



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:31 PM GMT

PDB ID : 1U0M
Title : Crystal Structure of 1,3,6,8-Tetrahydroxynaphthalene Synthase (THNS) from *Streptomyces coelicolor* A3(2): a Bacterial Type III Polyketide Synthase (PKS) Provides Insights into Enzymatic Control of Reactive Polyketide Intermediates
Authors : Austin, M.B.; Izumikawa, M.; Bowman, M.E.; Udvary, D.W.; Ferrer, J.L.; Moore, B.S.; Noel, J.P.
Deposited on : 2004-07-13
Resolution : 2.22 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

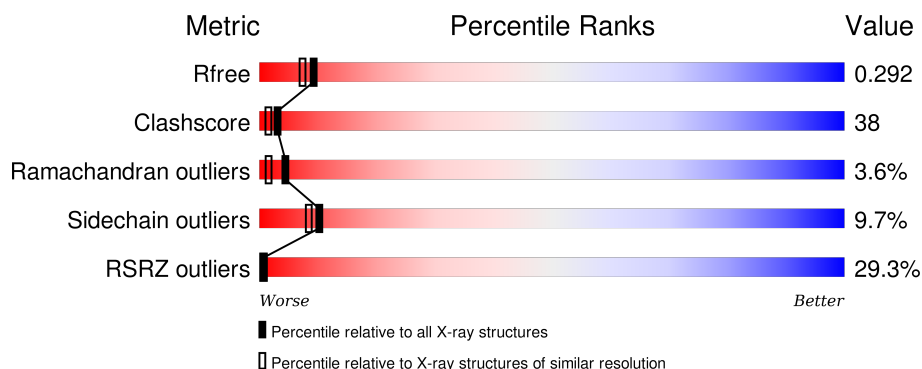
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	382	
1	B	382	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5504 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.

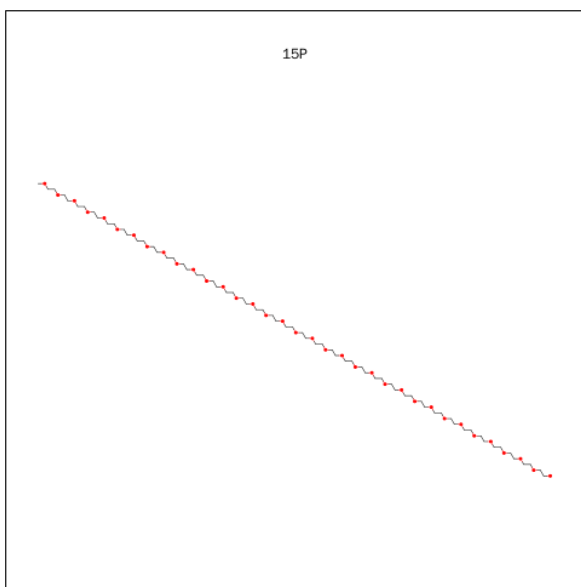
- Molecule 1 is a protein called putative polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2653	1676	459	502	16			
1	B	348	Total	C	N	O	S	0	0	0
			2653	1676	459	502	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	CLONING ARTIFACT	UNP Q9FCA7
A	-6	SER	-	CLONING ARTIFACT	UNP Q9FCA7
A	-5	HIS	-	CLONING ARTIFACT	UNP Q9FCA7
A	-4	GLY	-	CLONING ARTIFACT	UNP Q9FCA7
A	-3	GLY	-	CLONING ARTIFACT	UNP Q9FCA7
A	-2	SER	-	CLONING ARTIFACT	UNP Q9FCA7
A	-1	GLY	-	CLONING ARTIFACT	UNP Q9FCA7
A	0	PHE	-	CLONING ARTIFACT	UNP Q9FCA7
B	-7	GLY	-	CLONING ARTIFACT	UNP Q9FCA7
B	-6	SER	-	CLONING ARTIFACT	UNP Q9FCA7
B	-5	HIS	-	CLONING ARTIFACT	UNP Q9FCA7
B	-4	GLY	-	CLONING ARTIFACT	UNP Q9FCA7
B	-3	GLY	-	CLONING ARTIFACT	UNP Q9FCA7
B	-2	SER	-	CLONING ARTIFACT	UNP Q9FCA7
B	-1	GLY	-	CLONING ARTIFACT	UNP Q9FCA7
B	0	PHE	-	CLONING ARTIFACT	UNP Q9FCA7

- Molecule 2 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: C₆₉H₁₄₀O₃₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	12	7		
2	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total 70	O 70	0	0
4	B	78	Total 78	O 78	0	0

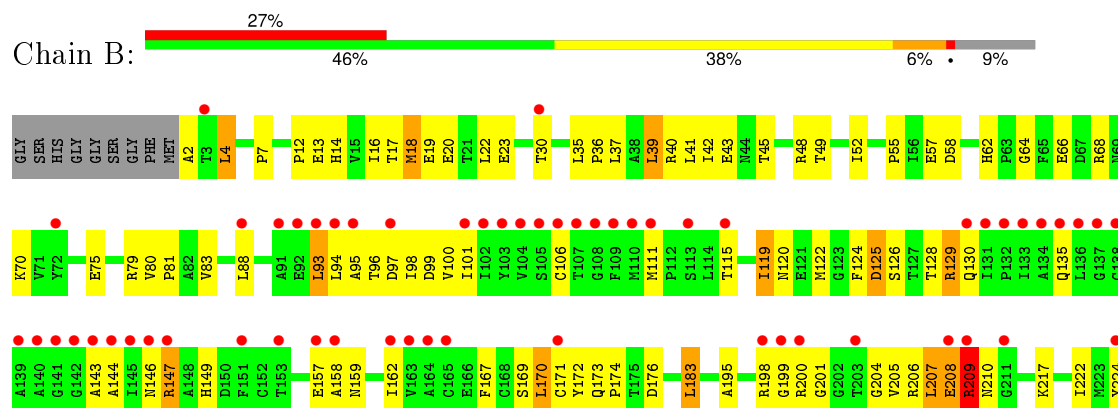
3 Residue-property plots

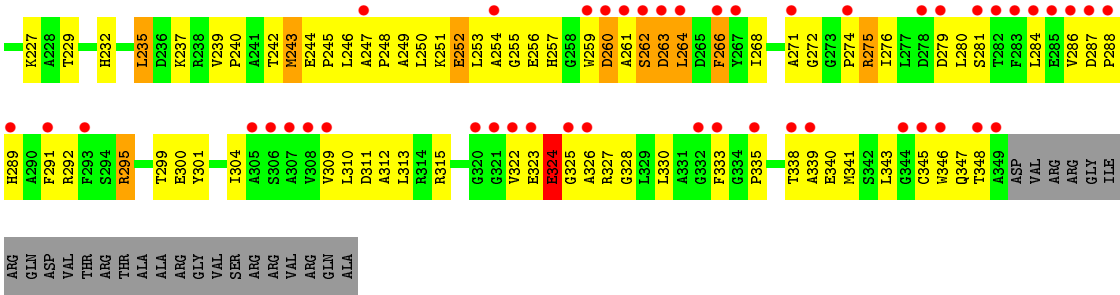
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: putative polyketide synthase



