA	1:A:311:ASP:HB3	1.95	0.49
1:B:324:PRO:HG3	1:B:362:LYS:HZ3	1.77	0.49
1:A:42:VAL:HG21	1:A:76:ILE:HG13	1.95	0.49
1:A:143:PRO:HA	1:A:146:THR:HG23	1.94	0.49
1:A:185:HIS:O	1:A:264:ASN:HB2	2.12	0.49
1:B:286:ASN:ND2	1:B:323:VAL:HB	2.28	0.49
1:B:157:VAL:C	1:B:159:VAL:H	2.21	0.49
1:A:252:LEU:O	1:A:253:ASP:O	2.30	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:SER:OG	1:B:155:SER:O	2.28	0.48
1:B:374:ARG:HA	1:B:378:ALA:HB3	1.94	0.48
1:B:395:LYS:HD3	1:B:418:HIS:CE1	2.48	0.48
1:B:464:ARG:HD2	1:B:464:ARG:HA	1.54	0.48
1:A:244:VAL:HA	1:A:247:ILE:HD13	1.94	0.48
1:B:33:LEU:HD23	1:B:35:HIS:O	2.13	0.48
1:A:188:SER:HB3	1:B:335:GLY:HA3	1.95	0.48
1:A:86:ASP:N	1:A:86:ASP:OD1	2.46	0.48
1:A:100:ARG:HB3	1:A:103:GLU:HG3	1.94	0.48
1:A:270:VAL:HG23	1:A:287:ASN:HB2	1.95	0.48
1:B:296:ASN:OD1	1:B:299:SER:OG	2.13	0.48
1:A:324:PRO:N	1:A:362:LYS:HD2	2.29	0.48
1:B:211:LEU:HD13	1:B:273:LEU:HB3	1.94	0.48
1:A:37:ARG:HA	1:A:37:ARG:HD3	1.62	0.48
1:A:150:VAL:HG13	1:A:193:ILE:CG2	2.43	0.48
1:B:21:ARG:HD2	1:B:202:TYR:OH	2.12	0.48
1:A:375:SER:OG	1:B:112:GLY:HA3	2.14	0.48
1:B:411:GLU:C	1:B:413:GLU:H	2.21	0.48
1:A:18:PRO:HB3	1:A:43:LEU:HB3	1.95	0.48
1:A:443:GLU:HG2	1:A:444:LYS:H	1.79	0.47
1:B:60:ASP:O	1:B:66:GLY:HA2	2.14	0.47
1:B:95:HIS:CG	1:B:133:GLY:HA3	2.48	0.47
1:B:401:LEU:C	1:B:403:LYS:H	2.21	0.47
1:B:323:VAL:HG22	1:B:325:GLY:H	1.79	0.47
1:B:370:ALA:O	1:B:372:ASN:N	2.47	0.47
1:A:80:TYR:O	1:A:84:ILE:HG13	2.14	0.47
1:A:42:VAL:HA	1:A:59:THR:HA	1.96	0.47
1:A:116:GLU:HB2	1:B:376:LEU:HD23	1.94	0.47
1:B:258:PHE:CE2	1:B:260:GLU:HB2	2.49	0.47
1:B:365:GLY:H	1:B:391:VAL:HA	1.79	0.47
1:B:308:ARG:HH12	1:B:350:GLU:CB	2.26	0.47
1:B:394:ALA:HB2	1:B:425:HIS:HB3	1.97	0.47
1:A:105:VAL:O	1:A:108:LEU:N	2.47	0.47
1:A:154:GLU:HA	1:A:156:ARG:HH22	1.80	0.47
1:A:186:LYS:O	1:A:188:SER:N	2.48	0.47
1:A:365:GLY:C	1:A:367:ALA:H	2.22	0.47
1:A:260:GLU:HA	1:A:272:GLY:HA2	1.97	0.47
1:A:267:PRO:HB2	1:A:290:ARG:HG3	1.97	0.47
1:A:445:ILE:HG21	1:A:453:LYS:HG3	1.96	0.47
1:A:431:GLY:O	1:A:434:SER:OG	2.31	0.47
1:B:324:PRO:HA	1:B:364:TYR:HD2	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ASP:HB2	1:B:448:ALA:O	2.15	0.46
1:B:132:VAL:HA	1:B:155:SER:HB3	1.97	0.46
