



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 07:55 PM EDT

PDB ID : 2NRB
Title : C28S Mutant of Succinyl-CoA:3-Ketoacid CoA Transferase from Pig Heart
Authors : Tammam, S.D.; Fraser, M.E.
Deposited on : 2006-11-01
Resolution : 2.00 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 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

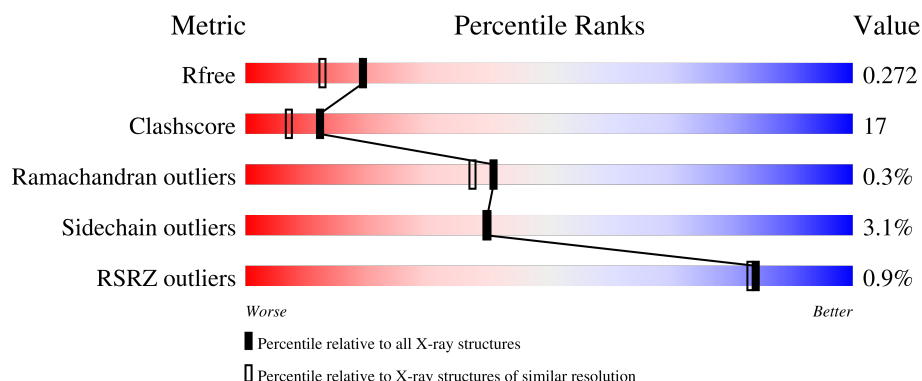
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	481	
1	B	481	
1	C	481	
1	D	481	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15104 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 Succinyl-CoA:3-ketoacid-coenzyme A transferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3561	2260	611	673	17			
1	B	470	Total	C	N	O	S	0	0	0
			3582	2271	614	680	17			
1	C	467	Total	C	N	O	S	0	0	0
			3561	2260	611	673	17			
1	D	469	Total	C	N	O	S	0	0	0
			3578	2269	613	679	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	SER	CYS	engineered mutation	UNP Q29551
B	28	SER	CYS	engineered mutation	UNP Q29551
C	28	SER	CYS	engineered mutation	UNP Q29551
D	28	SER	CYS	engineered mutation	UNP Q29551

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total	O	0	0
			169	169		
3	B	217	Total	O	0	0
			217	217		
3	C	242	Total	O	0	0
			242	242		

Continued on next page...

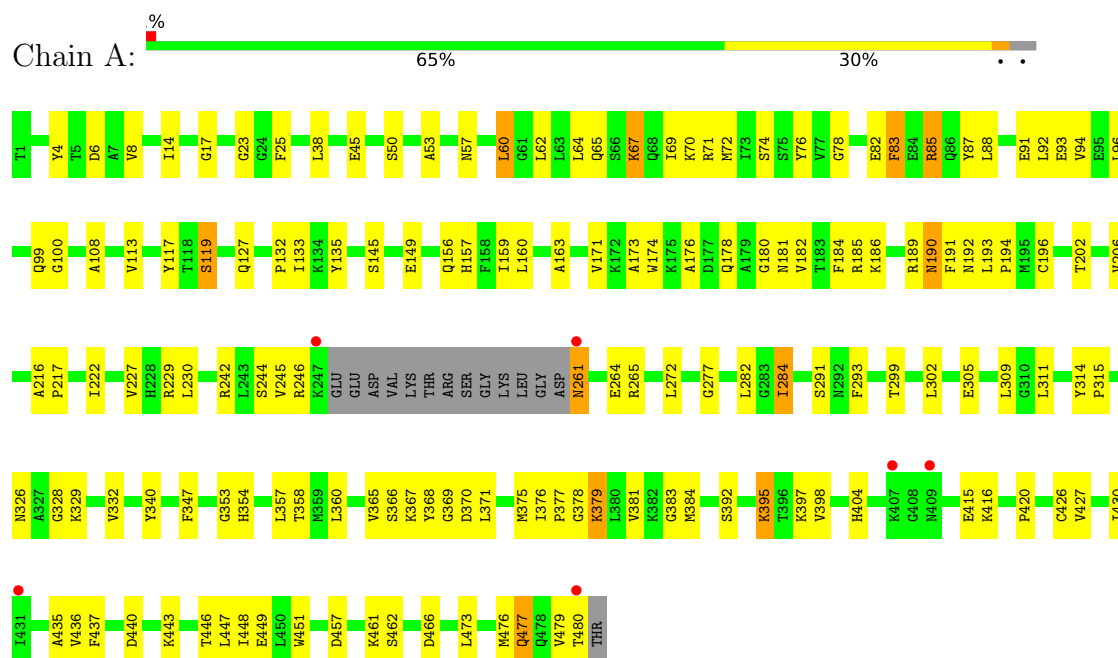
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	193	Total 193	O 193	0	0

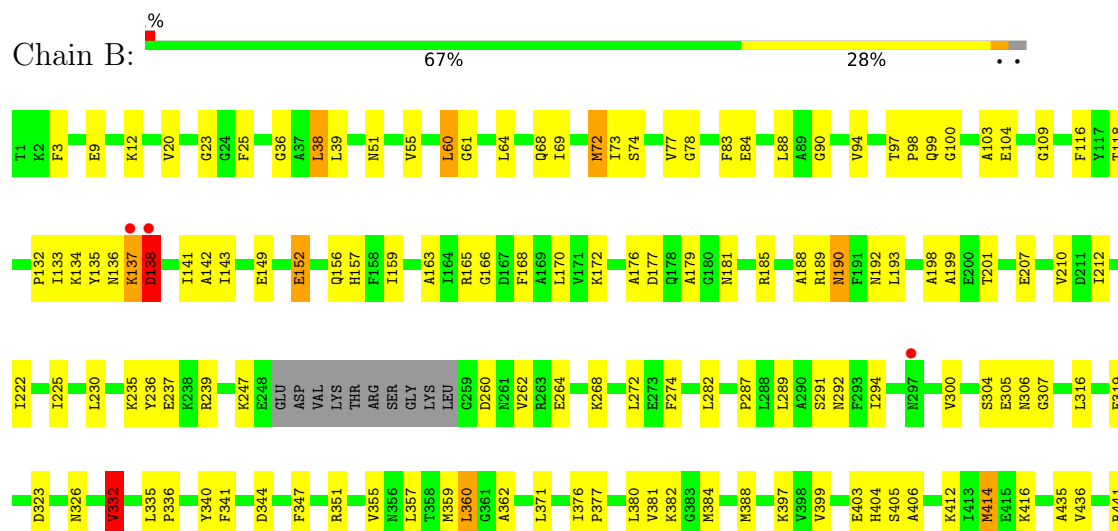
3 Residue-property plots

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: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1