- Molecule 1: putative polyketide synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.68Å 69.69Å 81.14Å 90.00° 95.42° 90.00°	Depositor
Resolution (Å)	40.39 – 2.22 40.39 – 2.22	Depositor EDS
% Data completeness (in resolution range)	87.9 (40.39-2.22) 88.0 (40.39-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.98 (at 2.22Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.253 , 0.292 0.253 , 0.292	Depositor DCC
R_{free} test set	1854 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 37126 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5504	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 15P

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	0.38	0/2710	0.66	0/3688
1	B	0.36	0/2710	0.65	0/3688
All	All	0.37	0/5420	0.65	0/7376

There are no bond length outliers.

There are no bond angle outliers.

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	2653	0	2601	221	0
1	B	2653	0	2601	198	0
2	A	19	0	24	1	0
2	B	19	0	24	1	0
3	A	6	0	8	2	0
3	B	6	0	8	3	0
4	A	70	0	0	2	0
4	B	78	0	0	3	0
All	All	5504	0	5266	407	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 38.

All (407) 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:260:ASP:OD1	1:A:261:ALA:N	1.83	1.12
1:B:93:LEU:HD12	1:B:97:ASP:HB2	1.30	1.10
1:B:275:ARG:HB2	1:B:275:ARG:HH11	1.18	1.04
1:A:148:ALA:HB1	1:A:197:VAL:HG21	1.41	1.02
1:A:266:PHE:HB3	1:A:328:GLY:HA2	1.40	1.02
1:B:323:GLU:HB2	1:B:326:ALA:HB2	1.46	0.97
1:A:2:ALA:HA	1:A:199:GLY:HA2	1.44	0.97
1:B:88:LEU:HD22	1:B:93:LEU:HD21	1.44	0.97
1:A:2:ALA:N	1:A:207:LEU:HD23	1.82	0.95
1:B:244:GLU:HB3	1:B:245:PRO:HD3	1.49	0.94
1:A:322:VAL:O	1:A:324:GLU:N	1.99	0.94
1:A:120:ASN:HD21	1:B:217:LYS:H	0.97	0.94
1:A:52:ILE:HD12	1:A:59:THR:HG21	1.46	0.94
1:A:2:ALA:O	1:A:207:LEU:HB3	1.70	0.90
1:A:37:LEU:O	1:A:41:LEU:HD13	1.69	0.90
1:B:266:PHE:CD2	1:B:328:GLY:HA3	2.08	0.89
1:A:206:ARG:HD3	1:A:347:GLN:NE2	1.88	0.89
1:A:254:ALA:O	1:A:260:ASP:HA	1.73	0.87
1:B:94:LEU:HG	1:B:96:THR:H	1.40	0.86
1:B:275:ARG:HB2	1:B:275:ARG:NH1	1.90	0.86
1:A:237:LYS:CD	1:A:237:LYS:H	1.87	0.86
1:A:209:ARG:NH1	1:A:209:ARG:HB2	1.91	0.85
1:A:244:GLU:HB3	1:A:245:PRO:HD3	1.59	0.84
1:B:93:LEU:HD12	1:B:97:ASP:CB	2.07	0.83
1:A:167:PHE:HB3	1:A:170:LEU:HD23	1.58	0.83
1:A:322:VAL:HG12	1:A:322:VAL:O	1.77	0.83
1:B:75:GLU:O	1:B:79:ARG:HG3	1.79	0.82
1:A:208:GLU:HB2	1:A:343:LEU:O	1.80	0.81
1:A:262:SER:O	1:A:264:LEU:HG	1.80	0.81
1:A:237:LYS:H	1:A:237:LYS:CE	1.93	0.81
1:B:93:LEU:CD1	1:B:97:ASP:HB2	2.10	0.81
1:A:66:GLU:HG2	1:A:70:LYS:HE2	1.63	0.81
1:B:119:ILE:HA	1:B:124:PHE:HB2	1.63	0.80
1:A:322:VAL:O	1:A:322:VAL:CG1	2.28	0.80
1:A:120:ASN:HD21	1:B:217:LYS:N	1.79	0.80
1:A:120:ASN:ND2	1:B:217:LYS:H	1.77	0.79
1:A:321:GLY:O	1:A:322:VAL:HB	1.82	0.79
1:A:237:LYS:HE3	1:A:237:LYS:H	1.48	0.79
1:A:111:MET:HE2	1:B:135:GLN:HA	1.64	0.79
1:A:206:ARG:NH1	1:A:208:GLU:OE1	2.15	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PHE:HD2	1:B:328:GLY:HA3	1.48	0.78
1:A:198:ARG:CZ	1:A:202:GLY:HA2	2.13	0.78
1:A:266:PHE:CB	1:A:328:GLY:HA2	2.12	0.78
1:B:62:HIS:HD2	1:B:64:GLY:H	1.32	0.77
1:B:243:MET:HE3	1:B:246:LEU:HD23	1.67	0.77
1:A:206:ARG:HB3	1:A:345:CYS:O	1.85	0.76
1:A:322:VAL:C	1:A:324:GLU:H	1.89	0.76
1:B:171:CYS:O	3:B:4000:GOL:H31	1.85	0.76
1:A:259:TRP:N	1:A:259:TRP:HE3	1.85	0.75
1:A:243:MET:CE	1:A:246:LEU:HD23	2.17	0.75
1:A:275:ARG:HG2	1:A:276:ILE:H	1.52	0.75
1:A:2:ALA:N	1:A:207:LEU:CD2	2.51	0.74
1:A:206:ARG:N	1:A:345:CYS:O	2.19	0.74
1:B:99:ASP:OD1	1:B:158:ALA:HA	1.86	0.74
1:A:275:ARG:HG2	1:A:276:ILE:N	2.02	0.73
1:A:254:ALA:HA	1:A:343:LEU:HD11	1.69	0.73
1:A:198:ARG:HD2	1:A:200:ARG:NH1	2.03	0.73
1:A:209:ARG:HB2	1:A:209:ARG:HH11	1.51	0.73
1:A:243:MET:HE3	1:A:246:LEU:HD23	1.71	0.72
1:A:247:ALA:HB3	1:A:248:PRO:HD3	1.71	0.72