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.80	0.46
1:B:336:GLY:O	1:B:340:ARG:HB2	2.15	0.46
1:A:116:GLU:OE1	1:A:120:ARG:NH1	2.48	0.46
1:B:114:VAL:O	1:B:118:MET:HG3	2.14	0.46
1:B:218:PHE:CD1	1:B:279:ARG:HB3	2.50	0.46
1:A:258:PHE:HA	1:A:259:ASP:C	2.41	0.46
1:A:438:ILE:HG23	1:B:106:ARG:NH1	2.30	0.46
1:B:157:VAL:O	1:B:159:VAL:HG23	2.16	0.46
1:B:275:ARG:NH1	1:B:280:THR:OG1	2.48	0.46
1:B:296:ASN:HD21	1:B:298:GLU:HB2	1.81	0.46
1:A:184:HIS:HA	1:A:188:SER:OG	2.15	0.46
1:A:398:VAL:HA	1:A:401:LEU:HD12	1.98	0.46
1:B:215:GLN:HA	1:B:280:THR:OG1	2.16	0.46
1:B:253:ASP:HB3	1:B:255:ASP:OD2	2.16	0.46
1:B:311:ASP:CG	1:B:352:THR:H	2.22	0.46
1:A:267:PRO:HB2	1:A:290:ARG:CB	2.46	0.46
1:B:26:PHE:HD2	1:B:31:VAL:HG22	1.80	0.46
1:B:347:ALA:O	1:B:351:CYS:HB2	2.15	0.46
1:B:367:ALA:HA	1:B:370:ALA:HB3	1.98	0.46
1:A:265:TRP:O	1:A:302:LYS:NZ	2.43	0.46
1:B:34:LEU:O	1:B:35:HIS:HB3	2.16	0.46
1:B:62:THR:OG1	1:B:63:VAL:N	2.48	0.46
1:B:303:ALA:O	1:B:307:VAL:HG23	2.16	0.46
1:A:394:ALA:O	1:A:396:ALA:HA	2.16	0.46
1:A:416:ALA:CB	1:A:417:LEU:HA	2.40	0.46
1:B:66:GLY:HA3	1:B:96:SER:HA	1.97	0.46
1:B:218:PHE:CE2	1:B:279:ARG:HD3	2.52	0.46
1:B:80:TYR:OH	1:B:118:MET:HG2	2.16	0.45
1:B:268:SER:OG	1:B:299:SER:OG	2.33	0.45
1:B:343:LYS:HA	1:B:343:LYS:HD2	1.55	0.45
1:B:106:ARG:O	1:B:110:ALA:N	2.49	0.45
1:B:405:LYS:C	1:B:407:ALA:H	2.22	0.45
1:A:301:GLU:H	1:A:301:GLU:HG2	1.50	0.45
1:A:342:ALA:HB1	1:B:145:LEU:CD2	2.47	0.45
1:A:410:PRO:HD2	1:A:411:GLU:H	1.81	0.45
1:B:417:LEU:HA	1:B:420:GLN:HB2	1.99	0.45
1:A:324:PRO:O	1:A:364:TYR:HB2	2.16	0.45
1:B:459:ALA:C	1:B:461:ALA:H	2.25	0.45
1:A:271:VAL:HA	1:A:284:LEU:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ALA:O	1:A:111:VAL:HG23	2.16	0.45
1:A:133:GLY:HA2	1:A:155:SER:HA	1.99	0.45
1:B:99:ALA:O	1:B:100:ARG:C	2.60	0.45
1:B:311:ASP:HA	1:B:353:VAL:HG13	1.99	0.45
1:A:33:LEU:HA	1:A:45:ALA:HA	1.99	0.45
1:A:117:ALA:HA	1:A:120:ARG:NH1	2.30	0.45
1:B:244:VAL:HB	1:B:288:PRO:HD2	1.99	0.45
1:B:399:GLY:O	1:B:401:LEU:N	2.46	0.45
1:A:67:ALA:HB3	1:A:100:ARG:HG3	1.99	0.44
1:B:391:VAL:HG22	1:B:392:MET:HG2	1.99	0.44
1:A:324:PRO:HG3	1:A:362:LYS:HZ3	1.82	0.44
1:B:111:VAL:HG11	1:B:138:GLY:HA3	1.99	0.44
1:B:307:VAL:O	1:B:310:CYS:N	2.50	0.44