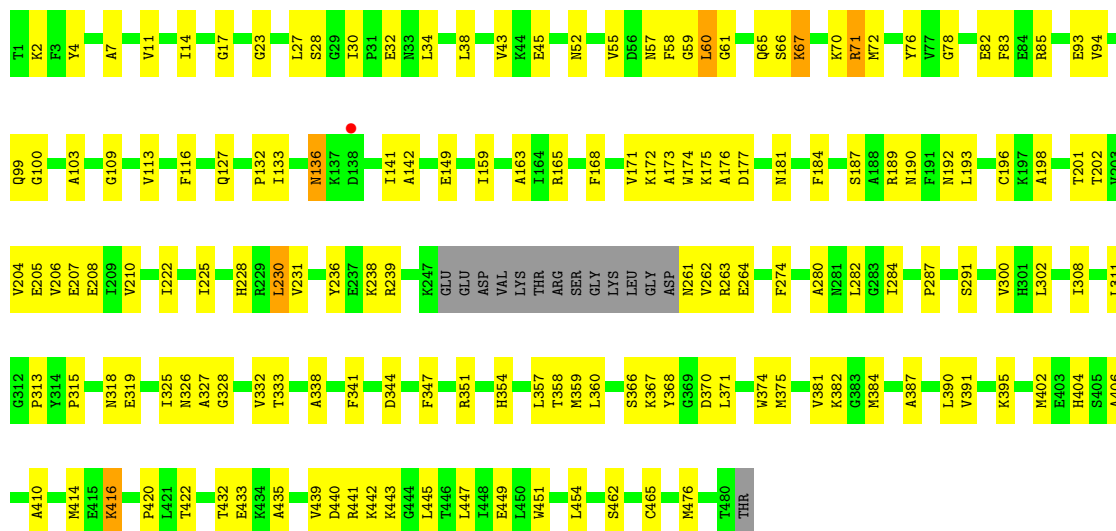
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1





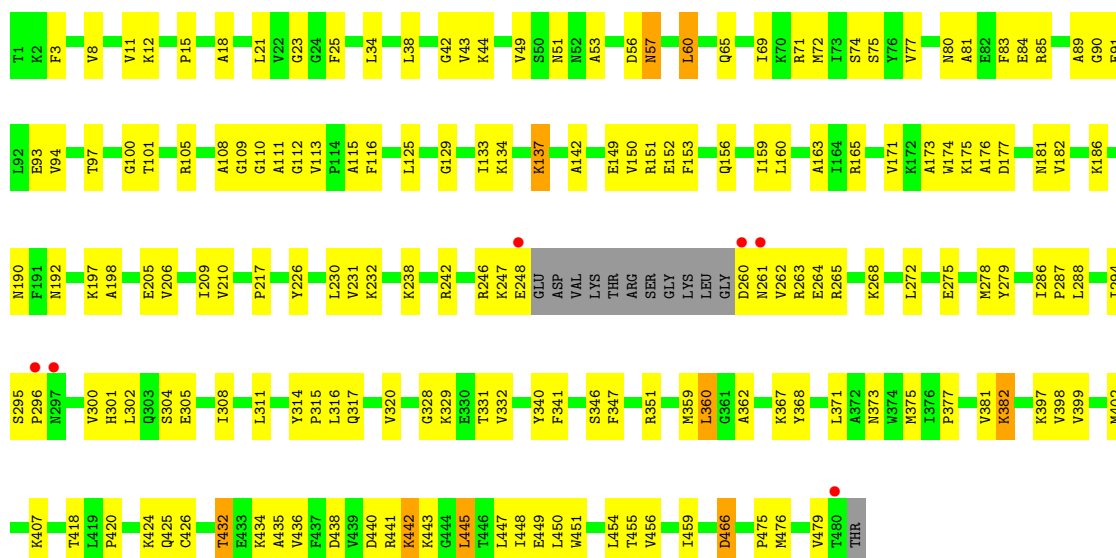
• Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1

Chain C: 65% 31% ..



• Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1

Chain D: 61% 34% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.97Å 264.43Å 61.42Å 90.00° 109.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.62 – 1.92	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-2.00) 88.5 (19.62-1.92)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.92Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.275 0.217 , 0.272	Depositor DCC
R_{free} test set	6267 reflections (5.49%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15104	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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	0.59	0/3619	0.82	1/4884 (0.0%)
1	B	0.66	0/3640	0.87	3/4912 (0.1%)
1	C	0.66	0/3619	0.85	2/4884 (0.0%)
1	D	0.61	0/3636	0.83	1/4907 (0.0%)
All	All	0.63	0/14514	0.84	7/19587 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	332	VAL	CB-CA-C	-5.85	100.29	111.40
1	A	216	ALA	N-CA-C	-5.58	95.93	111.00
1	B	73	ILE	N-CA-C	-5.45	96.29	111.00
1	D	316	LEU	N-CA-C	-5.41	96.38	111.00
1	C	136	ASN	N-CA-C	-5.17	97.05	111.00
1	C	71	ARG	CB-CG-CD	-5.06	98.44	111.60

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	3561	0	3636	112	0
1	B	3582	0	3649	114	0
1	C	3561	0	3636	120	0
1	D	3578	0	3646	158	0
2	A	1	0	0	0	0
3	A	169	0	0	3	0
3	B	217	0	0	7	0
3	C	242	0	0	8	0
3	D	193	0	0	6	0
All	All	15104	0	14567	491	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 17.

