



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:12 AM UTC

PDB ID : 2CFQ / pdb_00002cfq
Title : Sugar Free Lactose Permease at neutral pH
Authors : Mirza, O.; Guan, L.; Verner, G.; Iwata, S.; Kaback, H.R.
Deposited on : 2006-02-22
Resolution : 2.95 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

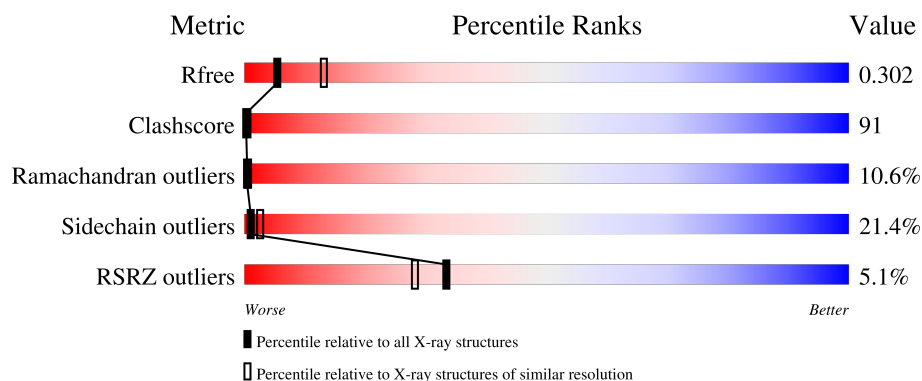
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	417	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3295 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 LACTOSE PERMEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	53	0	0
			3290	2222	506	541	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLY	CYS	engineered mutation	UNP P02920

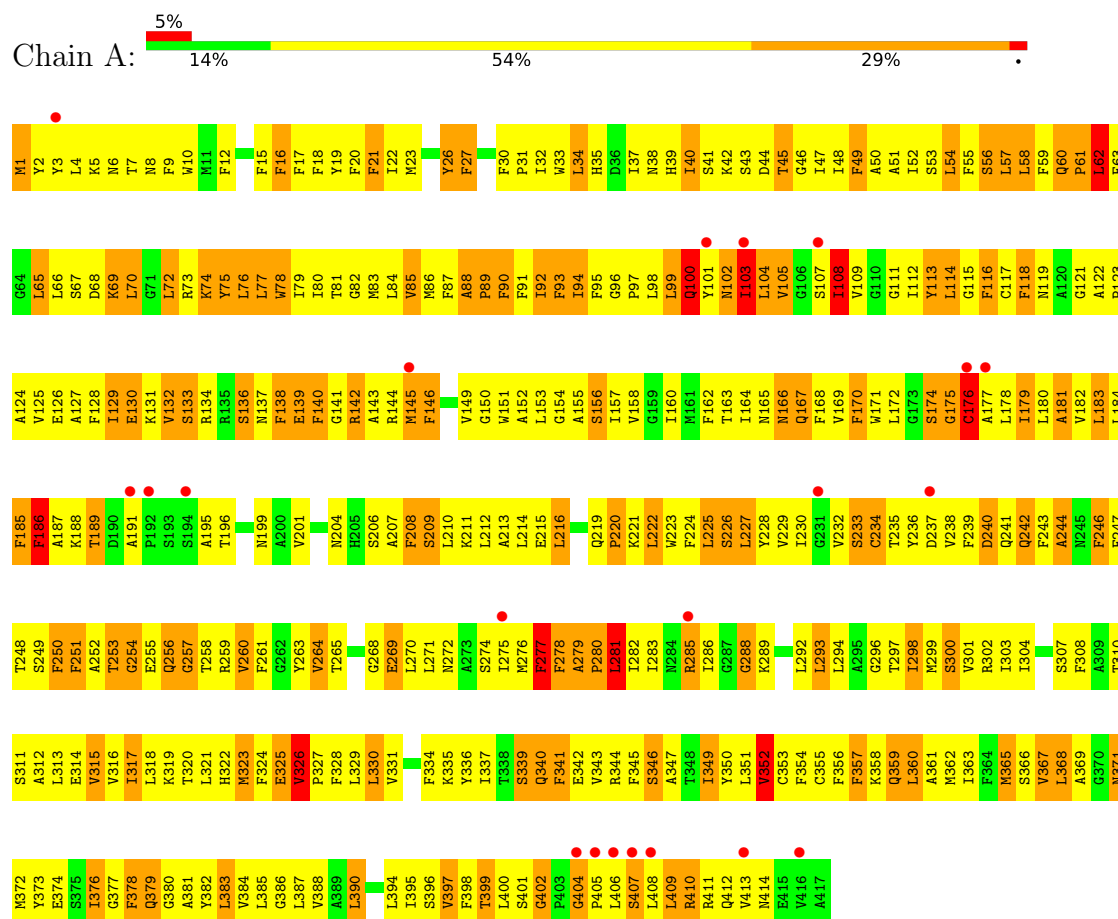
- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Hg	0	0
			5	5		

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: LACTOSE PERMEASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.47Å 122.47Å 187.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.99 – 2.95 9.99 – 2.95	Depositor EDS
% Data completeness (in resolution range)	82.6 (9.99-2.95) 81.6 (9.99-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.83Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.298 0.264 , 0.302	Depositor DCC
R_{free} test set	909 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 135.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3295	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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: HG

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	0.78	2/3387 (0.1%)	1.40	57/4588 (1.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	PHE	CA-C	5.97	1.60	1.52
1	A	185	PHE	CA-C	-5.47	1.45	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ILE	N-CA-C	-13.18	83.15	106.61
1	A	45	THR	N-CA-C	-12.43	98.12	113.28
1	A	108	ILE	N-CA-C	-10.66	101.54	111.45
1	A	105	VAL	N-CA-C	-10.51	100.65	110.53
1	A	114	LEU	N-CA-C	-10.03	100.98	113.02
1	A	317	ILE	N-CA-C	-9.98	104.23	113.71
1	A	85	VAL	N-CA-C	-9.50	99.42	113.39
1	A	254	GLY	N-CA-C	-9.46	100.69	113.37
1	A	145	MET	N-CA-C	-9.36	97.67	110.68
1	A	79	ILE	N-CA-C	-8.92	102.17	110.82
1	A	399	THR	N-CA-C	8.21	119.92	110.97
1	A	341	PHE	N-CA-C	7.74	121.51	109.52
1	A	246	PHE	N-CA-C	-7.50	103.39	112.54
1	A	367	VAL	N-CA-C	-7.41	104.56	111.45
1	A	285	ARG	N-CA-C	-7.21	104.47	113.55
1	A	2	TYR	N-CA-C	-7.14	104.56	113.20
1	A	225	LEU	N-CA-C	-7.12	103.58	112.90
1	A	113	TYR	N-CA-C	-6.85	105.86	114.56
1	A	132	VAL	N-CA-C	-6.83	105.94	111.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	PHE	N-CA-C	-6.79	104.00	112.90
1	A	404	GLY	CA-C-N	6.22	125.79	119.19
1	A	404	GLY	C-N-CA	6.22	125.79	119.19
1	A	56	SER	N-CA-C	-6.22	105.41	112.87
1	A	93	PHE	N-CA-C	6.19	120.97	113.17
1	A	365	MET	N-CA-C	6.16	118.50	111.11
1	A	253	THR	N-CA-C	-6.12	100.59	110.32
1	A	352	VAL	N-CA-C	6.12	116.29	110.42
1	A	152	ALA	N-CA-C	-6.08	103.29	112.04
1	A	260	VAL	CB-CA-C	-6.07	104.11	111.88
1	A	293	LEU	N-CA-C	-5.96	104.36	111.69
1	A	142	ARG	N-CA-C	-5.92	106.39	113.97
1	A	49	PHE	N-CA-C	-5.91	105.17	112.38
1	A	357	PHE	N-CA-C	5.84	118.53	111.40
1	A	251	PHE	N-CA-C	5.83	118.55	109.52
1	A	90	PHE	N-CA-C	5.75	117.24	110.97
1	A	139	GLU	N-CA-C	-5.73	98.55	108.52
1	A	269	GLU	N-CA-C	-5.66	104.11	111.02
1	A	100	GLN	N-CA-C	5.66	118.18	111.33
1	A	103	ILE	CA-C-N	-5.60	112.73	122.36
1	A	103	ILE	C-N-CA	-5.60	112.73	122.36
1	A	40	ILE	N-CA-C	5.59	116.78	108.46
1	A	7	THR	N-CA-C	5.51	118.13	111.40
1	A	176	CYS	CA-C-N	-5.51	113.50	122.26
1	A	176	CYS	C-N-CA	-5.51	113.50	122.26
1	A	96	GLY	CA-C-N	5.49	126.70	119.84
1	A	96	GLY	C-N-CA	5.49	126.70	119.84