1:A:363:THR:CG2	1:A:389:VAL:HG22	2.47	0.44
1:B:197:ASP:CG	1:B:200:ASP:HB3	2.43	0.44
1:A:271:VAL:HG22	1:A:302:LYS:HE2	1.99	0.44
1:B:143:PRO:HA	1:B:146:THR:OG1	2.18	0.44
1:B:267:PRO:O	1:B:287:ASN:ND2	2.44	0.44
1:A:266:ALA:CB	1:A:299:SER:HA	2.47	0.44
1:B:268:SER:HA	1:B:287:ASN:HB3	2.00	0.44
1:B:55:ILE:HG12	1:B:82:THR:HG22	2.00	0.44
1:B:227:ASP:CB	1:B:451:ARG:HB3	2.48	0.44
1:A:42:VAL:HG22	1:A:75:HIS:HD2	1.82	0.44
1:B:218:PHE:HE1	1:B:276:LEU:HB3	1.83	0.44
1:B:211:LEU:HD22	1:B:280:THR:HG23	2.00	0.43
1:B:286:ASN:OD1	1:B:322:ASP:N	2.40	0.43
1:B:204:ARG:O	1:B:208:LEU:HB2	2.19	0.43
1:B:270:VAL:O	1:B:284:LEU:HA	2.18	0.43
1:B:18:PRO:HG3	1:B:60:ASP:HA	2.00	0.43
1:B:33:LEU:HD11	1:B:43:LEU:HD11	2.00	0.43
1:B:212:PHE:O	1:B:215:GLN:HG3	2.19	0.43
1:B:344:LEU:HD12	1:B:344:LEU:HA	1.91	0.43
1:B:348:PHE:O	1:B:355:ARG:NH2	2.51	0.43
1:B:388:GLU:OE2	1:B:430:GLY:HA3	2.19	0.43
1:A:268:SER:HB2	1:A:293:GLY:C	2.43	0.43
1:A:84:ILE:HD11	1:A:121:ALA:HB2	2.01	0.43
1:B:88:SER:O	1:B:125:ILE:HD12	2.18	0.43
1:B:328:PRO:CA	1:B:337:VAL:HG11	2.49	0.43
1:A:260:GLU:HA	1:A:272:GLY:CA	2.49	0.43
1:B:258:PHE:O	1:B:260:GLU:N	2.51	0.43
1:B:38:ASP:HB2	1:B:39:ARG:H	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLY:O	1:B:75:HIS:N	2.49	0.43
1:B:294:CYS:SG	1:B:324:PRO:HD2	2.59	0.43
1:B:321:VAL:HG23	1:B:358:LEU:O	2.18	0.43
1:B:363:THR:HG23	1:B:389:VAL:HG13	2.01	0.43
1:B:337:VAL:H	1:B:337:VAL:HG13	1.56	0.43
1:A:31:VAL:HG12	1:A:32:GLU:O	2.18	0.43
1:A:54:THR:HG21	1:A:209:VAL:HG21	1.99	0.43
1:A:94:TRP:O	1:A:95:HIS:HB2	2.19	0.42
1:A:444:LYS:HB2	1:A:444:LYS:HE3	1.80	0.42
1:B:22:LEU:HD13	1:B:45:ALA:HB3	2.01	0.42
1:B:118:MET:O	1:B:121:ALA:HB3	2.18	0.42
1:B:384:TRP:O	1:B:386:ASP:N	2.52	0.42
1:A:66:GLY:O	1:A:67:ALA:C	2.62	0.42
1:A:235:PRO:HG3	1:A:242:TYR:CD2	2.54	0.42
1:A:151:MET:HG2	1:A:155:SER:OG	2.20	0.42
1:B:35:HIS:CE1	1:B:43:LEU:HD12	2.55	0.42
1:B:76:ILE:O	1:B:79:ALA:HB3	2.20	0.42
1:B:229:ASP:HA	1:B:448:ALA:HA	2.01	0.42
1:B:244:VAL:O	1:B:247:ILE:HG13	2.19	0.42
1:B:316:PRO:HB3	1:B:354:PRO:HB2	2.00	0.42
1:B:358:LEU:HD21	1:B:384:TRP:CZ2	2.54	0.42
1:B:395:LYS:CE	1:B:419:ASP:HA	2.48	0.42
1:A:141:TYR:O	1:A:142:GLY:C	2.63	0.42
1:A:339:ARG:O	1:A:341:GLY:N	2.52	0.42