All (491) 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:384:MET:SD	1:C:384:MET:CE	2.03	1.45
1:B:132:PRO:HB3	1:B:141:ILE:HG12	1.51	0.92
1:A:357:LEU:HD13	1:A:397:LYS:HE3	1.53	0.89
1:D:381:VAL:C	1:D:382:LYS:HE3	1.94	0.88
1:D:42:GLY:O	1:D:44:LYS:HE3	1.75	0.86
1:C:351:ARG:HD2	1:D:111:ALA:O	1.76	0.86
1:D:77:VAL:HG21	1:D:83:PHE:CE2	2.12	0.85
1:A:284:ILE:HD11	1:A:328:GLY:HA3	1.58	0.84
1:C:207:GLU:O	1:C:208:GLU:HG3	1.78	0.83
1:A:284:ILE:HD11	1:A:328:GLY:CA	2.10	0.81
1:C:57:ASN:CG	1:C:239:ARG:HH12	1.83	0.81
1:D:77:VAL:HG21	1:D:83:PHE:CZ	2.21	0.76
1:D:265:ARG:HD2	1:D:451:TRP:CZ2	2.21	0.75
1:D:260:ASP:OD2	1:D:262:VAL:HB	1.85	0.75
1:B:442:LYS:HE3	1:B:442:LYS:HA	1.69	0.74
1:D:238:LYS:HE2	1:D:238:LYS:HA	1.68	0.74
1:D:451:TRP:HB3	1:D:454:LEU:HD12	1.67	0.74
1:C:284:ILE:HD11	1:C:328:GLY:HA2	1.70	0.74
1:D:261:ASN:HA	1:D:264:GLU:HB3	1.70	0.73
1:C:371:LEU:HD23	1:C:391:VAL:HG11	1.69	0.73
1:D:302:LEU:HB2	1:D:311:LEU:HB2	1.71	0.73
1:C:94:VAL:O	1:C:133:ILE:HA	1.88	0.72
1:B:3:PHE:CE2	1:B:230:LEU:HD23	2.25	0.72
1:D:34:LEU:O	1:D:38:LEU:HD23	1.90	0.71
1:C:193:LEU:HG	1:C:222:ILE:HD11	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ASN:HB3	1:C:332:VAL:HG11	1.70	0.71
1:A:60:LEU:HD22	1:A:72:MET:HE1	1.71	0.71
1:A:245:VAL:HG12	1:A:246:ARG:H	1.56	0.71
1:B:436:VAL:HB	1:B:449:GLU:HB2	1.71	0.71
1:D:287:PRO:HG2	1:D:360:LEU:HA	1.73	0.70
1:C:176:ALA:HA	1:C:181:ASN:O	1.92	0.70
1:B:60:LEU:HD13	1:B:72:MET:HE1	1.75	0.69
1:B:176:ALA:CB	1:B:230:LEU:HD21	2.23	0.68
1:B:305:GLU:HG3	3:B:576:HOH:O	1.94	0.67
1:C:57:ASN:ND2	1:C:239:ARG:HH22	1.93	0.67
1:D:265:ARG:HD2	1:D:451:TRP:CH2	2.31	0.66
1:A:53:ALA:HB3	1:A:83:PHE:CD2	2.31	0.66
1:A:435:ALA:HB1	1:A:447:LEU:CD1	2.26	0.65
1:A:245:VAL:HG12	1:A:246:ARG:N	2.11	0.65
1:D:77:VAL:HG21	1:D:83:PHE:CD2	2.30	0.65
1:C:177:ASP:HA	1:C:210:VAL:O	1.96	0.65
1:C:7:ALA:O	1:C:11:VAL:HG22	1.97	0.65
1:D:351:ARG:HD3	3:D:548:HOH:O	1.96	0.65
1:B:152:GLU:OE1	1:B:157:HIS:ND1	2.30	0.64
1:C:60:LEU:CD1	1:C:72:MET:SD	2.85	0.64
1:B:60:LEU:HD22	1:B:69:ILE:HD11	1.78	0.64
1:C:132:PRO:HB3	1:C:141:ILE:HG12	1.78	0.64
1:A:360:LEU:HD11	1:A:371:LEU:HD21	1.80	0.64
1:B:36:GLY:O	1:B:39:LEU:HB2	1.98	0.64
1:D:77:VAL:HG22	1:D:77:VAL:O	1.97	0.64
1:C:208:GLU:HG2	3:C:625:HOH:O	1.99	0.63
1:B:384:MET:HG3	1:B:388:MET:HG3	1.80	0.63
1:B:134:LYS:HB3	1:B:143:ILE:HG13	1.81	0.62
1:C:57:ASN:ND2	1:C:239:ARG:HH12	1.96	0.62
1:B:60:LEU:HD22	1:B:69:ILE:CD1	2.28	0.62
1:C:14:ILE:HD12	1:C:38:LEU:HD21	1.81	0.62
1:B:23:GLY:HA3	1:B:192:ASN:OD1	1.99	0.62
1:B:177:ASP:HA	1:B:210:VAL:O	1.99	0.62
1:C:449:GLU:HB3	1:C:476:MET:HA	1.81	0.62
1:D:176:ALA:HB1	1:D:230:LEU:HD21	1.82	0.62
1:B:176:ALA:HB1	1:B:230:LEU:HD21	1.82	0.61
1:D:288:LEU:HD13	3:D:605:HOH:O	1.99	0.61
1:B:78:GLY:HA2	1:B:382:LYS:HD2	1.82	0.61
1:D:305:GLU:HB2	1:D:347:PHE:CZ	2.36	0.61
1:D:362:ALA:HB2	1:D:371:LEU:HD11	1.83	0.61
1:A:25:PHE:HE1	1:A:99:GLN:OE1	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:LYS:NZ	1:D:137:LYS:HB3	2.15	0.61
1:D:442:LYS:HE2	1:D:442:LYS:HA	1.82	0.61
1:B:94:VAL:O	1:B:133:ILE:HA	2.01	0.60
1:C:172:LYS:HE2	1:C:236:TYR:CE1	2.37	0.60
1:C:351:ARG:HG2	1:D:112:GLY:HA3	1.83	0.60
1:D:60:LEU:HD11	1:D:69:ILE:CD1	2.32	0.60
1:D:83:PHE:CZ	1:D:94:VAL:HG21	2.37	0.60
1:B:405:SER:C	1:B:412:LYS:HD2	2.22	0.60
1:D:315:PRO:HD3	1:D:332:VAL:HA	1.84	0.60
1:B:351:ARG:HD3	3:B:515:HOH:O	2.01	0.60
1:D:53:ALA:HB2	1:D:72:MET:CE	2.32	0.59
1:C:284:ILE:HD11	1:C:328:GLY:CA	2.31	0.59
1:A:436:VAL:HB	1:A:449:GLU:HB2	1.85	0.59
1:D:84:GLU:OE2	1:D:382:LYS:HD2	2.03	0.59
1:A:45:GLU:HA	1:A:70:LYS:HB2	1.85	0.59
1:A:173:ALA:HB3	1:A:206:VAL:HG12	1.85	0.59
1:A:282:LEU:CD1	1:A:291:SER:HB3	2.33	0.59
1:A:60:LEU:CD2	1:A:72:MET:SD	2.91	0.59
1:A:440:ASP:HB3	1:A:443:LYS:HG2	1.85	0.58
1:D:367:LYS:O	1:D:445:LEU:HD13	2.04	0.58
1:A:64:LEU:HD22	1:A:92:LEU:HD22	1.85	0.58
1:D:134:LYS:O	1:D:142:ALA:N	2.34	0.58
1:B:60:LEU:CD1	1:B:72:MET:CE	2.81	0.58
1:B:442:LYS:HA	1:B:442:LYS:CE	2.32	0.58
1:C:2:LYS:HD3	1:C:4:TYR:OH	2.04	0.58
1:D:177:ASP:HA	1:D:210:VAL:O	2.04	0.58
1:A:53:ALA:CB	1:A:83:PHE:CD2	2.87	0.58
1:C:168:PHE:HA	1:C:201:THR:O	2.04	0.58
1:C:205:GLU:HA	1:C:231:VAL:O	2.04	0.58
1:C:371:LEU:CD2	1:C:391:VAL:HG11	2.33	0.57
1:D:402:MET:O	1:D:432:THR:HA	2.04	0.57
1:A:305:GLU:HB2	1:A:347:PHE:CZ	2.39	0.57
1:C:406:ALA:HB3	1:C:410:ALA:HB3	1.85	0.57