1:A:208:GLU:HB3	1:A:257:HIS:NE2	2.04	0.72
1:A:237:LYS:HD3	1:A:237:LYS:H	1.53	0.71
1:B:2:ALA:HB3	1:B:207:LEU:HD23	1.71	0.71
1:B:37:LEU:O	1:B:41:LEU:HD13	1.91	0.71
1:A:268:ILE:HB	1:A:330:LEU:HD23	1.73	0.70
1:B:268:ILE:HB	1:B:330:LEU:HD23	1.73	0.70
1:A:267:TYR:CE2	1:A:286:VAL:HG21	2.26	0.70
1:B:35:LEU:O	1:B:39:LEU:HD22	1.92	0.70
1:B:88:LEU:HD22	1:B:93:LEU:CD2	2.22	0.70
1:A:209:ARG:HH11	1:A:209:ARG:CB	2.05	0.69
1:B:246:LEU:HD12	1:B:249:ALA:HB3	1.75	0.69
1:B:48:ARG:HG2	1:B:299:THR:HG23	1.74	0.69
1:A:143:ALA:HB2	1:A:340:GLU:HG3	1.75	0.68
1:A:171:CYS:O	3:A:2000:GOL:H31	1.93	0.68
1:A:200:ARG:HG2	1:A:201:GLY:N	2.07	0.68
1:B:280:LEU:HD12	1:B:291:PHE:CZ	2.27	0.68
1:A:62:HIS:HD2	1:A:64:GLY:H	1.42	0.68
1:B:122:MET:HB3	1:B:124:PHE:HD2	1.58	0.68
1:B:22:LEU:HD12	1:B:39:LEU:HD12	1.75	0.68
1:A:45:THR:HG22	1:A:47:VAL:H	1.58	0.68
1:B:286:VAL:HG12	1:B:287:ASP:N	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:CG	1:A:70:LYS:HE2	2.24	0.68
1:A:198:ARG:NE	1:A:202:GLY:HA2	2.09	0.68
1:B:311:ASP:O	1:B:315:ARG:HG2	1.95	0.67
1:B:93:LEU:HG	1:B:94:LEU:N	2.10	0.67
1:A:264:LEU:HB2	1:A:267:TYR:CE1	2.28	0.67
1:A:55:PRO:O	1:A:59:THR:HG22	1.94	0.67
1:B:266:PHE:HD2	1:B:328:GLY:CA	2.08	0.66
1:A:217:LYS:H	1:B:120:ASN:ND2	1.94	0.66
1:B:125:ASP:N	1:B:125:ASP:OD2	2.26	0.66
1:B:266:PHE:CD2	1:B:328:GLY:CA	2.79	0.66
1:A:237:LYS:HE3	1:A:237:LYS:N	2.10	0.66
1:B:18:MET:HA	1:B:18:MET:HE3	1.76	0.66
1:B:324:GLU:OE1	1:B:348:THR:N	2.29	0.66
1:B:248:PRO:O	1:B:252:GLU:HB2	1.96	0.66
1:A:150:ASP:O	1:A:153:THR:HG23	1.95	0.65
1:B:260:ASP:C	1:B:262:SER:H	1.99	0.65
1:A:246:LEU:HD21	1:A:333:PHE:CZ	2.32	0.65
1:A:266:PHE:HB2	1:A:327:ARG:O	1.95	0.65
1:B:288:PRO:O	1:B:295:ARG:NH2	2.31	0.64
1:B:173:GLN:HB2	3:B:4000:GOL:H11	1.78	0.64
1:B:323:GLU:CD	1:B:323:GLU:H	2.00	0.64
1:A:259:TRP:N	1:A:259:TRP:CE3	2.65	0.64
1:A:264:LEU:HB2	1:A:267:TYR:HE1	1.62	0.64
1:A:148:ALA:CB	1:A:197:VAL:HG21	2.21	0.64
1:A:149:HIS:CE1	1:A:207:LEU:HD13	2.32	0.64
1:B:143:ALA:O	1:B:147:ARG:HG2	1.98	0.63
1:A:255:GLY:HA2	1:A:260:ASP:HB2	1.80	0.63
1:A:286:VAL:HG12	1:A:287:ASP:N	2.13	0.63
1:A:94:LEU:HD12	1:A:96:THR:HB	1.79	0.63
1:A:122:MET:HB3	1:A:124:PHE:CD2	2.33	0.63
1:B:18:MET:HE2	1:B:42:ILE:HG22	1.78	0.63
1:B:255:GLY:N	1:B:260:ASP:HB2	2.14	0.63
1:A:42:ILE:O	1:A:45:THR:HB	1.99	0.63
1:B:143:ALA:HB2	1:B:340:GLU:HG3	1.81	0.63
1:B:289:HIS:CE1	1:B:292:ARG:HD3	2.34	0.63
1:A:280:LEU:HD12	1:A:291:PHE:CZ	2.33	0.62
1:B:122:MET:HG2	1:B:124:PHE:CE2	2.34	0.62
1:B:206:ARG:CZ	1:B:207:LEU:HD11	2.29	0.62
1:B:41:LEU:HB3	1:B:183:LEU:HD11	1.81	0.62
1:A:93:LEU:CD2	1:A:200:ARG:HH12	2.12	0.62
1:A:45:THR:HG23	1:A:47:VAL:HG23	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:MET:CE	1:B:246:LEU:HD23	2.29	0.62
1:A:93:LEU:HD21	1:A:200:ARG:HH12	1.65	0.62
1:A:13:GLU:CD	1:A:13:GLU:H	2.02	0.62
1:A:265:ASP:HB2	1:A:326:ALA:HB1	1.81	0.61
1:B:259:TRP:CH2	1:B:345:CYS:SG	2.92	0.61
1:A:93:LEU:HD21	1:A:200:ARG:NH1	2.15	0.61
1:A:262:SER:O	1:A:264:LEU:N	2.34	0.61
1:A:236:ASP:O	1:A:239:VAL:HG23	2.00	0.61
1:A:119:ILE:HA	1:A:124:PHE:HB2	1.83	0.61
1:A:309:VAL:HG23	1:A:310:LEU:HD13	1.81	0.61
1:A:159:ASN:ND2	1:A:198:ARG:HA	2.16	0.61
1:B:243:MET:HG3	1:B:280:LEU:HD23	1.82	0.61
1:B:35:LEU:HB3	1:B:36:PRO:HD3	1.82	0.61
1:A:267:TYR:CZ	1:A:286:VAL:HG21	2.36	0.60
1:B:17:THR:OG1	1:B:20:GLU:HG2	2.01	0.60
1:B:243:MET:CE	1:B:243:MET:HA	2.31	0.60
1:B:254:ALA:HB1	1:B:260:ASP:HA	1.84	0.60
1:A:207:LEU:O	1:A:207:LEU:HG	2.00	0.60
1:A:99:ASP:O	1:A:129:ARG:HG2	2.02	0.60
1:A:316:LEU:HD23	1:A:316:LEU:O	2.02	0.60
1:A:287:ASP:OD1	1:A:290:ALA:N	2.35	0.59
1:A:275:ARG:HG2	1:A:276:ILE:HG13	1.84	0.59
1:B:209:ARG:HB2	1:B:257:HIS:CD2	2.37	0.59
1:B:206:ARG:NH1	1:B:207:LEU:HD11	2.17	0.59
1:B:250:LEU:HD23	1:B:341:MET:SD	2.42	0.59
1:B:309:VAL:HG23	1:B:310:LEU:HD13	1.84	0.59