1:B:305:ARG:HB2	1:B:305:ARG:NH1	2.29	0.42
1:B:228:THR:OG1	1:B:230:ILE:HG12	2.19	0.42
1:B:353:VAL:O	1:B:355:ARG:HD3	2.19	0.42
1:B:380:LYS:HG3	1:B:442:ASP:CG	2.45	0.42
1:A:70:VAL:HA	1:A:110:ALA:CB	2.50	0.42
1:A:282:GLY:HA3	1:A:317:LEU:HD23	2.01	0.42
1:A:463:ALA:C	1:A:464:ARG:HG2	2.44	0.42
1:B:224:GLU:N	1:B:224:GLU:OE1	2.53	0.42
1:B:328:PRO:C	1:B:337:VAL:HG11	2.44	0.42
1:B:398:VAL:HG13	1:B:425:HIS:HE2	1.83	0.42
1:A:16:ARG:HA	1:A:21:ARG:CZ	2.50	0.42
1:A:115:PHE:CD2	1:B:345:LEU:HD13	2.54	0.42
1:A:262:GLN:OE1	1:A:302:LYS:HE3	2.19	0.42
1:B:27:ASP:OD1	1:B:49:VAL:HA	2.20	0.42
1:A:151:MET:HE2	1:A:155:SER:O	2.20	0.42
1:A:319:VAL:HB	1:A:357:THR:HG23	2.01	0.42
1:A:454:LEU:H	1:A:454:LEU:HD22	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:TYR:HA	1:A:90:ILE:HD13	2.02	0.42
1:B:70:VAL:HG21	1:B:106:ARG:HB3	2.02	0.42
1:B:392:MET:HE2	1:B:392:MET:HB3	1.93	0.42
1:A:192:HIS:C	1:A:193:ILE:HD12	2.45	0.41
1:A:207:ARG:O	1:A:211:LEU:HG	2.20	0.41
1:A:261:PHE:N	1:A:261:PHE:CD1	2.87	0.41
1:A:231:HIS:HA	1:A:384:TRP:CH2	2.55	0.41
1:B:16:ARG:HD3	1:B:95:HIS:CE1	2.56	0.41
1:B:379:THR:HB	1:B:380:LYS:H	1.66	0.41
1:A:141:TYR:HE1	1:B:338:VAL:HA	1.85	0.41
1:A:287:ASN:HA	1:A:288:PRO:HD3	1.77	0.41
1:A:349:GLY:HA3	1:B:119:ILE:HD13	2.00	0.41
1:B:222:LYS:HB3	1:B:277:SER:HA	2.02	0.41
1:B:291:LEU:O	1:B:327:LEU:HD11	2.20	0.41
1:A:35:HIS:HE1	1:A:42:VAL:O	2.04	0.41
1:A:67:ALA:CB	1:A:100:ARG:HG3	2.51	0.41
1:A:156:ARG:O	1:A:157:VAL:HG23	2.20	0.41
1:A:220:ARG:HG3	1:A:221:SER:N	2.34	0.41
1:B:26:PHE:CE1	1:B:54:THR:HG22	2.56	0.41
1:B:39:ARG:O	1:B:63:VAL:HG11	2.19	0.41
1:A:252:LEU:C	1:A:451:ARG:NH1	2.78	0.41
1:A:339:ARG:HH11	1:A:340:ARG:HE	1.68	0.41
1:A:392:MET:HB2	1:A:397:ALA:HB1	2.01	0.41
1:B:185:HIS:CD2	1:B:185:HIS:O	2.73	0.41
1:B:261:PHE:CD1	1:B:261:PHE:N	2.88	0.41
1:B:308:ARG:NH2	1:B:350:GLU:OE1	2.52	0.41
1:B:324:PRO:HA	1:B:364:TYR:CD2	2.56	0.41
1:B:403:LYS:C	1:B:405:LYS:H	2.28	0.41
1:B:434:SER:C	1:B:436:LEU:H	2.29	0.41
1:A:103:GLU:HB2	1:A:107:ALA:HB2	2.01	0.41
1:A:132:VAL:HA	1:A:152:ALA:CB	2.51	0.41
1:A:230:ILE:HG12	1:A:447:PRO:O	2.21	0.41
1:A:282:GLY:O	1:A:317:LEU:HA	2.21	0.41
1:A:296:ASN:H	1:A:299:SER:HG	1.61	0.41
1:A:324:PRO:CA	1:A:362:LYS:HD2	2.51	0.41