1	A	146	PHE	N-CA-C	-5.37	99.36	110.80
1	A	369	ALA	N-CA-C	-5.34	105.03	112.45
1	A	226	SER	N-CA-C	-5.32	106.05	112.54
1	A	244	ALA	N-CA-C	5.30	117.81	111.71
1	A	318	LEU	N-CA-C	-5.29	105.18	111.69
1	A	257	GLY	N-CA-C	-5.24	108.45	115.32
1	A	27	PHE	N-CA-C	5.23	121.37	109.81
1	A	371	ASN	N-CA-C	-5.23	106.00	112.38
1	A	58	LEU	N-CA-C	-5.13	107.08	113.38
1	A	195	ALA	N-CA-C	-5.10	99.94	110.80
1	A	60	GLN	N-CA-C	-5.05	106.43	113.45

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	3290	0	3332	596	0
2	A	5	0	0	0	0
All	All	3295	0	3332	596	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 91.

All (596) 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:85:VAL:HA	1:A:178:LEU:HG	1.26	1.13
1:A:330:LEU:HD23	1:A:331:VAL:HG23	1.42	1.02
1:A:358:LYS:O	1:A:362:MET:HG3	1.60	1.00
1:A:100:GLN:C	1:A:102:ASN:H	1.70	0.99
1:A:330:LEU:HD13	1:A:330:LEU:H	1.22	0.99
1:A:334:PHE:HD2	1:A:335:LYS:HD2	1.25	0.98
1:A:88:ALA:HB3	1:A:89:PRO:HD3	1.46	0.97
1:A:411:ARG:HE	1:A:411:ARG:HA	1.30	0.96
1:A:101:TYR:O	1:A:103:ILE:HG12	1.66	0.96
1:A:22:ILE:HG13	1:A:177:ALA:CB	1.96	0.96
1:A:85:VAL:HG22	1:A:178:LEU:HD11	1.47	0.96
1:A:330:LEU:HD22	1:A:331:VAL:H	1.29	0.95
1:A:180:LEU:N	1:A:180:LEU:HD12	1.80	0.94
1:A:234:CYS:SG	1:A:362:MET:HG2	2.08	0.93
1:A:1:MET:H2	1:A:4:LEU:HG	1.34	0.93
1:A:98:LEU:HB3	1:A:107:SER:HB2	1.51	0.93
1:A:209:SER:H	1:A:212:LEU:HD12	1.31	0.92
1:A:90:PHE:HA	1:A:94:ILE:HD12	1.52	0.92
1:A:337:ILE:HD12	1:A:349:ILE:HG21	1.51	0.90
1:A:54:LEU:HG	1:A:54:LEU:O	1.72	0.90
1:A:297:THR:O	1:A:301:VAL:HG23	1.72	0.89
1:A:92:ILE:HD12	1:A:92:ILE:H	1.36	0.89
1:A:51:ALA:HB3	1:A:112:ILE:HD12	1.55	0.89
1:A:85:VAL:CA	1:A:178:LEU:HG	2.01	0.89
1:A:51:ALA:HB3	1:A:112:ILE:CD1	2.03	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:SER:HB3	1:A:411:ARG:HB3	1.51	0.88
1:A:22:ILE:HG13	1:A:177:ALA:HB3	1.54	0.87
1:A:296:GLY:O	1:A:300:SER:HB2	1.75	0.87
1:A:74:LYS:H	1:A:74:LYS:HE3	1.40	0.87
1:A:394:LEU:O	1:A:397:VAL:HG23	1.74	0.86
1:A:330:LEU:CD2	1:A:331:VAL:HG23	2.05	0.86
1:A:409:LEU:HA	1:A:413:VAL:HB	1.57	0.85
1:A:12:PHE:HD2	1:A:129:ILE:HG12	1.41	0.85
1:A:342:GLU:HB2	1:A:345:PHE:CD1	2.10	0.85
1:A:334:PHE:CD2	1:A:335:LYS:HD2	2.12	0.84
1:A:279:ALA:O	1:A:283:ILE:HG12	1.77	0.84
1:A:178:LEU:HD13	1:A:179:ILE:N	1.94	0.82
1:A:54:LEU:O	1:A:57:LEU:HD22	1.79	0.82
1:A:74:LYS:HD3	1:A:188:LYS:HD2	1.59	0.82
1:A:238:VAL:O	1:A:241:GLN:HG2	1.80	0.82
1:A:116:PHE:HD2	1:A:117:CYS:N	1.78	0.81
1:A:224:PHE:CD2	1:A:399:THR:HB	2.15	0.81
1:A:246:PHE:HB2	1:A:378:PHE:CD2	2.16	0.81
1:A:92:ILE:HD12	1:A:92:ILE:N	1.95	0.81
1:A:77:LEU:HD21	1:A:185:PHE:CZ	2.15	0.81
1:A:282:ILE:HG23	1:A:285:ARG:HH21	1.46	0.80
1:A:172:LEU:O	1:A:176:CYS:HB3	1.82	0.79
1:A:92:ILE:H	1:A:92:ILE:CD1	1.95	0.79
1:A:154:GLY:O	1:A:158:VAL:HG23	1.82	0.79
1:A:311:SER:OG	1:A:314:GLU:HG3	1.82	0.79
1:A:210:LEU:O	1:A:214:LEU:HG	1.82	0.79
1:A:396:SER:C	1:A:398:PHE:H	1.86	0.79
1:A:180:LEU:C	1:A:182:VAL:H	1.89	0.79
1:A:8:ASN:ND2	1:A:189:THR:OG1	2.16	0.78
1:A:178:LEU:HD13	1:A:178:LEU:C	2.08	0.78
1:A:88:ALA:HB3	1:A:89:PRO:CD	2.13	0.78
1:A:139:GLU:O	1:A:142:ARG:N	2.16	0.78
1:A:62:LEU:O	1:A:66:LEU:HD12	1.84	0.77
1:A:278:PHE:HB3	1:A:282:ILE:HD11	1.65	0.77
1:A:100:GLN:C	1:A:102:ASN:N	2.41	0.77
1:A:85:VAL:HG13	1:A:178:LEU:HD12	1.67	0.77
1:A:22:ILE:CG1	1:A:177:ALA:HB3	2.15	0.76
1:A:91:PHE:HA	1:A:95:PHE:HB3	1.67	0.76
1:A:99:LEU:HD23	1:A:107:SER:OG	1.84	0.76
1:A:330:LEU:CD2	1:A:331:VAL:H	1.98	0.76
1:A:326:VAL:HG13	1:A:330:LEU:HD11	1.66	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:O	1:A:92:ILE:HD13	1.85	0.75
1:A:108:ILE:O	1:A:112:ILE:HG13	1.87	0.75
1:A:312:ALA:O	1:A:315:VAL:HG12	1.85	0.75