1:D:94:VAL:O	1:D:133:ILE:HA	2.04	0.57
1:A:284:ILE:HD11	1:A:328:GLY:HA2	1.86	0.57
1:B:136:ASN:HB2	1:B:138:ASP:OD1	2.04	0.57
1:D:176:ALA:CB	1:D:230:LEU:HD21	2.34	0.57
1:D:272:LEU:HD21	1:D:479:VAL:HA	1.87	0.57
1:B:172:LYS:HE2	1:B:236:TYR:CE1	2.40	0.57
1:B:60:LEU:HD13	1:B:72:MET:CE	2.34	0.56
1:C:52:ASN:HB2	3:C:484:HOH:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ILE:HD12	1:A:38:LEU:HD21	1.88	0.56
1:A:67:LYS:HD2	1:A:67:LYS:N	2.21	0.56
1:C:367:LYS:HE2	1:C:368:TYR:CE2	2.40	0.56
1:B:335:LEU:HB3	1:B:336:PRO:CD	2.35	0.56
1:D:53:ALA:HB2	1:D:72:MET:HE2	1.88	0.56
1:D:57:ASN:HA	1:D:65:GLN:NE2	2.21	0.56
1:C:60:LEU:HD13	1:C:72:MET:SD	2.46	0.55
1:D:449:GLU:HB3	1:D:476:MET:HA	1.86	0.55
1:B:149:GLU:O	1:B:159:ILE:HA	2.06	0.55
1:A:217:PRO:HB2	1:B:340:TYR:CD2	2.41	0.55
1:B:235:LYS:HE3	1:B:237:GLU:CG	2.36	0.55
1:D:247:LYS:O	1:D:248:GLU:HG3	2.07	0.55
1:B:472:LYS:HB3	3:B:658:HOH:O	2.05	0.55
3:B:484:HOH:O	1:C:65:GLN:HG2	2.06	0.55
1:C:366:SER:HA	1:C:414:MET:O	2.07	0.55
1:A:357:LEU:HD13	1:A:397:LYS:CE	2.32	0.55
1:B:403:GLU:OE1	1:C:67:LYS:HE3	2.06	0.55
1:C:30:ILE:HD11	1:C:32:GLU:HG2	1.89	0.55
1:D:34:LEU:HG	1:D:205:GLU:OE2	2.06	0.55
1:C:99:GLN:HG2	1:C:347:PHE:CE2	2.41	0.55
1:D:51:ASN:O	1:D:74:SER:HB3	2.06	0.55
1:D:115:ALA:HB1	1:D:160:LEU:HD11	1.88	0.54
1:A:315:PRO:HD3	1:A:332:VAL:HA	1.88	0.54
1:B:179:ALA:HB2	1:B:212:ILE:HG12	1.89	0.54
1:B:282:LEU:CD1	1:B:291:SER:HB3	2.37	0.54
1:B:406:ALA:N	1:B:412:LYS:HD2	2.23	0.54
1:C:280:ALA:HA	1:C:357:LEU:O	2.07	0.54
1:D:466:ASP:OD1	1:D:466:ASP:N	2.40	0.54
1:A:176:ALA:HA	1:A:181:ASN:O	2.08	0.54
1:C:27:LEU:HD22	1:C:58:PHE:HD2	1.73	0.54
1:B:55:VAL:O	1:B:61:GLY:HA3	2.08	0.54
1:D:151:ARG:HG2	1:D:153:PHE:CE2	2.43	0.54
1:A:60:LEU:HD22	1:A:72:MET:CE	2.38	0.53
1:A:449:GLU:OE1	1:A:477:GLN:HG3	2.08	0.53
1:B:100:GLY:HA2	1:B:347:PHE:CG	2.43	0.53
1:C:441:ARG:HG3	1:C:442:LYS:HG2	1.89	0.53
1:D:101:THR:O	1:D:105:ARG:HG3	2.09	0.53
1:D:436:VAL:HB	1:D:449:GLU:HB2	1.91	0.53
1:C:354:HIS:CD2	1:D:226:TYR:HE1	2.27	0.53
1:B:274:PHE:HE1	1:B:282:LEU:HD21	1.74	0.53
1:B:176:ALA:HA	1:B:181:ASN:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:PRO:HD3	3:C:665:HOH:O	2.07	0.53
1:C:136:ASN:OD1	1:C:142:ALA:HB2	2.09	0.53
1:D:265:ARG:HD2	1:D:451:TRP:CE2	2.44	0.53
1:D:83:PHE:CD1	1:D:83:PHE:C	2.82	0.52
1:B:289:LEU:HA	1:B:292:ASN:ND2	2.23	0.52
1:A:440:ASP:CB	1:A:443:LYS:HG2	2.38	0.52
1:B:260:ASP:HB3	1:C:66:SER:HB2	1.91	0.52
1:D:171:VAL:HG13	1:D:192:ASN:HB3	1.92	0.52
1:A:293:PHE:HB3	1:A:479:VAL:HG11	1.91	0.52
1:B:60:LEU:CD1	1:B:72:MET:HE1	2.37	0.52
1:D:152:GLU:HA	1:D:156:GLN:O	2.10	0.51
1:D:125:LEU:O	1:D:129:GLY:N	2.40	0.51
1:C:196:CYS:O	1:C:202:THR:HG21	2.10	0.51
1:C:439:VAL:HG22	1:C:445:LEU:CD2	2.40	0.51
1:C:28:SER:HB3	1:C:325:ILE:CD1	2.41	0.51
1:D:176:ALA:HB2	1:D:206:VAL:HG11	1.93	0.51
1:C:28:SER:HA	3:C:619:HOH:O	2.11	0.51
1:D:108:ALA:HB1	1:D:113:VAL:O	2.10	0.51
1:A:100:GLY:HA2	1:A:347:PHE:CG	2.45	0.51
1:C:83:PHE:C	1:C:83:PHE:CD1	2.84	0.51
1:A:193:LEU:HG	1:A:222:ILE:HD11	1.93	0.51
1:B:289:LEU:O	1:B:292:ASN:HB2	2.10	0.51
1:D:15:PRO:HG2	1:D:18:ALA:HB2	1.92	0.51
1:D:447:LEU:HD11	1:D:449:GLU:O	2.09	0.51
1:A:76:TYR:CE2	1:A:78:GLY:HA2	2.45	0.51
1:C:172:LYS:HE3	3:C:486:HOH:O	2.11	0.50
1:A:8:VAL:HG23	3:A:1020:HOH:O	2.10	0.50
1:A:60:LEU:HD21	1:A:69:ILE:HD13	1.93	0.50
1:B:135:TYR:OH	1:B:381:VAL:HG11	2.10	0.50
1:B:381:VAL:HG23	1:B:381:VAL:O	2.10	0.50
1:C:57:ASN:ND2	1:C:239:ARG:NH2	2.58	0.50
1:B:362:ALA:HB2	1:B:371:LEU:HD11	1.94	0.50
1:D:57:ASN:HA	1:D:65:GLN:HE22	1.75	0.50
1:A:119:SER:HB2	1:A:156:GLN:HE21	1.76	0.50
1:D:381:VAL:H	1:D:382:LYS:HE3	1.77	0.50
1:B:435:ALA:N	1:B:476:MET:HE1	2.27	0.50
1:D:375:MET:O	1:D:420:PRO:HD2	2.12	0.50
1:C:82:GLU:OE1	1:C:85:ARG:NH1	2.44	0.50
1:D:176:ALA:HA	1:D:181:ASN:O	2.12	0.50
1:A:186:LYS:HA	1:A:340:TYR:CD2	2.47	0.49
1:A:360:LEU:HD23	1:A:360:LEU:H	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:GLY:HA2	1:C:163:ALA:HB1	1.94	0.49
1:D:77:VAL:HG21	1:D:83:PHE:CE1	2.46	0.49
1:A:457:ASP:O	1:A:461:LYS:HG2	2.12	0.49
1:C:287:PRO:HB3	1:C:359:MET:HG2	1.94	0.49
1:A:443:LYS:HE3	3:A:1066:HOH:O	2.13	0.49
1:A:302:LEU:HB2	1:A:311:LEU:HB2	1.95	0.49
1:C:57:ASN:ND2	1:C:239:ARG:NH1	2.60	0.49
1:A:448:ILE:C	1:A:473:LEU:HD12	2.32	0.49
1:B:189:ARG:O	1:B:190:ASN:C	2.51	0.49
1:B:316:LEU:HB2	1:B:319:GLU:HG3	1.94	0.49