1:B:45:THR:O	1:B:274:PRO:HG3	2.03	0.59
1:A:258:GLY:C	1:A:260:ASP:N	2.57	0.58
1:A:92:GLU:C	1:A:93:LEU:HD22	2.22	0.58
1:A:254:ALA:C	1:A:260:ASP:HA	2.24	0.58
1:A:41:LEU:HD23	1:A:183:LEU:HD21	1.85	0.58
1:A:237:LYS:CD	1:A:237:LYS:N	2.63	0.58
1:B:167:PHE:HB3	1:B:170:LEU:HD22	1.85	0.58
1:B:235:LEU:CD2	1:B:239:VAL:HG11	2.33	0.58
1:B:206:ARG:O	1:B:207:LEU:O	2.21	0.58
1:A:160:ALA:HB3	1:A:197:VAL:CG2	2.33	0.57
1:B:66:GLU:O	1:B:70:LYS:HG2	2.04	0.57
1:A:26:ARG:HG3	1:A:39:LEU:HD21	1.87	0.57
1:A:217:LYS:H	1:B:120:ASN:HD21	1.51	0.57
1:B:122:MET:HG2	1:B:124:PHE:HE2	1.70	0.57
1:B:208:GLU:O	1:B:209:ARG:HB2	2.02	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:CD2	1:A:183:LEU:HD21	2.35	0.57
1:B:4:LEU:O	1:B:204:GLY:HA3	2.05	0.57
1:B:7:PRO:HB3	1:B:195:ALA:HB2	1.87	0.57
1:B:206:ARG:HB2	1:B:347:GLN:NE2	2.19	0.56
1:B:13:GLU:H	1:B:13:GLU:CD	2.08	0.56
1:A:255:GLY:C	1:A:257:HIS:H	2.09	0.56
1:A:280:LEU:HD13	1:A:280:LEU:O	2.06	0.56
1:B:246:LEU:O	1:B:246:LEU:HD12	2.04	0.56
1:A:45:THR:CG2	1:A:47:VAL:HG23	2.35	0.56
1:B:19:GLU:O	1:B:23:GLU:HG3	2.05	0.56
1:A:207:LEU:HD12	1:A:208:GLU:N	2.20	0.56
1:A:148:ALA:HB1	1:A:197:VAL:CG2	2.25	0.56
1:A:2:ALA:CA	1:A:199:GLY:HA2	2.29	0.56
1:B:40:ARG:HD2	4:B:4057:HOH:O	2.05	0.56
1:A:257:HIS:HE1	1:A:259:TRP:CE2	2.23	0.56
1:A:229:THR:OG1	1:A:232:HIS:HE1	1.88	0.56
1:B:243:MET:HE1	1:B:333:PHE:CE1	2.41	0.55
1:A:62:HIS:HE1	1:A:173:GLN:HE22	1.52	0.55
1:B:229:THR:OG1	1:B:232:HIS:HE1	1.88	0.55
1:A:18:MET:HE1	1:A:42:ILE:HG22	1.87	0.55
1:B:146:ASN:OD1	1:B:210:ASN:HB2	2.06	0.55
1:A:227:LYS:HD2	1:A:232:HIS:CE1	2.41	0.55
1:A:149:HIS:NE2	1:A:207:LEU:HD13	2.22	0.55
1:A:197:VAL:O	1:A:197:VAL:HG23	2.06	0.55
1:A:268:ILE:HD11	1:A:316:LEU:HD12	1.88	0.55
1:B:22:LEU:CD1	1:B:39:LEU:HD12	2.36	0.55
1:B:323:GLU:O	1:B:325:GLY:N	2.40	0.55
1:A:237:LYS:N	1:A:237:LYS:HD3	2.19	0.55
1:B:229:THR:OG1	1:B:232:HIS:CE1	2.59	0.55
1:A:137:GLY:H	1:B:111:MET:CE	2.20	0.55
1:A:260:ASP:CG	1:A:261:ALA:N	2.60	0.55
1:A:48:ARG:HE	1:A:49:THR:HG23	1.72	0.55
1:B:207:LEU:CD1	1:B:208:GLU:H	2.19	0.54
1:B:18:MET:SD	1:B:43:GLU:HA	2.47	0.54
1:B:243:MET:HE2	1:B:243:MET:HA	1.89	0.54
1:B:167:PHE:CB	1:B:170:LEU:HD22	2.37	0.54
1:B:280:LEU:HD13	1:B:280:LEU:O	2.08	0.54
1:A:266:PHE:CE1	1:A:316:LEU:HD11	2.42	0.54
1:B:247:ALA:N	1:B:248:PRO:HD2	2.22	0.54
1:A:137:GLY:H	1:B:111:MET:HE1	1.72	0.54
1:A:96:THR:O	1:A:96:THR:HG22	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:VAL:CG1	1:B:287:ASP:N	2.71	0.53
1:B:253:LEU:HD13	1:B:343:LEU:HD11	1.90	0.53
1:A:265:ASP:CB	1:A:326:ALA:HB1	2.38	0.52
1:B:205:VAL:HG21	1:B:266:PHE:HZ	1.74	0.52
1:A:4:LEU:HD13	1:A:313:LEU:HD11	1.92	0.52
1:A:32:HIS:CE1	1:A:34:GLN:HB2	2.44	0.52
1:A:162:ILE:O	1:A:194:ALA:HA	2.10	0.52
1:B:97:ASP:O	1:B:159:ASN:HB2	2.09	0.52
1:A:293:PHE:CE1	1:A:316:LEU:HA	2.45	0.52
1:B:18:MET:HG3	1:B:22:LEU:HD23	1.92	0.52
1:A:48:ARG:NE	1:A:49:THR:HG23	2.23	0.52
1:A:321:GLY:O	1:A:322:VAL:CB	2.57	0.52
1:B:115:THR:O	1:B:119:ILE:HG12	2.09	0.52
1:B:338:THR:HG22	1:B:339:ALA:N	2.25	0.52
1:A:170:LEU:N	1:A:170:LEU:HD22	2.24	0.52
1:B:100:VAL:HG23	1:B:129:ARG:HB2	1.91	0.52
1:B:115:THR:OG1	1:B:130:GLN:NE2	2.43	0.51
1:A:97:ASP:O	1:A:159:ASN:HB2	2.10	0.51
1:B:57:GLU:CD	1:B:57:GLU:H	2.14	0.51
1:A:81:PRO:HB3	1:A:122:MET:HE2	1.93	0.51
1:B:144:ALA:HB1	1:B:162:ILE:HG23	1.92	0.51
1:A:3:THR:HG23	1:A:205:VAL:O	2.10	0.51
1:A:149:HIS:O	1:A:153:THR:HG22	2.11	0.51
1:A:255:GLY:O	1:A:257:HIS:N	2.44	0.51
1:A:275:ARG:HD2	1:A:275:ARG:H	1.76	0.51
1:B:207:LEU:HD12	1:B:208:GLU:N	2.24	0.51
1:B:93:LEU:HD23	1:B:93:LEU:C	2.31	0.51
1:B:93:LEU:HG	1:B:94:LEU:O	2.11	0.51
1:A:41:LEU:HB3	1:A:183:LEU:HD11	1.92	0.51
1:B:260:ASP:O	1:B:262:SER:N	2.43	0.51
1:B:239:VAL:HG23	1:B:240:PRO:HD3	1.93	0.51
1:A:207:LEU:HD12	1:A:207:LEU:C	2.32	0.50
1:B:254:ALA:HB3	1:B:260:ASP:HB2	1.93	0.50