1:A:46:GLY:O	1:A:50:ALA:HB2	1.87	0.75
1:A:351:LEU:C	1:A:351:LEU:HD23	2.11	0.75
1:A:264:VAL:HB	1:A:319:LYS:HD2	1.68	0.74
1:A:85:VAL:HG22	1:A:178:LEU:CD1	2.18	0.74
1:A:210:LEU:HG	1:A:214:LEU:HD11	1.68	0.74
1:A:70:LEU:CD2	1:A:73:ARG:HB2	2.18	0.74
1:A:74:LYS:CD	1:A:188:LYS:HD2	2.18	0.74
1:A:221:LYS:NZ	1:A:340:GLN:O	2.20	0.73
1:A:178:LEU:O	1:A:182:VAL:HG12	1.89	0.73
1:A:316:VAL:HG12	1:A:316:VAL:O	1.89	0.72
1:A:93:PHE:C	1:A:94:ILE:HG13	2.13	0.72
1:A:302:ARG:HH21	1:A:319:LYS:HA	1.55	0.72
1:A:408:LEU:O	1:A:413:VAL:HG23	1.90	0.72
1:A:368:LEU:O	1:A:372:MET:HB2	1.89	0.71
1:A:410:ARG:HA	1:A:410:ARG:HH11	1.55	0.71
1:A:57:LEU:HD23	1:A:57:LEU:C	2.15	0.71
1:A:411:ARG:HH21	1:A:414:ASN:HD21	1.39	0.71
1:A:77:LEU:O	1:A:81:THR:HG23	1.91	0.71
1:A:35:HIS:O	1:A:39:HIS:HA	1.90	0.70
1:A:85:VAL:HB	1:A:86:MET:HE2	1.71	0.70
1:A:62:LEU:C	1:A:62:LEU:HD23	2.16	0.70
1:A:136:SER:HB3	1:A:138:PHE:CE1	2.27	0.70
1:A:294:LEU:O	1:A:298:ILE:HG12	1.91	0.70
1:A:307:SER:C	1:A:379:GLN:HE21	1.98	0.70
1:A:368:LEU:O	1:A:368:LEU:HD12	1.91	0.70
1:A:396:SER:C	1:A:398:PHE:N	2.45	0.70
1:A:410:ARG:HA	1:A:410:ARG:NH1	2.06	0.70
1:A:241:GLN:HE21	1:A:366:SER:HB2	1.57	0.69
1:A:271:LEU:HD21	1:A:324:PHE:CE1	2.26	0.69
1:A:68:ASP:C	1:A:70:LEU:H	2.01	0.69
1:A:225:LEU:HD12	1:A:336:TYR:CE2	2.27	0.69
1:A:121:GLY:O	1:A:125:VAL:HG23	1.93	0.69
1:A:1:MET:N	1:A:4:LEU:HG	2.06	0.69
1:A:185:PHE:O	1:A:188:LYS:HD3	1.92	0.69
1:A:74:LYS:H	1:A:74:LYS:CE	2.05	0.68
1:A:293:LEU:HD13	1:A:397:VAL:HG13	1.74	0.68
1:A:409:LEU:C	1:A:410:ARG:HD2	2.18	0.68
1:A:41:SER:HB3	1:A:44:ASP:HB2	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:MET:SD	1:A:117:CYS:SG	2.91	0.68
1:A:280:PRO:O	1:A:281:LEU:C	2.36	0.68
1:A:90:PHE:HA	1:A:94:ILE:CD1	2.24	0.68
1:A:330:LEU:HD22	1:A:331:VAL:N	2.08	0.68
1:A:84:LEU:HD21	1:A:117:CYS:SG	2.34	0.67
1:A:185:PHE:O	1:A:187:ALA:N	2.28	0.67
1:A:47:ILE:HD13	1:A:367:VAL:HG22	1.76	0.67
1:A:180:LEU:HD12	1:A:180:LEU:H	1.54	0.67
1:A:54:LEU:N	1:A:363:ILE:CD1	2.57	0.67
1:A:116:PHE:C	1:A:116:PHE:CD2	2.73	0.66
1:A:172:LEU:HG	1:A:176:CYS:HB3	1.77	0.66
1:A:208:PHE:HD1	1:A:208:PHE:N	1.93	0.66
1:A:233:SER:O	1:A:236:TYR:N	2.28	0.66
1:A:170:PHE:HD1	1:A:170:PHE:H	1.44	0.66
1:A:88:ALA:C	1:A:92:ILE:HD13	2.20	0.66
1:A:238:VAL:HA	1:A:241:GLN:HG2	1.78	0.66
1:A:233:SER:O	1:A:234:CYS:C	2.38	0.66
1:A:282:ILE:HA	1:A:285:ARG:HE	1.61	0.66
1:A:298:ILE:O	1:A:299:MET:C	2.39	0.66
1:A:335:LYS:O	1:A:339:SER:OG	2.12	0.65
1:A:260:VAL:O	1:A:264:VAL:HG23	1.97	0.65
1:A:278:PHE:H	1:A:278:PHE:HD1	1.43	0.65
1:A:52:ILE:HD13	1:A:112:ILE:HG23	1.78	0.65
1:A:325:GLU:OE2	1:A:326:VAL:N	2.29	0.65
1:A:230:ILE:HD11	1:A:357:PHE:HB3	1.78	0.65
1:A:32:ILE:CG2	1:A:162:PHE:HE2	2.09	0.65
1:A:165:ASN:OD1	1:A:167:GLN:N	2.30	0.65
1:A:208:PHE:N	1:A:208:PHE:CD1	2.62	0.65
1:A:51:ALA:CB	1:A:112:ILE:HD12	2.27	0.65
1:A:90:PHE:CE2	1:A:95:PHE:HB2	2.32	0.64
1:A:282:ILE:O	1:A:286:ILE:HG22	1.98	0.64
1:A:12:PHE:CD2	1:A:129:ILE:HG12	2.30	0.64
1:A:38:ASN:HB2	1:A:40:ILE:HD11	1.79	0.64
1:A:206:SER:OG	1:A:207:ALA:N	2.28	0.64
1:A:279:ALA:C	1:A:283:ILE:HG12	2.23	0.64
1:A:38:ASN:HA	1:A:100:GLN:HE22	1.63	0.63
1:A:88:ALA:O	1:A:89:PRO:C	2.42	0.63
1:A:185:PHE:O	1:A:186:PHE:C	2.40	0.63
1:A:279:ALA:O	1:A:280:PRO:C	2.40	0.63
1:A:342:GLU:OE1	1:A:344:ARG:HD3	1.97	0.63
1:A:330:LEU:CD2	1:A:331:VAL:N	2.61	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:SER:O	1:A:178:LEU:HB3	1.99	0.63
1:A:30:PHE:HB3	1:A:31:PRO:HD3	1.79	0.63
1:A:278:PHE:O	1:A:281:LEU:HB3	1.99	0.62
1:A:85:VAL:HG13	1:A:178:LEU:CD1	2.29	0.62
1:A:180:LEU:N	1:A:180:LEU:CD1	2.55	0.62
1:A:68:ASP:C	1:A:70:LEU:N	2.56	0.62
1:A:92:ILE:HD11	1:A:170:PHE:CB	2.29	0.62
1:A:232:VAL:HG12	1:A:299:MET:SD	2.40	0.62