1:C:302:LEU:HB2	1:C:311:LEU:HB2	1.95	0.49
1:C:451:TRP:HB3	1:C:454:LEU:HD12	1.95	0.49
1:A:23:GLY:HA3	1:A:192:ASN:OD1	2.12	0.48
1:A:132:PRO:HG2	3:A:1058:HOH:O	2.12	0.48
1:B:83:PHE:CD1	1:B:83:PHE:C	2.85	0.48
1:B:272:LEU:HD21	1:B:479:VAL:HA	1.94	0.48
1:D:149:GLU:O	1:D:159:ILE:HA	2.12	0.48
1:C:52:ASN:HA	1:C:76:TYR:O	2.12	0.48
1:C:404:HIS:CD2	1:C:462:SER:O	2.67	0.48
1:D:367:LYS:HE2	1:D:368:TYR:CZ	2.47	0.48
1:A:437:PHE:HA	1:A:446:THR:O	2.12	0.48
1:B:357:LEU:HD12	1:B:397:LYS:O	2.12	0.48
1:B:359:MET:HA	1:B:399:VAL:O	2.13	0.48
1:C:263:ARG:HG2	3:C:530:HOH:O	2.13	0.48
1:D:176:ALA:HB2	1:D:182:VAL:HG22	1.95	0.48
1:A:65:GLN:NE2	1:A:82:GLU:HG2	2.28	0.48
1:C:367:LYS:HG3	1:C:465:CYS:SG	2.53	0.48
1:D:71:ARG:HD2	1:D:93:GLU:OE1	2.14	0.48
1:B:376:ILE:O	1:B:377:PRO:C	2.52	0.48
1:B:166:GLY:O	1:B:199:ALA:HA	2.14	0.48
1:B:60:LEU:CD2	1:B:69:ILE:HD11	2.42	0.48
1:B:305:GLU:HB2	1:B:347:PHE:CZ	2.48	0.48
1:C:201:THR:HA	1:C:228:HIS:ND1	2.29	0.48
1:D:72:MET:HG3	1:D:83:PHE:HE2	1.78	0.48
1:D:315:PRO:HD3	1:D:332:VAL:CA	2.42	0.48
1:B:100:GLY:CA	1:B:347:PHE:CG	2.97	0.48
1:D:109:GLY:HA2	1:D:163:ALA:HB1	1.96	0.48
1:D:435:ALA:N	1:D:476:MET:HE1	2.29	0.48
1:A:174:TRP:CE2	1:A:185:ARG:HD2	2.48	0.47
1:B:51:ASN:OD1	1:B:99:GLN:HG3	2.14	0.47
1:B:360:LEU:N	1:B:360:LEU:CD2	2.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:VAL:HB	1:C:433:GLU:HG3	1.95	0.47
1:D:186:LYS:HA	1:D:340:TYR:CD2	2.48	0.47
1:D:359:MET:HA	1:D:399:VAL:O	2.14	0.47
1:A:277:GLY:N	1:A:299:THR:O	2.43	0.47
1:C:149:GLU:O	1:C:159:ILE:HA	2.14	0.47
1:B:335:LEU:HB3	1:B:336:PRO:HD2	1.95	0.47
1:D:8:VAL:O	1:D:12:LYS:N	2.45	0.47
1:D:362:ALA:HB2	1:D:371:LEU:CD1	2.43	0.47
1:A:4:TYR:CZ	1:A:229:ARG:HD3	2.50	0.47
1:B:185:ARG:O	1:B:188:ALA:HB3	2.14	0.47
1:C:93:GLU:HA	1:C:133:ILE:O	2.15	0.47
1:D:407:LYS:HG3	3:D:632:HOH:O	2.15	0.47
1:A:245:VAL:CG1	1:A:246:ARG:H	2.24	0.47
1:B:235:LYS:HE3	1:B:237:GLU:HG2	1.97	0.47
1:B:260:ASP:OD2	1:B:262:VAL:HB	2.15	0.47
1:B:274:PHE:CE1	1:B:282:LEU:HD21	2.50	0.47
1:D:80:ASN:HB3	1:D:83:PHE:HB3	1.97	0.47
1:D:89:ALA:O	1:D:137:LYS:HE2	2.15	0.47
1:D:165:ARG:HG3	1:D:198:ALA:O	2.15	0.47
1:A:94:VAL:O	1:A:133:ILE:HA	2.14	0.47
1:C:225:ILE:HG13	1:D:279:TYR:CD2	2.50	0.47
1:D:434:LYS:HB3	1:D:454:LEU:HD13	1.97	0.47
1:A:353:GLY:HA3	1:A:395:LYS:HG2	1.97	0.47
1:B:168:PHE:HA	1:B:201:THR:O	2.15	0.47
1:C:225:ILE:HG13	1:D:279:TYR:CG	2.50	0.47
1:D:424:LYS:O	1:D:425:GLN:C	2.52	0.47
1:A:96:LEU:HD13	1:A:383:GLY:HA2	1.96	0.46
1:D:23:GLY:HA3	1:D:192:ASN:OD1	2.15	0.46
1:D:38:LEU:HD12	1:D:43:VAL:CG1	2.45	0.46
1:D:137:LYS:HB3	1:D:137:LYS:HZ2	1.79	0.46
1:A:196:CYS:O	1:A:202:THR:HG21	2.15	0.46
1:A:354:HIS:O	1:B:225:ILE:HD11	2.16	0.46
1:A:367:LYS:HE3	1:A:466:ASP:OD1	2.15	0.46
1:A:360:LEU:HD23	1:A:360:LEU:N	2.30	0.46
1:C:100:GLY:HA2	1:C:347:PHE:CG	2.50	0.46
1:C:189:ARG:HD3	1:C:193:LEU:HD13	1.97	0.46
1:B:60:LEU:HD11	1:B:72:MET:HE2	1.97	0.46
1:B:90:GLY:HA2	3:B:550:HOH:O	2.14	0.46
1:C:28:SER:OG	1:C:325:ILE:HD11	2.15	0.46
1:D:174:TRP:CZ2	1:D:175:LYS:HE3	2.50	0.46
1:A:184:PHE:CG	1:A:189:ARG:HG3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:GLU:OE2	1:D:268:LYS:HE2	2.15	0.46
1:A:67:LYS:N	1:A:67:LYS:CD	2.78	0.46
1:B:305:GLU:C	1:B:307:GLY:H	2.19	0.46
1:D:60:LEU:CD1	1:D:69:ILE:CD1	2.94	0.46
1:D:246:ARG:NH1	1:D:314:TYR:O	2.48	0.46
1:B:176:ALA:HB3	1:B:230:LEU:HD21	1.95	0.46
1:A:245:VAL:CG1	1:A:246:ARG:N	2.78	0.46
1:A:357:LEU:CD1	1:A:397:LYS:HE3	2.35	0.45
1:C:113:VAL:O	1:C:163:ALA:HB2	2.16	0.45
1:A:378:GLY:O	1:A:379:LYS:HB2	2.17	0.45
1:A:449:GLU:HB3	1:A:476:MET:HA	1.98	0.45
1:B:9:GLU:O	1:B:12:LYS:HG2	2.16	0.45
1:B:118:THR:OG1	1:B:351:ARG:HD2	2.16	0.45
1:C:358:THR:HG21	1:C:390:LEU:HB3	1.97	0.45
1:D:177:ASP:OD2	1:D:181:ASN:HB2	2.16	0.45
1:D:434:LYS:HB3	1:D:459:ILE:HD11	1.97	0.45
1:A:265:ARG:HD2	1:A:451:TRP:CZ2	2.51	0.45
1:B:222:ILE:O	1:B:222:ILE:HG22	2.16	0.45
1:C:173:ALA:HB3	1:C:206:VAL:HG12	1.97	0.45
1:A:244:SER:O	1:A:314:TYR:HB3	2.17	0.45
1:B:84:GLU:O	1:B:88:LEU:HG	2.17	0.45
1:B:103:ALA:HB1	1:B:344:ASP:HA	1.98	0.45
1:D:186:LYS:HA	1:D:340:TYR:CE2	2.52	0.45
1:D:448:ILE:HG13	1:D:449:GLU:HG3	1.97	0.45
1:A:6:ASP:OD1	1:A:8:VAL:N	2.50	0.45
1:B:239:ARG:HD3	3:C:608:HOH:O	2.16	0.45
1:C:43:VAL:O	1:C:43:VAL:HG13	2.15	0.45
1:D:3:PHE:CE2	1:D:230:LEU:HD23	2.52	0.45
1:D:150:VAL:HG22	1:D:159:ILE:HG22	1.97	0.45