1:A:208:GLU:OE2	1:A:257:HIS:NE2	2.44	0.50
1:A:281:SER:HB3	1:A:291:PHE:HE1	1.75	0.50
1:A:289:HIS:CE1	1:A:292:ARG:HD3	2.46	0.50
1:B:281:SER:O	1:B:286:VAL:O	2.29	0.50
1:B:251:LYS:HA	1:B:260:ASP:OD1	2.12	0.50
1:A:12:PRO:HG2	1:A:51:HIS:HB3	1.93	0.50
1:B:18:MET:CE	1:B:42:ILE:HG22	2.40	0.50
1:A:309:VAL:HG23	1:A:310:LEU:CD1	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:GLU:HG2	1:B:301:TYR:CD2	2.47	0.49
1:B:122:MET:HB3	1:B:124:PHE:CD2	2.43	0.49
1:A:280:LEU:HD12	1:A:291:PHE:CE2	2.46	0.49
1:B:207:LEU:CD1	1:B:208:GLU:N	2.75	0.49
1:B:2:ALA:HA	1:B:198:ARG:O	2.11	0.49
1:A:235:LEU:CD1	1:A:239:VAL:HG21	2.42	0.49
1:A:48:ARG:HG3	1:A:49:THR:N	2.27	0.49
1:B:266:PHE:CE2	1:B:328:GLY:HA3	2.46	0.49
1:A:94:LEU:CD1	1:A:96:THR:HB	2.42	0.49
1:A:229:THR:OG1	1:A:232:HIS:CE1	2.66	0.49
1:B:41:LEU:CB	1:B:183:LEU:HD21	2.42	0.49
1:A:56:ILE:HA	1:A:59:THR:HG23	1.95	0.49
1:B:254:ALA:CB	1:B:260:ASP:HA	2.42	0.49
1:B:300:GLU:HG2	1:B:301:TYR:CE2	2.48	0.49
1:A:169:SER:HA	2:A:1000:15P:H132	1.95	0.49
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.77	0.49
1:B:264:LEU:HD12	1:B:327:ARG:CB	2.43	0.49
1:A:18:MET:O	1:A:18:MET:HE2	2.13	0.48
1:B:2:ALA:HA	1:B:199:GLY:HA2	1.95	0.48
1:B:80:VAL:HB	1:B:81:PRO:HD3	1.96	0.48
1:A:209:ARG:NH1	1:A:257:HIS:CD2	2.82	0.48
1:A:257:HIS:CE1	1:A:259:TRP:CE2	3.01	0.48
1:B:239:VAL:N	1:B:240:PRO:HD2	2.28	0.48
1:B:146:ASN:O	1:B:149:HIS:HB3	2.14	0.48
1:A:255:GLY:HA2	1:A:260:ASP:CB	2.43	0.48
1:B:287:ASP:OD2	1:B:288:PRO:HD2	2.14	0.48
1:A:239:VAL:N	1:A:240:PRO:HD2	2.29	0.48
1:A:198:ARG:HB2	1:A:200:ARG:HD3	1.94	0.48
1:A:206:ARG:HG2	1:A:345:CYS:HB2	1.96	0.48
1:A:268:ILE:HG23	1:A:312:ALA:HB3	1.94	0.48
1:B:30:THR:HG22	4:B:4028:HOH:O	2.12	0.48
1:A:198:ARG:NE	1:A:202:GLY:CA	2.77	0.48
1:A:125:ASP:C	1:A:127:THR:H	2.17	0.48
1:B:206:ARG:HH11	1:B:206:ARG:HG3	1.79	0.47
1:A:81:PRO:HB2	4:A:2059:HOH:O	2.14	0.47
1:A:284:LEU:O	1:A:285:GLU:HB2	2.14	0.47
1:A:275:ARG:HH11	1:A:275:ARG:HG3	1.79	0.47
1:A:80:VAL:HB	1:A:81:PRO:HD3	1.97	0.47
1:B:227:LYS:HD2	1:B:232:HIS:CE1	2.49	0.47
1:B:96:THR:HG22	1:B:96:THR:O	2.14	0.47
1:A:94:LEU:HD12	1:A:96:THR:CB	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ASP:OD2	1:A:232:HIS:HD2	1.97	0.47
1:A:284:LEU:O	1:A:285:GLU:CB	2.61	0.47
1:A:235:LEU:HD12	1:A:239:VAL:HG21	1.96	0.47
1:B:49:THR:HG23	1:B:300:GLU:O	2.15	0.47
1:A:338:THR:HG22	1:A:339:ALA:N	2.28	0.47
1:A:242:THR:O	1:A:245:PRO:HD2	2.14	0.47
1:B:79:ARG:O	1:B:83:VAL:HG23	2.14	0.47
1:A:286:VAL:HG12	1:A:287:ASP:H	1.78	0.47
1:B:98:ILE:HB	1:B:124:PHE:HE1	1.80	0.47
1:A:173:GLN:HB2	3:A:2000:GOL:H11	1.97	0.47
1:B:253:LEU:O	1:B:253:LEU:HD13	2.15	0.47
1:A:319:GLU:O	1:A:320:GLY:C	2.53	0.47
1:A:214:LEU:HD22	1:A:337:ILE:O	2.14	0.47
1:B:261:ALA:O	1:B:262:SER:HB3	2.14	0.47
1:A:295:ARG:HB2	1:A:295:ARG:NH1	2.30	0.47
1:A:59:THR:HB	4:A:2016:HOH:O	2.15	0.46
1:B:12:PRO:HB2	1:B:52:ILE:O	2.15	0.46
1:A:243:MET:CE	1:A:280:LEU:HD23	2.45	0.46
1:A:209:ARG:NH1	1:A:257:HIS:HD2	2.14	0.46
1:A:329:LEU:HD23	1:A:343:LEU:HD23	1.96	0.46
1:A:106:CYS:CB	1:B:111:MET:HE1	2.45	0.46
1:A:284:LEU:C	1:A:285:GLU:HG3	2.35	0.46
1:B:18:MET:HE3	1:B:18:MET:CA	2.43	0.46
1:B:260:ASP:C	1:B:262:SER:N	2.68	0.46
1:A:284:LEU:HD23	1:A:286:VAL:HG23	1.97	0.46
1:A:129:ARG:NH1	1:A:129:ARG:HG3	2.31	0.46
1:A:254:ALA:O	1:A:260:ASP:CA	2.56	0.46
1:B:271:ALA:HB1	1:B:276:ILE:CG2	2.46	0.46
1:B:149:HIS:CD2	1:B:210:ASN:HD22	2.34	0.45
1:A:62:HIS:CE1	1:A:173:GLN:HE22	2.33	0.45
1:B:157:GLU:HG3	1:B:200:ARG:HH21	1.81	0.45
1:B:280:LEU:HD12	1:B:291:PHE:HZ	1.77	0.45
1:B:286:VAL:HG12	1:B:287:ASP:H	1.80	0.45
1:B:206:ARG:HB2	1:B:347:GLN:HE21	1.81	0.45
1:B:255:GLY:C	1:B:257:HIS:H	2.19	0.45
1:B:263:ASP:CG	1:B:263:ASP:O	2.54	0.45
1:A:281:SER:HB3	1:A:291:PHE:CE1	2.51	0.45
1:B:119:ILE:HD12	1:B:128:THR:HB	1.98	0.45