1:B:227:ASP:HB3	1:B:451:ARG:HB3	2.03	0.41
1:A:319:VAL:O	1:A:358:LEU:HD23	2.22	0.40
1:B:445:ILE:CG2	1:B:453:LYS:HG2	2.50	0.40
1:A:99:ALA:HB2	1:A:111:VAL:HG21	2.03	0.40
1:A:131:VAL:HG11	1:A:135:ALA:HB2	2.04	0.40
1:B:107:ALA:O	1:B:110:ALA:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PHE:CD2	1:A:76:ILE:HG12	2.55	0.40
1:A:284:LEU:HD21	1:A:307:VAL:HG23	2.03	0.40
1:A:438:ILE:HG21	1:B:106:ARG:HG2	2.02	0.40
1:B:185:HIS:CD2	1:B:264:ASN:H	2.40	0.40
1:B:289:LEU:HB3	1:B:290:ARG:H	1.62	0.40
1:B:297:SER:O	1:B:301:GLU:HG3	2.21	0.40
1:A:48:THR:HA	1:A:53:ARG:HA	2.02	0.40
1:A:410:PRO:HB2	1:A:412:HIS:H	1.86	0.40
1:A:28:ASP:HB2	1:A:29:GLY:H	1.71	0.40
1:A:86:ASP:O	1:A:88:SER:N	2.55	0.40
1:B:186:LYS:C	1:B:188:SER:H	2.30	0.40
1:B:242:TYR:CG	1:B:243:ASP:N	2.89	0.40
1:B:311:ASP:HA	1:B:353:VAL:CG1	2.51	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:A:102:ALA:O	1:A:405:LYS:NZ[2_555]	2.06	0.14

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	427/473 (90%)	321 (75%)	76 (18%)	30 (7%)	1	4
1	B	419/473 (89%)	309 (74%)	84 (20%)	26 (6%)	1	6
All	All	846/946 (89%)	630 (74%)	160 (19%)	56 (7%)	1	5

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	87	GLN
1	A	95	HIS
1	A	122	SER
1	A	253	ASP
1	A	257	PRO
1	A	258	PHE
1	A	332	GLN
1	A	337	VAL
1	A	406	LEU
1	A	410	PRO
1	A	419	ASP
1	A	430	GLY
1	A	432	VAL
1	B	263	ALA
1	B	289	LEU
1	B	328	PRO
1	B	400	ILE
1	B	403	LYS
1	A	39	ARG
1	A	238	SER
1	A	239	ARG
1	A	262	GLN
1	A	363	THR
1	A	418	HIS
1	A	468	HIS
1	B	30	SER
1	B	35	HIS
1	B	100	ARG
1	B	242	TYR
1	B	322	ASP
1	B	412	HIS
1	B	435	ALA
1	A	27	ASP
1	B	62	THR
1	B	97	GLY
1	B	155	SER
1	B	225	ALA
1	B	406	LEU
1	B	426	GLU
1	A	146	THR
1	A	236	GLU
1	A	322	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	340	ARG
1	A	429	ALA
1	B	63	VAL
1	B	147	ASP
1	B	224	GLU
1	A	405	LYS
1	B	153	PRO
1	B	226	GLY
1	B	385	PRO
1	B	425	HIS
1	A	324	PRO
1	A	338	VAL
1	B	288	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/362 (83%)	235 (78%)	66 (22%)	1	5
1	B	296/362 (82%)	222 (75%)	74 (25%)	0	3
All	All	597/724 (82%)	457 (76%)	140 (24%)	1	4

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	24	ASN
1	A	27	ASP
1	A	28	ASP
1	A	30	SER
1	A	32	GLU
1	A	33	LEU
1	A	37	ARG
1	A	42	VAL