1:D:279:TYR:CD1	1:D:301:HIS:HB2	2.51	0.45
1:A:60:LEU:HD22	1:A:72:MET:SD	2.56	0.45
1:C:261:ASN:HB2	1:C:264:GLU:HB2	1.98	0.45
1:C:435:ALA:HB1	1:C:447:LEU:CD1	2.47	0.45
1:D:25:PHE:CD1	1:D:51:ASN:ND2	2.84	0.45
1:B:282:LEU:HD13	1:B:287:PRO:O	2.17	0.45
1:C:225:ILE:HA	1:D:279:TYR:CZ	2.52	0.45
1:D:328:GLY:O	1:D:329:LYS:HB2	2.17	0.45
1:B:20:VAL:CG1	1:B:170:LEU:HG	2.47	0.45
1:C:338:ALA:O	1:D:217:PRO:HB3	2.17	0.45
1:D:302:LEU:CB	1:D:311:LEU:HB2	2.44	0.45
1:A:60:LEU:HD21	1:A:72:MET:SD	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TYR:O	1:A:135:TYR:HD2	2.00	0.44
1:A:180:GLY:O	1:A:227:VAL:HG21	2.16	0.44
1:A:358:THR:O	1:A:398:VAL:HA	2.17	0.44
1:C:71:ARG:HD2	1:C:93:GLU:HB2	1.99	0.44
1:B:445:LEU:HD22	1:B:465:CYS:SG	2.57	0.44
1:D:275:GLU:O	1:D:278:MET:HB3	2.17	0.44
1:C:78:GLY:HA2	1:C:382:LYS:HD3	2.00	0.44
1:A:57:ASN:O	1:A:62:LEU:HD21	2.18	0.44
1:A:71:ARG:HD2	1:A:93:GLU:OE1	2.18	0.44
1:D:442:LYS:HA	1:D:442:LYS:CE	2.48	0.44
1:A:85:ARG:NH2	1:A:91:GLU:OE2	2.50	0.44
1:B:109:GLY:HA2	1:B:163:ALA:HB1	1.99	0.44
1:D:425:GLN:HB3	1:D:441:ARG:HG2	1.99	0.44
1:B:450:LEU:O	1:B:475:PRO:HA	2.18	0.44
1:C:127:GLN:HG3	1:C:159:ILE:CG2	2.47	0.44
1:D:294:ILE:HD13	1:D:300:VAL:HG21	1.99	0.44
1:C:78:GLY:CA	1:C:382:LYS:HD3	2.48	0.44
1:C:274:PHE:HB3	1:C:300:VAL:HG21	1.99	0.44
1:A:242:ARG:HB2	1:A:329:LYS:O	2.18	0.44
1:D:21:LEU:HA	1:D:49:VAL:HB	2.00	0.44
1:D:261:ASN:O	1:D:265:ARG:HB2	2.18	0.44
1:D:397:LYS:CE	3:D:633:HOH:O	2.65	0.44
1:A:17:GLY:HA2	1:A:45:GLU:O	2.17	0.43
1:B:60:LEU:CD1	1:B:72:MET:HE2	2.47	0.43
1:B:132:PRO:HB3	1:B:141:ILE:CG1	2.35	0.43
1:B:326:ASN:N	1:B:332:VAL:CG2	2.81	0.43
1:C:204:VAL:HB	1:C:230:LEU:HD12	1.99	0.43
1:C:315:PRO:HB2	1:C:319:GLU:HB2	2.00	0.43
1:D:125:LEU:HD23	1:D:125:LEU:HA	1.83	0.43
1:D:286:ILE:HB	1:D:287:PRO:HD3	2.00	0.43
1:D:341:PHE:CE1	1:D:346:SER:HA	2.52	0.43
1:A:60:LEU:CD2	1:A:69:ILE:CD1	2.96	0.43
1:C:55:VAL:O	1:C:61:GLY:HA3	2.18	0.43
1:D:56:ASP:O	1:D:65:GLN:NE2	2.51	0.43
1:D:436:VAL:HG23	1:D:476:MET:CE	2.48	0.43
1:D:450:LEU:O	1:D:475:PRO:HA	2.18	0.43
1:B:287:PRO:HA	1:B:359:MET:CE	2.48	0.43
1:D:263:ARG:HG3	1:D:263:ARG:HH11	1.83	0.43
1:D:440:ASP:HB3	1:D:443:LYS:HG2	1.99	0.43
1:D:455:THR:O	1:D:456:VAL:C	2.55	0.43
1:B:99:GLN:NE2	3:B:486:HOH:O	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLU:HG2	1:B:116:PHE:CE2	2.54	0.43
1:C:313:PRO:O	1:C:333:THR:HG23	2.19	0.43
1:A:366:SER:OG	1:A:370:ASP:HB2	2.19	0.43
1:A:367:LYS:HD2	1:A:415:GLU:OE2	2.19	0.43
1:D:238:LYS:HE2	3:D:665:HOH:O	2.19	0.43
1:D:264:GLU:HG2	1:D:268:LYS:HE2	1.99	0.43
1:A:367:LYS:HD3	1:A:368:TYR:CZ	2.54	0.43
1:B:177:ASP:OD2	1:B:181:ASN:HB2	2.18	0.43
1:C:28:SER:HB3	1:C:325:ILE:HD13	2.00	0.43
1:C:193:LEU:HG	1:C:222:ILE:CD1	2.44	0.43
1:D:381:VAL:H	1:D:382:LYS:NZ	2.17	0.43
1:A:119:SER:HB2	1:A:156:GLN:NE2	2.33	0.43
1:A:326:ASN:HB3	1:A:332:VAL:HG11	2.00	0.43
1:D:382:LYS:HE3	1:D:382:LYS:N	2.34	0.43
1:B:39:LEU:HD23	1:B:68:GLN:OE1	2.17	0.43
1:B:355:VAL:HB	3:B:612:HOH:O	2.18	0.43
1:C:236:TYR:HB3	1:C:238:LYS:HG3	2.00	0.43
1:C:375:MET:O	1:C:420:PRO:HD2	2.19	0.43
1:C:395:LYS:NZ	1:D:165:ARG:CZ	2.82	0.43
1:D:53:ALA:HB2	1:D:72:MET:HE1	2.01	0.43
1:D:113:VAL:O	1:D:163:ALA:HB2	2.18	0.43
1:D:295:SER:HA	1:D:296:PRO:HD3	1.93	0.43
1:D:397:LYS:HE3	3:D:633:HOH:O	2.18	0.43
1:A:127:GLN:HG3	1:A:159:ILE:CG2	2.49	0.43
1:A:156:GLN:HG2	1:A:157:HIS:N	2.33	0.42
1:B:185:ARG:NH1	1:B:323:ASP:OD2	2.45	0.42
1:B:193:LEU:C	1:B:193:LEU:HD23	2.40	0.42
1:C:282:LEU:CD1	1:C:291:SER:HB3	2.49	0.42
1:D:11:VAL:HG21	1:D:38:LEU:HD22	2.00	0.42
1:A:50:SER:O	1:A:74:SER:CB	2.67	0.42
1:A:272:LEU:CD1	1:A:477:GLN:HB2	2.50	0.42
1:C:187:SER:HB3	1:C:308:ILE:HD11	2.00	0.42
1:D:85:ARG:HH12	1:D:91:GLU:CD	2.23	0.42
1:A:189:ARG:O	1:A:190:ASN:C	2.56	0.42
1:A:117:TYR:CZ	1:A:160:LEU:HD13	2.53	0.42
1:B:156:GLN:HG2	1:B:157:HIS:N	2.34	0.42
1:B:414:MET:HG3	1:B:416:LYS:O	2.20	0.42
1:D:60:LEU:HD13	1:D:60:LEU:O	2.18	0.42
1:D:320:VAL:HG13	1:D:331:THR:HG21	2.00	0.42
1:D:360:LEU:N	1:D:360:LEU:CD2	2.83	0.42
1:C:23:GLY:HA3	1:C:192:ASN:OD1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:GLY:CA	1:C:163:ALA:HB1	2.50	0.42
1:D:56:ASP:OD2	1:D:81:ALA:HB3	2.19	0.42
1:D:100:GLY:CA	1:D:347:PHE:CG	3.02	0.42
1:D:381:VAL:CA	1:D:382:LYS:HE3	2.48	0.42
1:B:360:LEU:HD23	1:B:360:LEU:H	1.84	0.42
1:C:165:ARG:HA	1:C:198:ALA:O	2.18	0.42
1:D:110:GLY:HA3	1:D:197:LYS:O	2.19	0.42