1:B:323:GLU:N	1:B:323:GLU:CD	2.68	0.45
1:B:222:ILE:O	1:B:335:PRO:HB3	2.17	0.45
1:A:209:ARG:HH11	1:A:257:HIS:HD2	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ARG:NH2	1:B:207:LEU:HD11	2.32	0.45
1:B:286:VAL:CG1	1:B:287:ASP:H	2.30	0.45
1:B:322:VAL:HG11	1:B:346:TRP:CD2	2.51	0.45
1:B:41:LEU:HD23	1:B:183:LEU:HD21	2.00	0.44
1:A:217:LYS:HA	1:A:217:LYS:HD3	1.81	0.44
1:B:149:HIS:CG	1:B:210:ASN:HD22	2.35	0.44
1:B:262:SER:OG	1:B:284:LEU:O	2.35	0.44
1:B:239:VAL:HG23	1:B:240:PRO:CD	2.48	0.44
1:B:309:VAL:HG23	1:B:310:LEU:CD1	2.45	0.44
1:B:93:LEU:CG	1:B:94:LEU:N	2.79	0.44
1:A:55:PRO:HD2	1:A:58:ASP:OD2	2.18	0.44
1:A:4:LEU:HD13	1:A:313:LEU:CD1	2.48	0.44
1:B:75:GLU:OE1	1:B:79:ARG:HD2	2.17	0.44
1:A:18:MET:HE1	1:A:22:LEU:CD1	2.47	0.44
1:A:125:ASP:OD1	1:A:125:ASP:N	2.41	0.44
1:B:313:LEU:HA	1:B:313:LEU:HD23	1.90	0.43
1:A:135:GLN:C	1:B:111:MET:HE2	2.38	0.43
1:A:258:GLY:C	1:A:260:ASP:H	2.18	0.43
1:B:255:GLY:C	1:B:257:HIS:N	2.71	0.43
1:A:4:LEU:O	1:A:204:GLY:HA3	2.18	0.43
1:A:111:MET:CE	1:B:106:CYS:HB2	2.48	0.43
1:A:94:LEU:HG	1:A:97:ASP:OD2	2.18	0.43
1:B:4:LEU:HD13	1:B:313:LEU:CD1	2.49	0.43
1:A:76:ALA:O	1:A:80:VAL:HG23	2.19	0.43
1:B:176:ASP:OD2	1:B:232:HIS:HD2	2.01	0.43
1:B:237:LYS:HE3	4:B:4076:HOH:O	2.18	0.43
1:B:243:MET:CE	1:B:280:LEU:HD23	2.49	0.43
1:A:206:ARG:NH1	1:A:206:ARG:HG2	2.34	0.43
1:B:260:ASP:CG	1:B:261:ALA:N	2.70	0.43
1:B:4:LEU:HD13	1:B:313:LEU:HD11	1.99	0.43
1:B:312:ALA:O	1:B:315:ARG:HB2	2.18	0.43
1:A:81:PRO:HB3	1:A:122:MET:CE	2.49	0.43
1:A:309:VAL:HG23	1:A:310:LEU:N	2.34	0.43
1:A:208:GLU:HB3	1:A:257:HIS:CD2	2.53	0.43
1:B:41:LEU:CD2	1:B:183:LEU:HD21	2.48	0.43
1:A:309:VAL:HG23	1:A:310:LEU:H	1.84	0.43
1:B:222:ILE:HB	1:B:335:PRO:HA	2.01	0.43
1:B:264:LEU:HA	1:B:264:LEU:HD13	1.85	0.42
1:A:198:ARG:NH2	1:A:201:GLY:O	2.50	0.42
1:A:219:GLU:HA	1:A:336:GLY:O	2.19	0.42
1:A:147:ARG:HD3	1:A:147:ARG:HA	1.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:O	1:A:93:LEU:HD22	2.18	0.42
1:B:169:SER:HA	2:B:3000:15P:H121	2.01	0.42
1:A:243:MET:HE2	1:A:280:LEU:HD23	2.01	0.42
1:A:32:HIS:HE1	1:A:34:GLN:HB2	1.81	0.42
1:B:100:VAL:HG22	1:B:101:ILE:N	2.33	0.42
1:B:172:TYR:CE2	1:B:174:PRO:HG3	2.55	0.42
1:B:16:ILE:HG13	1:B:20:GLU:HG3	2.00	0.42
1:B:246:LEU:O	1:B:249:ALA:HB3	2.20	0.42
1:A:331:ALA:HA	1:A:340:GLU:O	2.20	0.42
1:B:254:ALA:HB3	1:B:260:ASP:CB	2.50	0.42
1:A:15:VAL:HG22	1:A:51:HIS:CD2	2.55	0.42
1:B:149:HIS:NE2	1:B:207:LEU:HB2	2.34	0.41
1:B:147:ARG:HA	1:B:147:ARG:HD3	1.74	0.41
1:B:240:PRO:O	1:B:243:MET:HB2	2.20	0.41
1:B:173:GLN:CG	3:B:4000:GOL:H32	2.50	0.41
1:B:235:LEU:HD22	1:B:239:VAL:HG21	2.01	0.41
1:A:47:VAL:HG22	1:A:298:LEU:O	2.19	0.41
1:A:178:GLY:O	1:A:182:LEU:HD13	2.20	0.41
1:A:330:LEU:O	1:A:342:SER:N	2.53	0.41
1:A:242:THR:C	1:A:245:PRO:HD2	2.41	0.41
1:B:62:HIS:HD2	1:B:64:GLY:N	2.09	0.41
1:B:208:GLU:O	1:B:209:ARG:CB	2.67	0.41
1:B:268:ILE:HD12	1:B:313:LEU:HA	2.02	0.41
1:B:14:HIS:HB2	1:B:52:ILE:HG13	2.02	0.41
1:B:55:PRO:HD2	1:B:58:ASP:OD2	2.19	0.41
1:B:239:VAL:HA	1:B:242:THR:HG23	2.02	0.41
1:A:300:GLU:HG2	1:A:301:TYR:CD2	2.56	0.41
1:A:106:CYS:HB3	1:B:111:MET:HE1	2.02	0.41
1:B:268:ILE:O	1:B:268:ILE:HG22	2.21	0.41
1:A:206:ARG:HG2	1:A:206:ARG:HH11	1.85	0.40
1:A:205:VAL:HG22	1:A:266:PHE:HE2	1.85	0.40
1:A:275:ARG:NH1	1:A:275:ARG:HG3	2.36	0.40
1:B:209:ARG:HD2	1:B:257:HIS:HB2	2.04	0.40
1:A:143:ALA:CB	1:A:340:GLU:HG3	2.46	0.40
1:A:169:SER:OG	1:A:170:LEU:HD22	2.21	0.40
1:B:205:VAL:HG21	1:B:266:PHE:CZ	2.56	0.40
1:B:207:LEU:HD13	1:B:208:GLU:H	1.85	0.40
1:B:119:ILE:CD1	1:B:128:THR:HB	2.51	0.40
1:A:12:PRO:O	1:A:51:HIS:CD2	2.74	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	346/382 (91%)	311 (90%)	23 (7%)	12 (4%)	4	2
1	B	346/382 (91%)	306 (88%)	27 (8%)	13 (4%)	4	1
All	All	692/764 (91%)	617 (89%)	50 (7%)	25 (4%)	4	1