1:A:73:ARG:HB3	1:A:75:TYR:CD1	2.35	0.61
1:A:122:ALA:N	1:A:123:PRO:HD2	2.15	0.61
1:A:180:LEU:C	1:A:182:VAL:N	2.59	0.61
1:A:180:LEU:O	1:A:182:VAL:N	2.33	0.61
1:A:34:LEU:O	1:A:38:ASN:HB2	2.00	0.61
1:A:246:PHE:HB2	1:A:378:PHE:CE2	2.34	0.61
1:A:100:GLN:O	1:A:102:ASN:N	2.31	0.61
1:A:298:ILE:HD13	1:A:298:ILE:N	2.14	0.61
1:A:307:SER:C	1:A:308:PHE:HD1	2.08	0.61
1:A:313:LEU:O	1:A:317:ILE:HG12	1.99	0.61
1:A:407:SER:HB3	1:A:411:ARG:CB	2.30	0.61
1:A:170:PHE:O	1:A:174:SER:HB2	2.01	0.61
1:A:89:PRO:O	1:A:93:PHE:HB2	2.00	0.60
1:A:210:LEU:HG	1:A:214:LEU:CD1	2.31	0.60
1:A:238:VAL:O	1:A:241:GLN:CG	2.49	0.60
1:A:65:LEU:O	1:A:69:LYS:HB3	2.00	0.60
1:A:182:VAL:HG13	1:A:183:LEU:N	2.17	0.60
1:A:225:LEU:O	1:A:229:VAL:HG23	2.01	0.60
1:A:282:ILE:HA	1:A:285:ARG:NE	2.16	0.60
1:A:356:PHE:O	1:A:360:LEU:HB2	2.01	0.60
1:A:323:MET:O	1:A:327:PRO:HD2	2.01	0.60
1:A:376:ILE:HD12	1:A:380:GLY:HA3	1.83	0.60
1:A:337:ILE:HD12	1:A:349:ILE:CG2	2.28	0.59
1:A:178:LEU:CD1	1:A:179:ILE:N	2.65	0.59
1:A:280:PRO:HG2	1:A:281:LEU:H	1.67	0.59
1:A:146:PHE:O	1:A:149:VAL:HG12	2.01	0.59
1:A:278:PHE:CB	1:A:282:ILE:HD11	2.31	0.59
1:A:108:ILE:HB	1:A:112:ILE:HD11	1.84	0.59
1:A:236:TYR:CG	1:A:299:MET:HG2	2.37	0.59
1:A:59:PHE:CD2	1:A:116:PHE:HB2	2.38	0.59
1:A:112:ILE:HG22	1:A:112:ILE:O	2.02	0.59
1:A:179:ILE:C	1:A:182:VAL:HG12	2.27	0.59
1:A:38:ASN:CA	1:A:100:GLN:HE22	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:O	1:A:108:ILE:HG13	2.02	0.59
1:A:307:SER:C	1:A:379:GLN:NE2	2.60	0.59
1:A:359:GLN:O	1:A:363:ILE:HG12	2.02	0.59
1:A:269:GLU:C	1:A:271:LEU:H	2.11	0.59
1:A:88:ALA:HA	1:A:92:ILE:HD13	1.84	0.59
1:A:23:MET:HE1	1:A:122:ALA:CB	2.32	0.58
1:A:238:VAL:C	1:A:241:GLN:HG2	2.28	0.58
1:A:211:LYS:O	1:A:215:GLU:N	2.36	0.58
1:A:82:GLY:HA2	1:A:85:VAL:HG23	1.85	0.58
1:A:89:PRO:O	1:A:94:ILE:HD12	2.03	0.58
1:A:241:GLN:NE2	1:A:366:SER:HB2	2.16	0.58
1:A:233:SER:O	1:A:235:THR:N	2.36	0.58
1:A:258:THR:O	1:A:261:PHE:N	2.35	0.58
1:A:41:SER:HB3	1:A:44:ASP:CB	2.33	0.58
1:A:83:MET:C	1:A:84:LEU:HD23	2.28	0.58
1:A:178:LEU:HD13	1:A:179:ILE:CA	2.33	0.58
1:A:54:LEU:HA	1:A:363:ILE:HD11	1.86	0.58
1:A:236:TYR:O	1:A:239:PHE:HB3	2.04	0.58
1:A:45:THR:HA	1:A:48:ILE:HD12	1.86	0.57
1:A:93:PHE:O	1:A:94:ILE:HG13	2.04	0.57
1:A:48:ILE:HG12	1:A:108:ILE:CG2	2.34	0.57
1:A:160:ILE:HD11	1:A:263:TYR:CZ	2.39	0.57
1:A:15:PHE:HA	1:A:184:LEU:HD12	1.85	0.57
1:A:21:PHE:CE1	1:A:154:GLY:HA2	2.40	0.57
1:A:41:SER:HB3	1:A:44:ASP:CG	2.30	0.57
1:A:88:ALA:CB	1:A:89:PRO:HD3	2.28	0.57
1:A:139:GLU:O	1:A:140:PHE:C	2.45	0.57
1:A:326:VAL:HG12	1:A:327:PRO:N	2.19	0.57
1:A:271:LEU:HD23	1:A:323:MET:CB	2.34	0.57
1:A:383:LEU:HD23	1:A:387:LEU:HD11	1.86	0.57
1:A:186:PHE:C	1:A:186:PHE:CD1	2.81	0.57
1:A:280:PRO:O	1:A:283:ILE:N	2.38	0.57
1:A:186:PHE:HD1	1:A:187:ALA:N	2.03	0.57
1:A:33:TRP:HA	1:A:37:ILE:HD13	1.86	0.56
1:A:55:PHE:C	1:A:57:LEU:H	2.11	0.56
1:A:260:VAL:HA	1:A:263:TYR:CD1	2.40	0.56
1:A:26:TYR:CE1	1:A:27:PHE:HD1	2.22	0.56
1:A:32:ILE:HG22	1:A:162:PHE:HE2	1.68	0.56
1:A:54:LEU:N	1:A:363:ILE:HD12	2.20	0.56
1:A:85:VAL:HA	1:A:178:LEU:CG	2.18	0.56
1:A:186:PHE:CD1	1:A:187:ALA:N	2.73	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG22	1:A:255:GLU:H	1.70	0.56
1:A:271:LEU:HD21	1:A:324:PHE:HE1	1.69	0.56
1:A:282:ILE:HA	1:A:285:ARG:HH21	1.70	0.56
1:A:325:GLU:O	1:A:326:VAL:C	2.47	0.56
1:A:65:LEU:HD23	1:A:65:LEU:N	2.20	0.56
1:A:74:LYS:HE3	1:A:74:LYS:N	2.15	0.56
1:A:88:ALA:CB	1:A:89:PRO:CD	2.83	0.56
1:A:126:GLU:OE2	1:A:144:ARG:NE	2.36	0.56
1:A:12:PHE:CE2	1:A:128:PHE:HE1	2.24	0.56
1:A:376:ILE:HG23	1:A:376:ILE:O	2.06	0.56
1:A:26:TYR:CD1	1:A:26:TYR:C	2.83	0.56
1:A:48:ILE:HG12	1:A:108:ILE:HG21	1.87	0.56
1:A:282:ILE:HA	1:A:285:ARG:NH2	2.21	0.56