1:D:304:SER:HB3	1:D:308:ILE:HB	2.02	0.42
1:D:440:ASP:CB	1:D:443:LYS:HG2	2.50	0.42
1:A:171:VAL:HG13	1:A:192:ASN:HB3	2.01	0.42
1:A:404:HIS:CD2	1:A:462:SER:O	2.73	0.42
1:B:294:ILE:HD13	1:B:300:VAL:HG21	2.01	0.42
1:D:60:LEU:CD1	1:D:69:ILE:HD12	2.49	0.42
1:D:368:TYR:HE1	1:D:442:LYS:O	2.02	0.42
1:D:443:LYS:HE2	1:D:443:LYS:HB3	1.81	0.42
1:A:53:ALA:HB2	1:A:83:PHE:CE2	2.55	0.42
1:A:261:ASN:O	1:A:264:GLU:HB3	2.20	0.42
1:B:289:LEU:HA	1:B:292:ASN:HD22	1.84	0.42
1:B:404:HIS:CD2	1:B:462:SER:O	2.73	0.42
1:B:449:GLU:OE2	1:B:477:GLN:NE2	2.51	0.42
1:C:71:ARG:HD2	1:C:93:GLU:CB	2.49	0.42
1:C:440:ASP:HB3	1:C:443:LYS:HB2	2.02	0.42
1:D:435:ALA:HB1	1:D:447:LEU:CD1	2.50	0.42
1:A:173:ALA:HB1	1:A:182:VAL:CG1	2.49	0.42
1:A:369:GLY:O	1:A:427:VAL:HG23	2.20	0.42
1:C:11:VAL:HB	1:C:14:ILE:HD12	2.01	0.42
1:C:57:ASN:OD1	1:C:239:ARG:NH1	2.40	0.42
1:D:77:VAL:HG11	1:D:83:PHE:CE1	2.54	0.42
1:C:30:ILE:HD13	1:C:59:GLY:HA2	2.00	0.42
1:D:398:VAL:HB	1:D:426:CYS:O	2.20	0.42
1:A:113:VAL:O	1:A:163:ALA:HB2	2.20	0.41
1:B:64:LEU:HD23	1:B:64:LEU:HA	1.85	0.41
1:C:327:ALA:HB3	3:C:582:HOH:O	2.19	0.41
1:A:119:SER:OG	1:A:392:SER:HB2	2.19	0.41
1:A:127:GLN:HG3	1:A:159:ILE:HG21	2.02	0.41
1:A:173:ALA:HB1	1:A:182:VAL:HG13	2.00	0.41
1:D:75:SER:HA	1:D:97:THR:O	2.19	0.41
1:C:381:VAL:HG23	1:C:381:VAL:O	2.20	0.41
1:D:38:LEU:CD1	1:D:43:VAL:HG11	2.50	0.41
1:D:242:ARG:HB2	1:D:329:LYS:O	2.20	0.41
1:B:134:LYS:O	1:B:142:ALA:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:NZ	1:B:207:GLU:OE2	2.50	0.41
1:B:357:LEU:HD11	1:B:399:VAL:HG23	2.02	0.41
1:C:384:MET:CE	1:C:384:MET:CG	2.93	0.41
1:B:60:LEU:HD11	1:B:72:MET:CE	2.50	0.41
1:D:77:VAL:CG2	1:D:83:PHE:CD2	3.01	0.41
1:B:264:GLU:O	1:B:268:LYS:HG3	2.21	0.41
1:B:357:LEU:HD11	1:B:399:VAL:CG2	2.51	0.41
1:C:174:TRP:CZ2	1:C:175:LYS:HE3	2.55	0.41
1:D:438:ASP:CG	1:D:448:ILE:HD13	2.41	0.41
1:B:137:LYS:H	1:B:137:LYS:HD2	1.86	0.41
1:D:176:ALA:O	1:D:209:ILE:HA	2.20	0.41
1:A:190:ASN:OD1	1:A:191:PHE:N	2.50	0.41
1:B:326:ASN:N	1:B:332:VAL:HG22	2.36	0.41
1:C:172:LYS:CE	1:C:236:TYR:CE1	3.03	0.41
1:D:100:GLY:HA2	1:D:347:PHE:CG	2.56	0.41
1:D:381:VAL:H	1:D:382:LYS:CE	2.34	0.41
1:A:99:GLN:HE21	1:A:99:GLN:HB2	1.70	0.41
1:A:149:GLU:O	1:A:159:ILE:HA	2.21	0.41
1:A:375:MET:O	1:A:420:PRO:HD2	2.21	0.41
1:B:97:THR:HA	1:B:98:PRO:HD3	1.96	0.41
1:B:247:LYS:HE2	1:B:247:LYS:HB2	1.96	0.41
1:C:94:VAL:N	1:C:133:ILE:O	2.43	0.41
1:D:173:ALA:HB1	1:D:182:VAL:CG1	2.51	0.41
1:D:231:VAL:HG22	1:D:232:LYS:O	2.21	0.41
1:A:435:ALA:HB1	1:A:447:LEU:HD11	2.02	0.41
1:C:184:PHE:CG	1:C:189:ARG:HG3	2.57	0.40
1:C:222:ILE:HD13	1:C:222:ILE:HA	1.88	0.40
1:D:60:LEU:HD11	1:D:69:ILE:HD12	2.03	0.40
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.90	0.40
1:B:441:ARG:O	1:B:442:LYS:HD2	2.20	0.40
1:C:17:GLY:HA2	1:C:45:GLU:O	2.20	0.40
1:C:103:ALA:HB1	1:C:344:ASP:HA	2.03	0.40
1:C:116:PHE:HA	1:D:116:PHE:HA	2.03	0.40
1:C:171:VAL:HG13	1:C:192:ASN:HB3	2.04	0.40
1:C:387:ALA:HB1	1:C:422:THR:HG21	2.02	0.40
1:A:25:PHE:CE1	1:A:99:GLN:OE1	2.69	0.40
1:A:133:ILE:HD11	1:A:145:SER:HA	2.03	0.40
1:C:34:LEU:HA	1:C:34:LEU:HD23	1.79	0.40
1:C:370:ASP:OD2	1:C:416:LYS:HE3	2.21	0.40
1:C:374:TRP:HB2	1:C:384:MET:HA	2.03	0.40
1:A:88:LEU:HD21	1:A:381:VAL:HG21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ALA:HB1	1:A:113:VAL:O	2.21	0.40
1:A:365:VAL:HG11	1:A:430:ILE:HD11	2.04	0.40
1:A:398:VAL:HB	1:A:426:CYS:O	2.21	0.40
1:B:165:ARG:HG3	1:B:198:ALA:O	2.22	0.40
1:C:45:GLU:HA	1:C:70:LYS:HB2	2.04	0.40
1:C:85:ARG:HH11	1:C:85:ARG:HD3	1.72	0.40
1:D:362:ALA:HA	1:D:373:ASN:CB	2.51	0.40
1:A:193:LEU:HB3	1:A:194:PRO:CD	2.51	0.40
1:A:376:ILE:O	1:A:377:PRO:C	2.58	0.40
1:B:25:PHE:CE2	1:B:306:ASN:HB3	2.57	0.40
1:B:77:VAL:HG21	1:B:83:PHE:CZ	2.56	0.40
1:C:127:GLN:HG3	1:C:159:ILE:HG21	2.04	0.40
1:C:402:MET:O	1:C:432:THR:HA	2.22	0.40
1:D:90:GLY:O	1:D:134:LYS:HE3	2.21	0.40
1:D:381:VAL:N	1:D:382:LYS:HE3	2.35	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	463/481 (96%)	446 (96%)	15 (3%)	2 (0%)	34	30
1	B	466/481 (97%)	452 (97%)	12 (3%)	2 (0%)	34	30
1	C	463/481 (96%)	450 (97%)	12 (3%)	1 (0%)	47	44
1	D	465/481 (97%)	450 (97%)	14 (3%)	1 (0%)	47	44
All	All	1857/1924 (96%)	1798 (97%)	53 (3%)	6 (0%)	41	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	LYS
1	B	138	ASP
1	B	190	ASN
1	C	190	ASN
1	D	190	ASN
1	A	190	ASN