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	ASP
1	A	263	ASP
1	A	320	GLY
1	A	322	VAL
1	A	323	GLU
1	A	327	ARG
1	B	207	LEU
1	B	260	ASP
1	A	256	GLU
1	A	285	GLU
1	A	289	HIS
1	A	324	GLU
1	B	324	GLU
1	B	95	ALA
1	B	126	SER
1	B	209	ARG
1	B	263	ASP
1	B	262	SER
1	A	286	VAL
1	B	208	GLU
1	B	272	GLY
1	B	201	GLY
1	A	201	GLY
1	B	119	ILE
1	B	304	ILE

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	277/304 (91%)	245 (88%)	32 (12%)	7	5
1	B	277/304 (91%)	255 (92%)	22 (8%)	15	14
All	All	554/608 (91%)	500 (90%)	54 (10%)	10	8

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	GLU
1	A	39	LEU
1	A	45	THR
1	A	59	THR
1	A	68	ARG
1	A	70	LYS
1	A	90	ASP
1	A	94	LEU
1	A	114	LEU
1	A	121	GLU
1	A	122	MET
1	A	125	ASP
1	A	129	ARG
1	A	147	ARG
1	A	153	THR
1	A	183	LEU
1	A	198	ARG
1	A	200	ARG
1	A	206	ARG
1	A	207	LEU
1	A	224	TYR
1	A	229	THR
1	A	237	LYS
1	A	252	GLU
1	A	259	TRP
1	A	260	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	266	PHE
1	A	275	ARG
1	A	324	GLU
1	A	347	GLN
1	A	348	THR
1	B	4	LEU
1	B	18	MET
1	B	39	LEU
1	B	68	ARG
1	B	93	LEU
1	B	125	ASP
1	B	129	ARG
1	B	147	ARG
1	B	170	LEU
1	B	183	LEU
1	B	209	ARG
1	B	224	TYR
1	B	235	LEU
1	B	243	MET
1	B	252	GLU
1	B	256	GLU
1	B	264	LEU
1	B	266	PHE
1	B	275	ARG
1	B	279	ASP
1	B	295	ARG
1	B	324	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	51	HIS
1	A	62	HIS
1	A	120	ASN
1	A	159	ASN
1	A	173	GLN
1	A	232	HIS
1	A	289	HIS
1	A	347	GLN
1	B	14	HIS
1	B	51	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	62	HIS
1	B	85	GLN
1	B	120	ASN
1	B	210	ASN
1	B	232	HIS
1	B	289	HIS
1	B	347	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	15P	A	1000	-	18,18,103	0.85	0	17,17,102	0.77	0
3	GOL	A	2000	-	5,5,5	0.26	0	5,5,5	0.80	0
2	15P	B	3000	-	18,18,103	0.83	0	17,17,102	0.76	0
3	GOL	B	4000	-	5,5,5	0.43	0	5,5,5	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	15P	A	1000	-	-	0/16/16/101	0/0/0/0
3	GOL	A	2000	-	-	0/4/4/4	0/0/0/0
2	15P	B	3000	-	-	0/16/16/101	0/0/0/0
3	GOL	B	4000	-	-	0/4/4/4	0/0/0/0