1:A:172:LEU:HG	1:A:176:CYS:CB	2.35	0.56
1:A:238:VAL:CA	1:A:241:GLN:HG2	2.35	0.56
1:A:136:SER:O	1:A:137:ASN:CG	2.49	0.56
1:A:228:TYR:CD1	1:A:228:TYR:C	2.84	0.55
1:A:409:LEU:HA	1:A:413:VAL:CB	2.32	0.55
1:A:127:ALA:O	1:A:128:PHE:C	2.50	0.55
1:A:51:ALA:HB3	1:A:112:ILE:HD13	1.86	0.55
1:A:339:SER:O	1:A:340:GLN:NE2	2.39	0.55
1:A:216:LEU:O	1:A:219:GLN:N	2.40	0.55
1:A:170:PHE:N	1:A:170:PHE:CD1	2.74	0.55
1:A:178:LEU:C	1:A:178:LEU:CD1	2.78	0.55
1:A:327:PRO:O	1:A:330:LEU:HD22	2.06	0.55
1:A:12:PHE:HE2	1:A:128:PHE:CE1	2.24	0.55
1:A:60:GLN:N	1:A:61:PRO:CD	2.70	0.55
1:A:258:THR:O	1:A:259:ARG:C	2.49	0.55
1:A:225:LEU:HD21	1:A:354:PHE:HE1	1.71	0.55
1:A:15:PHE:HE2	1:A:125:VAL:HG13	1.72	0.55
1:A:26:TYR:HB2	1:A:87:PHE:CZ	2.41	0.55
1:A:34:LEU:HA	1:A:38:ASN:HD22	1.72	0.55
1:A:324:PHE:N	1:A:324:PHE:CD1	2.75	0.55
1:A:77:LEU:HD21	1:A:185:PHE:HZ	1.71	0.54
1:A:410:ARG:HA	1:A:414:ASN:HB3	1.88	0.54
1:A:70:LEU:HD21	1:A:73:ARG:HB2	1.89	0.54
1:A:183:LEU:C	1:A:183:LEU:HD23	2.32	0.54
1:A:98:LEU:HB3	1:A:107:SER:CB	2.32	0.54
1:A:209:SER:N	1:A:212:LEU:HD12	2.13	0.54
1:A:279:ALA:HA	1:A:282:ILE:HD12	1.88	0.54
1:A:282:ILE:CG2	1:A:285:ARG:HH21	2.19	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HB	1:A:112:ILE:CD1	2.38	0.54
1:A:47:ILE:CD1	1:A:367:VAL:HG22	2.37	0.54
1:A:91:PHE:CD1	1:A:91:PHE:N	2.76	0.54
1:A:381:ALA:O	1:A:385:LEU:HG	2.07	0.54
1:A:55:PHE:C	1:A:57:LEU:N	2.64	0.54
1:A:175:GLY:O	1:A:176:CYS:C	2.50	0.54
1:A:153:LEU:N	1:A:153:LEU:HD12	2.23	0.53
1:A:35:HIS:HA	1:A:40:ILE:H	1.74	0.53
1:A:278:PHE:N	1:A:278:PHE:CD1	2.76	0.53
1:A:279:ALA:HB3	1:A:280:PRO:CD	2.38	0.53
1:A:57:LEU:CD2	1:A:58:LEU:HG	2.38	0.53
1:A:153:LEU:O	1:A:157:ILE:HD13	2.08	0.53
1:A:157:ILE:HG22	1:A:158:VAL:N	2.23	0.53
1:A:247:PHE:CE1	1:A:315:VAL:HG13	2.43	0.53
1:A:253:THR:H	1:A:256:GLN:HG2	1.74	0.53
1:A:22:ILE:HG13	1:A:177:ALA:HB1	1.87	0.53
1:A:351:LEU:C	1:A:351:LEU:CD2	2.81	0.53
1:A:272:ASN:OD1	1:A:327:PRO:HG3	2.09	0.53
1:A:282:ILE:HG23	1:A:285:ARG:NH2	2.20	0.53
1:A:66:LEU:O	1:A:70:LEU:HB2	2.07	0.53
1:A:300:SER:OG	1:A:390:LEU:HB2	2.09	0.53
1:A:178:LEU:HD13	1:A:179:ILE:HA	1.90	0.53
1:A:289:LYS:HD2	1:A:402:GLY:HA2	1.91	0.53
1:A:326:VAL:HG12	1:A:327:PRO:CD	2.38	0.53
1:A:410:ARG:HD2	1:A:410:ARG:N	2.24	0.53
1:A:116:PHE:HD2	1:A:116:PHE:C	2.16	0.53
1:A:116:PHE:CD2	1:A:117:CYS:N	2.66	0.53
1:A:282:ILE:HG12	1:A:285:ARG:NH2	2.25	0.53
1:A:289:LYS:HE2	1:A:400:LEU:O	2.09	0.52
1:A:57:LEU:HD23	1:A:58:LEU:HG	1.91	0.52
1:A:324:PHE:N	1:A:324:PHE:HD1	2.05	0.52
1:A:46:GLY:O	1:A:50:ALA:CB	2.57	0.52
1:A:74:LYS:O	1:A:75:TYR:C	2.51	0.52
1:A:271:LEU:HD23	1:A:323:MET:HB2	1.92	0.52
1:A:26:TYR:HE1	1:A:27:PHE:HD1	1.57	0.52
1:A:127:ALA:O	1:A:130:GLU:N	2.41	0.52
1:A:54:LEU:CA	1:A:363:ILE:CD1	2.88	0.52
1:A:88:ALA:CA	1:A:92:ILE:HD13	2.39	0.52
1:A:177:ALA:O	1:A:181:ALA:HB3	2.10	0.52
1:A:326:VAL:HG12	1:A:327:PRO:HD3	1.92	0.52
1:A:16:PHE:CE1	1:A:129:ILE:HG21	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:CA	1:A:94:ILE:HD12	2.33	0.52
1:A:279:ALA:O	1:A:280:PRO:O	2.27	0.52
1:A:323:MET:O	1:A:327:PRO:CD	2.57	0.52
1:A:54:LEU:N	1:A:363:ILE:HD11	2.25	0.52
1:A:238:VAL:HA	1:A:241:GLN:CG	2.39	0.52
1:A:85:VAL:HG22	1:A:178:LEU:CG	2.40	0.52
1:A:122:ALA:N	1:A:123:PRO:CD	2.73	0.52
1:A:123:PRO:HG2	1:A:124:ALA:H	1.74	0.52
1:A:153:LEU:N	1:A:153:LEU:CD1	2.73	0.52
1:A:77:LEU:HD21	1:A:185:PHE:CE2	2.45	0.51
1:A:38:ASN:CB	1:A:40:ILE:HD11	2.39	0.51
1:A:80:ILE:O	1:A:84:LEU:HG	2.10	0.51
1:A:56:SER:CB	1:A:119:ASN:HB3	2.40	0.51
1:A:97:PRO:O	1:A:98:LEU:C	2.51	0.51
1:A:66:LEU:HB3	1:A:76:LEU:HD13	1.92	0.51
1:A:225:LEU:HD12	1:A:336:TYR:HE2	1.75	0.51
1:A:326:VAL:O	1:A:327:PRO:C	2.51	0.51