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	381/393 (97%)	367 (96%)	14 (4%)	34	32
1	B	383/393 (98%)	369 (96%)	14 (4%)	34	32
1	C	381/393 (97%)	374 (98%)	7 (2%)	59	63
1	D	383/393 (98%)	371 (97%)	12 (3%)	40	40
All	All	1528/1572 (97%)	1481 (97%)	47 (3%)	40	40

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	67	LYS
1	A	83	PHE
1	A	85	ARG
1	A	119	SER
1	A	178	GLN
1	A	230	LEU
1	A	261	ASN
1	A	284	ILE
1	A	384	MET
1	A	395	LYS
1	A	416	LYS
1	A	477	GLN
1	A	480	THR
1	B	38	LEU
1	B	60	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	72	MET
1	B	74	SER
1	B	137	LYS
1	B	138	ASP
1	B	152	GLU
1	B	304	SER
1	B	332	VAL
1	B	341	PHE
1	B	360	LEU
1	B	380	LEU
1	B	414	MET
1	B	466	ASP
1	C	60	LEU
1	C	67	LYS
1	C	230	LEU
1	C	318	ASN
1	C	341	PHE
1	C	360	LEU
1	C	416	LYS
1	D	57	ASN
1	D	60	LEU
1	D	137	LYS
1	D	317	GLN
1	D	360	LEU
1	D	377	PRO
1	D	382	LYS
1	D	418	THR
1	D	432	THR
1	D	442	LYS
1	D	445	LEU
1	D	466	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	425	GLN
1	B	292	ASN
1	B	297	ASN
1	C	65	GLN
1	C	99	GLN
1	C	156	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	301	HIS
1	C	317	GLN
1	D	65	GLN
1	D	99	GLN
1	D	292	ASN
1	D	297	ASN
1	D	317	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 1 ligands modelled in this entry, 1 is 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 [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	467/481 (97%)	-0.15	6 (1%) 77 76	15, 27, 42, 56	0
1	B	470/481 (97%)	-0.32	3 (0%) 89 88	13, 23, 36, 51	0
1	C	467/481 (97%)	-0.34	1 (0%) 95 94	13, 23, 36, 47	0
1	D	469/481 (97%)	-0.10	6 (1%) 77 76	14, 27, 41, 60	0
All	All	1873/1924 (97%)	-0.23	16 (0%) 84 83	13, 25, 40, 60	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	260	ASP	3.6
1	D	248	GLU	3.4
1	A	480	THR	3.0
1	A	407	LYS	2.9
1	D	297	ASN	2.7
1	B	297	ASN	2.7
1	A	247	LYS	2.7
1	B	138	ASP	2.6
1	A	409	ASN	2.5
1	D	296	PRO	2.4
1	A	431	ILE	2.4
1	D	480	THR	2.3
1	B	137	LYS	2.3
1	D	261	ASN	2.3
1	C	138	ASP	2.2
1	A	261	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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(\AA^2)	Q<0.9
2	CL	A	901	1/1	0.99	0.03	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.