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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	15P	1	0
3	A	2000	GOL	2	0
2	B	3000	15P	1	0
3	B	4000	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	348/382 (91%)	1.46	100 (28%) 1 0	26, 49, 89, 99	0
1	B	348/382 (91%)	1.44	104 (29%) 1 0	25, 51, 86, 96	0
All	All	696/764 (91%)	1.45	204 (29%) 1 0	25, 50, 88, 99	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	VAL	7.5
1	A	260	ASP	7.1
1	B	133	ILE	7.0
1	A	104	VAL	6.7
1	A	266	PHE	6.6
1	A	259	TRP	6.0
1	A	132	PRO	6.0
1	A	328	GLY	6.0
1	B	322	VAL	5.9
1	B	104	VAL	5.9
1	B	261	ALA	5.9
1	A	133	ILE	5.6
1	B	132	PRO	5.6
1	B	131	ILE	5.6
1	B	260	ASP	5.4
1	B	267	TYR	5.3
1	B	140	ALA	5.3
1	A	131	ILE	5.3
1	B	321	GLY	5.3
1	B	165	CYS	5.3
1	A	283	PHE	5.3
1	A	287	ASP	5.2
1	A	136	LEU	5.2
1	B	263	ASP	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	134	ALA	5.1
1	A	327	ARG	5.0
1	B	283	PHE	5.0
1	A	320	GLY	4.9
1	B	134	ALA	4.8
1	A	207	LEU	4.7
1	B	164	ALA	4.6
1	A	255	GLY	4.6
1	A	284	LEU	4.6
1	B	139	ALA	4.5
1	A	140	ALA	4.4
1	A	203	THR	4.3
1	B	288	PRO	4.3
1	A	139	ALA	4.3
1	A	322	VAL	4.3
1	A	138	CYS	4.3
1	B	262	SER	4.3
1	B	102	ILE	4.2
1	A	164	ALA	4.2
1	A	291	PHE	4.2
1	B	106	CYS	4.2
1	B	109	PHE	4.1
1	A	285	GLU	4.1
1	B	138	CYS	4.1
1	A	262	SER	4.1
1	B	157	GLU	4.1
1	B	285	GLU	4.1
1	B	203	THR	4.1
1	B	346	TRP	4.0
1	B	264	LEU	4.0
1	B	105	SER	4.0
1	A	103	TYR	4.0
1	A	105	SER	4.0
1	A	106	CYS	3.9
1	B	91	ALA	3.9
1	A	325	GLY	3.8
1	A	109	PHE	3.8
1	A	324	GLU	3.8
1	B	266	PHE	3.7
1	A	163	VAL	3.7
1	B	93	LEU	3.7
1	B	143	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	323	GLU	3.7
1	A	165	CYS	3.7
1	A	135	GLN	3.6
1	A	280	LEU	3.6
1	A	323	GLU	3.6
1	A	263	ASP	3.6
1	B	247	ALA	3.6
1	B	163	VAL	3.5
1	B	110	MET	3.5
1	A	252	GLU	3.5
1	B	144	ALA	3.5
1	B	284	LEU	3.5
1	B	158	ALA	3.5
1	B	141	GLY	3.4
1	B	307	ALA	3.4
1	A	102	ILE	3.4
1	A	108	GLY	3.4
1	A	110	MET	3.4
1	A	333	PHE	3.4
1	B	92	GLU	3.4
1	B	136	LEU	3.4
1	B	137	GLY	3.3
1	A	144	ALA	3.3
1	B	115	THR	3.3
1	B	348	THR	3.3
1	A	206	ARG	3.3
1	B	208	GLU	3.3
1	A	113	SER	3.3
1	B	281	SER	3.3
1	B	94	LEU	3.3
1	A	261	ALA	3.2
1	A	272	GLY	3.2
1	B	103	TYR	3.2
1	B	130	GLN	3.1
1	B	344	GLY	3.1
1	B	97	ASP	3.1
1	A	267	TYR	3.1
1	B	147	ARG	3.1
1	A	346	TRP	3.1
1	B	200	ARG	3.0
1	B	309	VAL	3.0
1	B	306	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	137	GLY	3.0
1	A	125	ASP	3.0
1	B	108	GLY	2.9
1	A	338	THR	2.9
1	B	305	ALA	2.9
1	B	291	PHE	2.9
1	A	107	THR	2.9
1	A	115	THR	2.9
1	B	274	PRO	2.9
1	A	258	GLY	2.8
1	B	3	THR	2.8
1	A	279	ASP	2.8
1	B	135	GLN	2.8
1	B	259	TRP	2.8
1	A	48	ARG	2.7
1	A	264	LEU	2.7
1	B	107	THR	2.7
1	B	113	SER	2.7
1	A	94	LEU	2.7
1	B	325	GLY	2.7
1	A	147	ARG	2.7
1	B	101	ILE	2.7
1	B	198	ARG	2.7
1	B	287	ASP	2.7
1	A	209	ARG	2.7
1	A	111	MET	2.6
1	B	145	ILE	2.6
1	A	200	ARG	2.6
1	B	146	ASN	2.6
1	A	307	ALA	2.6
1	B	111	MET	2.6
1	B	254	ALA	2.6
1	B	282	THR	2.6
1	A	156	PRO	2.6
1	B	349	ALA	2.6
1	A	201	GLY	2.5
1	B	30	THR	2.5
1	A	208	GLU	2.5
1	B	162	ILE	2.5
1	B	151	PHE	2.5
1	B	293	PHE	2.5
1	A	257	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	333	PHE	2.5
1	B	286	VAL	2.4
1	B	142	GLY	2.4
1	A	347	GLN	2.4
1	A	332	GLY	2.4
1	B	338	THR	2.4
1	A	253	LEU	2.4
1	A	141	GLY	2.4
1	A	171	CYS	2.4
1	A	3	THR	2.3
1	B	339	ALA	2.3
1	A	154	ALA	2.3
1	B	211	GLY	2.3
1	B	332	GLY	2.3
1	A	282	THR	2.3
1	B	271	ALA	2.3
1	A	274	PRO	2.2
1	B	95	ALA	2.2
1	B	345	CYS	2.2
1	B	320	GLY	2.2
1	B	335	PRO	2.2
1	A	265	ASP	2.2
1	A	306	SER	2.2
1	B	289	HIS	2.2
1	A	345	CYS	2.2
1	B	209	ARG	2.2
1	A	305	ALA	2.2
1	A	251	LYS	2.2
1	A	288	PRO	2.1
1	A	162	ILE	2.1
1	A	88	LEU	2.1
1	A	198	ARG	2.1
1	A	242	THR	2.1
1	A	339	ALA	2.1
1	B	308	VAL	2.1
1	A	231	PHE	2.1
1	A	143	ALA	2.1
1	B	326	ALA	2.1
1	A	112	PRO	2.1
1	B	72	TYR	2.1
1	A	290	ALA	2.1
1	B	199	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	278	ASP	2.1
1	B	279	ASP	2.1
1	B	153	THR	2.0
1	A	329	LEU	2.0
1	B	171	CYS	2.0
1	A	304	ILE	2.0
1	A	243	MET	2.0
1	B	88	LEU	2.0
1	A	256	GLU	2.0
1	B	224	TYR	2.0
1	A	270	HIS	2.0
1	A	145	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	15P	A	1000	19/104	0.81	0.23	0.76	43,47,57,58	0
2	15P	B	3000	19/104	0.80	0.20	0.50	38,47,53,54	0
3	GOL	A	2000	6/6	0.91	0.18	0.36	35,44,47,49	0
3	GOL	B	4000	6/6	0.94	0.16	0.20	26,38,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.