1:A:57:LEU:HD23	1:A:58:LEU:N	2.25	0.51
1:A:160:ILE:HD11	1:A:263:TYR:OH	2.10	0.51
1:A:26:TYR:HB2	1:A:87:PHE:HZ	1.76	0.51
1:A:283:ILE:HA	1:A:286:ILE:CG2	2.41	0.51
1:A:411:ARG:NH2	1:A:414:ASN:HD21	2.08	0.51
1:A:133:SER:HA	1:A:138:PHE:CD2	2.46	0.51
1:A:160:ILE:HD11	1:A:263:TYR:CE2	2.45	0.51
1:A:324:PHE:HD1	1:A:324:PHE:H	1.59	0.51
1:A:330:LEU:HD13	1:A:330:LEU:N	2.06	0.51
1:A:70:LEU:O	1:A:70:LEU:HD23	2.11	0.50
1:A:77:LEU:O	1:A:77:LEU:HG	2.11	0.50
1:A:246:PHE:HD2	1:A:378:PHE:HD2	1.58	0.50
1:A:85:VAL:CG2	1:A:178:LEU:HD11	2.32	0.50
1:A:210:LEU:O	1:A:213:ALA:HB3	2.11	0.50
1:A:293:LEU:HD13	1:A:397:VAL:CG1	2.41	0.50
1:A:394:LEU:O	1:A:397:VAL:CG2	2.54	0.50
1:A:9:PHE:CZ	1:A:142:ARG:HG2	2.47	0.50
1:A:59:PHE:O	1:A:60:GLN:C	2.55	0.50
1:A:77:LEU:HA	1:A:80:ILE:HD12	1.93	0.50
1:A:316:VAL:O	1:A:317:ILE:HD13	2.12	0.50
1:A:378:PHE:O	1:A:380:GLY:N	2.45	0.49
1:A:112:ILE:O	1:A:113:TYR:CD2	2.66	0.49
1:A:185:PHE:C	1:A:187:ALA:N	2.71	0.49
1:A:278:PHE:HD1	1:A:278:PHE:N	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:O	1:A:409:LEU:HD23	2.12	0.49
1:A:410:ARG:HH11	1:A:410:ARG:CA	2.22	0.49
1:A:23:MET:HE1	1:A:122:ALA:HB1	1.93	0.49
1:A:32:ILE:N	1:A:32:ILE:HD12	2.27	0.49
1:A:91:PHE:HD1	1:A:91:PHE:H	1.60	0.49
1:A:304:ILE:HD11	1:A:386:GLY:C	2.38	0.49
1:A:88:ALA:O	1:A:90:PHE:N	2.45	0.49
1:A:242:GLN:HE21	1:A:373:TYR:HD2	1.58	0.49
1:A:372:MET:HE1	1:A:384:VAL:HG11	1.94	0.49
1:A:22:ILE:CG1	1:A:177:ALA:CB	2.77	0.49
1:A:108:ILE:HD12	1:A:109:VAL:N	2.28	0.49
1:A:224:PHE:CD2	1:A:399:THR:CB	2.92	0.49
1:A:23:MET:HE1	1:A:122:ALA:HB2	1.95	0.49
1:A:92:ILE:HG22	1:A:93:PHE:CD1	2.47	0.49
1:A:253:THR:HB	1:A:256:GLN:HB3	1.94	0.49
1:A:373:TYR:O	1:A:377:GLY:HA2	2.13	0.49
1:A:69:LYS:O	1:A:69:LYS:CG	2.60	0.49
1:A:93:PHE:N	1:A:93:PHE:HD1	2.11	0.49
1:A:409:LEU:CA	1:A:413:VAL:HB	2.37	0.49
1:A:86:MET:O	1:A:87:PHE:C	2.55	0.49
1:A:373:TYR:CE1	1:A:382:TYR:HE1	2.30	0.49
1:A:48:ILE:C	1:A:50:ALA:N	2.70	0.49
1:A:303:ILE:HG21	1:A:386:GLY:N	2.28	0.49
1:A:89:PRO:C	1:A:94:ILE:HD12	2.38	0.48
1:A:236:TYR:CD1	1:A:299:MET:HG2	2.48	0.48
1:A:75:TYR:O	1:A:78:TRP:HB2	2.13	0.48
1:A:66:LEU:O	1:A:68:ASP:N	2.47	0.48
1:A:141:GLY:O	1:A:145:MET:HG3	2.12	0.48
1:A:56:SER:HB2	1:A:119:ASN:HB3	1.95	0.48
1:A:62:LEU:HD23	1:A:63:PHE:N	2.28	0.48
1:A:10:TRP:HA	1:A:10:TRP:CE3	2.48	0.48
1:A:183:LEU:C	1:A:185:PHE:H	2.22	0.48
1:A:60:GLN:HB2	1:A:61:PRO:HD3	1.96	0.48
1:A:66:LEU:CB	1:A:76:LEU:HD13	2.44	0.48
1:A:334:PHE:CD2	1:A:334:PHE:C	2.91	0.48
1:A:352:VAL:HG12	1:A:353:CYS:N	2.27	0.48
1:A:143:ALA:O	1:A:146:PHE:CB	2.61	0.48
1:A:220:PRO:O	1:A:223:TRP:N	2.47	0.48
1:A:240:ASP:OD1	1:A:302:ARG:NH1	2.47	0.48
1:A:61:PRO:O	1:A:63:PHE:N	2.47	0.48
1:A:43:SER:HB2	1:A:371:ASN:HD22	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:CA	1:A:363:ILE:HD11	2.44	0.48
1:A:297:THR:C	1:A:298:ILE:HD13	2.38	0.48
1:A:143:ALA:O	1:A:146:PHE:HB3	2.14	0.47
1:A:246:PHE:HE2	1:A:379:GLN:HG2	1.79	0.47
1:A:32:ILE:CD1	1:A:32:ILE:H	2.27	0.47
1:A:47:ILE:O	1:A:47:ILE:CG2	2.62	0.47
1:A:66:LEU:O	1:A:70:LEU:CB	2.62	0.47
1:A:91:PHE:CD2	1:A:170:PHE:HE2	2.32	0.47
1:A:166:ASN:ND2	1:A:167:GLN:N	2.61	0.47
1:A:175:GLY:O	1:A:178:LEU:N	2.47	0.47
1:A:233:SER:OG	1:A:358:LYS:HE3	2.15	0.47
1:A:242:GLN:O	1:A:244:ALA:N	2.48	0.47
1:A:404:GLY:N	1:A:405:PRO:HD3	2.28	0.47
1:A:179:ILE:HA	1:A:182:VAL:CG1	2.43	0.47
1:A:260:VAL:O	1:A:263:TYR:HB2	2.14	0.47
1:A:73:ARG:HD2	1:A:73:ARG:N	2.29	0.47
1:A:108:ILE:O	1:A:109:VAL:C	2.57	0.47
1:A:132:VAL:HG12	1:A:138:PHE:CZ	2.50	0.47
1:A:269:GLU:O	1:A:271:LEU:N	2.48	0.47
1:A:361:ALA:O	1:A:365:MET:HG3	2.14	0.47
1:A:10:TRP:HA	1:A:10:TRP:HE3	1.79	0.47
1:A:19:TYR:HD2	1:A:20:PHE:CD1	2.32	0.47
1:A:93:PHE:CD1	1:A:93:PHE:N	2.80	0.47