1	A	48	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	54	THR
1	A	58	CYS
1	A	62	THR
1	A	68	MET
1	A	71	GLU
1	A	75	HIS
1	A	84	ILE
1	A	86	ASP
1	A	88	SER
1	A	108	LEU
1	A	118	MET
1	A	129	SER
1	A	155	SER
1	A	157	VAL
1	A	159	VAL
1	A	191	CYS
1	A	193	ILE
1	A	206	ARG
1	A	209	VAL
1	A	215	GLN
1	A	221	SER
1	A	230	ILE
1	A	236	GLU
1	A	240	ARG
1	A	242	TYR
1	A	245	ARG
1	A	249	THR
1	A	251	ILE
1	A	253	ASP
1	A	258	PHE
1	A	262	GLN
1	A	281	VAL
1	A	286	ASN
1	A	301	GLU
1	A	327	LEU
1	A	337	VAL
1	A	350	GLU
1	A	351	CYS
1	A	358	LEU
1	A	359	VAL
1	A	363	THR
1	A	368	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	400	ILE
1	A	401	LEU
1	A	404	LYS
1	A	425	HIS
1	A	426	GLU
1	A	427	ARG
1	A	434	SER
1	A	436	LEU
1	A	437	ASP
1	A	438	ILE
1	A	450	THR
1	A	452	SER
1	A	456	GLU
1	A	464	ARG
1	B	21	ARG
1	B	22	LEU
1	B	33	LEU
1	B	34	LEU
1	B	38	ASP
1	B	52	VAL
1	B	54	THR
1	B	55	ILE
1	B	58	CYS
1	B	63	VAL
1	B	64	MET
1	B	75	HIS
1	B	77	VAL
1	B	82	THR
1	B	87	GLN
1	B	90	ILE
1	B	101	LEU
1	B	111	VAL
1	B	130	VAL
1	B	141	TYR
1	B	156	ARG
1	B	157	VAL
1	B	159	VAL
1	B	160	THR
1	B	183	THR
1	B	190	VAL
1	B	193	ILE
1	B	194	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	196	ASP
1	B	200	ASP
1	B	208	LEU
1	B	209	VAL
1	B	221	SER
1	B	224	GLU
1	B	227	ASP
1	B	228	THR
1	B	229	ASP
1	B	245	ARG
1	B	251	ILE
1	B	255	ASP
1	B	259	ASP
1	B	271	VAL
1	B	277	SER
1	B	279	ARG
1	B	281	VAL
1	B	284	LEU
1	B	289	LEU
1	B	291	LEU
1	B	295	LEU
1	B	305	ARG
1	B	320	VAL
1	B	321	VAL
1	B	337	VAL
1	B	338	VAL
1	B	343	LYS
1	B	346	HIS
1	B	350	GLU
1	B	355	ARG
1	B	368	TYR
1	B	389	VAL
1	B	391	VAL
1	B	398	VAL
1	B	418	HIS
1	B	420	GLN
1	B	421	LEU
1	B	424	GLU
1	B	425	HIS
1	B	432	VAL
1	B	436	LEU
1	B	437	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	438	ILE
1	B	443	GLU
1	B	450	THR
1	B	464	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	127	GLN
1	A	346	HIS
1	A	449	HIS
1	B	87	GLN
1	B	113	GLN
1	B	214	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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	435/473 (91%)	-0.92	0 100 100	13, 50, 87, 139	0
1	B	427/473 (90%)	-1.00	0 100 100	6, 44, 89, 123	0
All	All	862/946 (91%)	-0.96	0 100 100	6, 47, 88, 139	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.