1:A:98:LEU:O	1:A:99:LEU:C	2.54	0.47
1:A:282:ILE:HA	1:A:285:ARG:CZ	2.44	0.47
1:A:77:LEU:C	1:A:77:LEU:HD23	2.39	0.47
1:A:53:SER:C	1:A:363:ILE:HD11	2.40	0.47
1:A:130:GLU:OE2	1:A:131:LYS:HG2	2.15	0.47
1:A:349:ILE:HG22	1:A:350:TYR:N	2.29	0.47
1:A:73:ARG:HB3	1:A:75:TYR:HD1	1.78	0.47
1:A:408:LEU:O	1:A:412:GLN:HB3	2.15	0.47
1:A:69:LYS:O	1:A:69:LYS:HG3	2.15	0.46
1:A:113:TYR:C	1:A:115:GLY:H	2.22	0.46
1:A:220:PRO:C	1:A:222:LEU:N	2.73	0.46
1:A:272:ASN:O	1:A:276:MET:HB2	2.14	0.46
1:A:260:VAL:HA	1:A:263:TYR:HD1	1.79	0.46
1:A:345:PHE:O	1:A:346:SER:C	2.57	0.46
1:A:66:LEU:HD13	1:A:76:LEU:CD1	2.45	0.46
1:A:169:VAL:C	1:A:171:TRP:N	2.70	0.46
1:A:321:LEU:C	1:A:323:MET:N	2.71	0.46
1:A:368:LEU:HA	1:A:371:ASN:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:HD13	1:A:395:ILE:HA	1.82	0.46
1:A:47:ILE:O	1:A:47:ILE:HG22	2.15	0.46
1:A:105:VAL:C	1:A:107:SER:H	2.24	0.46
1:A:303:ILE:HG22	1:A:382:TYR:O	2.16	0.46
1:A:340:GLN:HB3	1:A:341:PHE:CE1	2.51	0.46
1:A:49:PHE:HB3	1:A:241:GLN:NE2	2.31	0.46
1:A:166:ASN:ND2	1:A:166:ASN:C	2.74	0.46
1:A:91:PHE:N	1:A:91:PHE:HD1	2.13	0.46
1:A:250:PHE:CD2	1:A:311:SER:O	2.69	0.46
1:A:342:GLU:CD	1:A:344:ARG:HH11	2.24	0.46
1:A:12:PHE:CE2	1:A:128:PHE:CE1	3.02	0.45
1:A:127:ALA:O	1:A:130:GLU:OE1	2.33	0.45
1:A:378:PHE:O	1:A:381:ALA:N	2.49	0.45
1:A:139:GLU:O	1:A:141:GLY:N	2.49	0.45
1:A:227:LEU:HA	1:A:227:LEU:HD22	1.47	0.45
1:A:274:SER:O	1:A:277:PHE:HB2	2.15	0.45
1:A:340:GLN:C	1:A:341:PHE:CD1	2.95	0.45
1:A:16:PHE:CE1	1:A:144:ARG:HG2	2.52	0.45
1:A:17:PHE:O	1:A:17:PHE:CG	2.70	0.45
1:A:41:SER:C	1:A:43:SER:H	2.24	0.45
1:A:17:PHE:CE1	1:A:150:GLY:HA2	2.51	0.45
1:A:38:ASN:O	1:A:100:GLN:NE2	2.50	0.45
1:A:54:LEU:CA	1:A:363:ILE:HD12	2.46	0.45
1:A:240:ASP:O	1:A:241:GLN:C	2.58	0.45
1:A:1:MET:C	1:A:3:TYR:H	2.24	0.45
1:A:32:ILE:HG21	1:A:162:PHE:HE2	1.78	0.45
1:A:365:MET:HB3	1:A:365:MET:HE3	1.57	0.45
1:A:342:GLU:O	1:A:345:PHE:HB2	2.16	0.45
1:A:47:ILE:HD13	1:A:367:VAL:CG2	2.44	0.45
1:A:182:VAL:CG1	1:A:183:LEU:N	2.79	0.45
1:A:283:ILE:HA	1:A:286:ILE:HG22	1.99	0.45
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.87	0.45
1:A:383:LEU:HD23	1:A:387:LEU:CD1	2.46	0.45
1:A:3:TYR:HA	1:A:6:ASN:HB3	1.97	0.45
1:A:157:ILE:N	1:A:157:ILE:HD12	2.32	0.45
1:A:62:LEU:C	1:A:62:LEU:CD2	2.83	0.45
1:A:74:LYS:HG2	1:A:185:PHE:CE2	2.51	0.45
1:A:175:GLY:C	1:A:177:ALA:N	2.74	0.45
1:A:355:CYS:O	1:A:359:GLN:HB2	2.16	0.45
1:A:9:PHE:CE1	1:A:143:ALA:HB2	2.51	0.45
1:A:75:TYR:O	1:A:78:TRP:N	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:HB2	1:A:170:PHE:O	2.17	0.44
1:A:283:ILE:CA	1:A:286:ILE:HG22	2.47	0.44
1:A:54:LEU:HA	1:A:363:ILE:CD1	2.47	0.44
1:A:288:GLY:O	1:A:289:LYS:C	2.60	0.44
1:A:289:LYS:CE	1:A:402:GLY:HA2	2.47	0.44
1:A:42:LYS:HB3	1:A:374:GLU:OE1	2.17	0.44
1:A:330:LEU:H	1:A:330:LEU:CD1	2.02	0.44
1:A:3:TYR:HA	1:A:6:ASN:CB	2.46	0.44
1:A:61:PRO:C	1:A:63:PHE:N	2.75	0.44
1:A:401:SER:O	1:A:402:GLY:O	2.36	0.44
1:A:56:SER:O	1:A:60:GLN:HG3	2.18	0.44
1:A:100:GLN:HE21	1:A:100:GLN:HB2	1.51	0.44
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.84	0.44
1:A:113:TYR:O	1:A:116:PHE:HB3	2.18	0.44
1:A:269:GLU:C	1:A:271:LEU:N	2.72	0.44
1:A:38:ASN:HB2	1:A:40:ILE:CD1	2.47	0.44
1:A:256:GLN:HE21	1:A:256:GLN:HB2	1.47	0.44
1:A:130:GLU:CD	1:A:131:LYS:N	2.76	0.43
1:A:178:LEU:C	1:A:180:LEU:N	2.76	0.43
1:A:167:GLN:O	1:A:169:VAL:N	2.41	0.43
1:A:282:ILE:H	1:A:282:ILE:HG13	1.42	0.43
1:A:30:PHE:N	1:A:31:PRO:CD	2.81	0.43
1:A:83:MET:O	1:A:84:LEU:HD23	2.18	0.43
1:A:360:LEU:C	1:A:362:MET:N	2.76	0.43
1:A:73:ARG:N	1:A:73:ARG:CD	2.81	0.43
1:A:172:LEU:O	1:A:176:CYS:N	2.51	0.43
1:A:183:LEU:HD23	1:A:184:LEU:HD23	2.01	0.43
1:A:316:VAL:O	1:A:316:VAL:CG1	2.60	0.43
1:A:6:ASN:ND2	1:A:137:ASN:OD1	2.51	0.43
1:A:321:LEU:C	1:A:323:MET:H	2.27	0.43
1:A:149:VAL:O	1:A:153:LEU:HD13	2.19	0.43
1:A:15:PHE:CA	1:A:184:LEU:HD12	2.48	0.43
1:A:178:LEU:O	1:A:180:LEU:N	2.52	0.43
1:A:48:ILE:C	1:A:50:ALA:H	2.26	0.42
1:A:75:TYR:O	1:A:76:LEU:C	2.62	0.42
1:A:41:SER:C	1:A:43:SER:N	2.76	0.42
1:A:413:VAL:HG12	1:A:413:VAL:O	2.19	0.42
1:A:155:ALA:O	1:A:156:SER:C	2.62	0.42
1:A:248:THR:HG22	1:A:257:GLY:O	2.19	0.42
1:A:360:LEU:C	1:A:362:MET:H	2.25	0.42
1:A:411:ARG:HE	1:A:411:ARG:CA	2.12	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LYS:HE3	1:A:42:LYS:HB2	1.88	0.42
1:A:254:GLY:C	1:A:256:GLN:H	2.27	0.42
1:A:264:VAL:HG11	1:A:319:LYS:HB3	2.01	0.42
1:A:294:LEU:HD12	1:A:294:LEU:HA	1.81	0.42
1:A:346:SER:OG	1:A:347:ALA:N	2.52	0.42
1:A:5:LYS:O	1:A:5:LYS:HD3	2.20	0.42
1:A:49:PHE:HB3	1:A:241:GLN:HE22	1.84	0.42
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.82	0.42
1:A:249:SER:C	1:A:251:PHE:H	2.27	0.42
1:A:302:ARG:CZ	1:A:322:HIS:HB2	2.50	0.42
1:A:101:TYR:O	1:A:103:ILE:CG1	2.52	0.42
1:A:108:ILE:O	1:A:112:ILE:N	2.52	0.42
1:A:209:SER:OG	1:A:210:LEU:N	2.50	0.42
1:A:313:LEU:HD12	1:A:313:LEU:HA	1.74	0.42
1:A:32:ILE:N	1:A:32:ILE:CD1	2.83	0.42
1:A:82:GLY:HA2	1:A:85:VAL:CG2	2.49	0.42
1:A:271:LEU:O	1:A:275:ILE:HG12	2.19	0.42
1:A:281:LEU:O	1:A:285:ARG:HG3	2.19	0.42
1:A:91:PHE:HB2	1:A:92:ILE:HD12	2.01	0.41
1:A:224:PHE:CG	1:A:399:THR:HB	2.53	0.41
1:A:299:MET:HE3	1:A:325:GLU:OE1	2.20	0.41
1:A:340:GLN:HB3	1:A:341:PHE:CD1	2.55	0.41
1:A:410:ARG:CA	1:A:414:ASN:HB3	2.49	0.41
1:A:77:LEU:O	1:A:77:LEU:CG	2.68	0.41
1:A:219:GLN:O	1:A:222:LEU:HB3	2.20	0.41
1:A:32:ILE:HG22	1:A:162:PHE:CE2	2.51	0.41
1:A:157:ILE:H	1:A:157:ILE:CD1	2.33	0.41
1:A:307:SER:O	1:A:379:GLN:NE2	2.53	0.41
1:A:390:LEU:O	1:A:390:LEU:HG	2.19	0.41
1:A:88:ALA:HA	1:A:170:PHE:HB3	2.02	0.41
1:A:47:ILE:HD13	1:A:47:ILE:HA	1.76	0.41
1:A:88:ALA:HA	1:A:92:ILE:CD1	2.48	0.41
1:A:163:THR:OG1	1:A:164:ILE:N	2.52	0.41
1:A:180:LEU:H	1:A:180:LEU:CD1	2.25	0.41
1:A:90:PHE:HD2	1:A:91:PHE:CE1	2.39	0.41
1:A:179:ILE:C	1:A:182:VAL:CG1	2.94	0.41
1:A:185:PHE:O	1:A:188:LYS:CD	2.67	0.41
1:A:303:ILE:HG21	1:A:386:GLY:CA	2.50	0.41
1:A:117:CYS:O	1:A:118:PHE:CG	2.74	0.41
1:A:241:GLN:HB2	1:A:242:GLN:H	1.59	0.41
1:A:90:PHE:HD2	1:A:91:PHE:CD1	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:N	1:A:224:PHE:CD1	2.88	0.41
1:A:233:SER:C	1:A:235:THR:N	2.79	0.41
1:A:341:PHE:CD1	1:A:341:PHE:N	2.89	0.41
1:A:3:TYR:HE2	1:A:138:PHE:HA	1.86	0.41
1:A:17:PHE:CD2	1:A:18:PHE:CE1	3.08	0.41
1:A:82:GLY:CA	1:A:85:VAL:HG23	2.50	0.41
1:A:92:ILE:HD11	1:A:170:PHE:HB2	2.02	0.41
1:A:108:ILE:HG13	1:A:108:ILE:H	1.58	0.41
1:A:256:GLN:HG3	1:A:257:GLY:N	2.33	0.41
1:A:297:THR:O	1:A:301:VAL:CG2	2.56	0.41
1:A:314:GLU:O	1:A:317:ILE:HB	2.20	0.41
1:A:326:VAL:O	1:A:330:LEU:HD13	2.21	0.41
1:A:342:GLU:O	1:A:345:PHE:N	2.53	0.41
1:A:35:HIS:O	1:A:39:HIS:CA	2.66	0.41
1:A:143:ALA:O	1:A:146:PHE:HB2	2.21	0.41
1:A:304:ILE:HD11	1:A:386:GLY:O	2.20	0.41
1:A:32:ILE:HD12	1:A:32:ILE:H	1.85	0.40
1:A:108:ILE:HG13	1:A:109:VAL:H	1.85	0.40
1:A:123:PRO:HG2	1:A:124:ALA:N	2.36	0.40
1:A:130:GLU:C	1:A:132:VAL:H	2.29	0.40
1:A:246:PHE:HD2	1:A:378:PHE:CD2	2.38	0.40
1:A:342:GLU:HB3	1:A:344:ARG:HG2	2.02	0.40
1:A:165:ASN:OD1	1:A:165:ASN:C	2.64	0.40
1:A:219:GLN:HA	1:A:220:PRO:HD3	1.75	0.40
1:A:104:LEU:HA	1:A:107:SER:OG	2.22	0.40
1:A:268:GLY:O	1:A:269:GLU:C	2.63	0.40
1:A:327:PRO:O	1:A:331:VAL:HB	2.21	0.40
1:A:349:ILE:HG22	1:A:350:TYR:CD1	2.57	0.40
1:A:19:TYR:HD2	1:A:20:PHE:CE1	2.39	0.40
1:A:59:PHE:C	1:A:61:PRO:N	2.78	0.40
1:A:92:ILE:HG22	1:A:93:PHE:HD1	1.85	0.40
1:A:174:SER:C	1:A:178:LEU:HB3	2.47	0.40
1:A:241:GLN:NE2	1:A:366:SER:CB	2.84	0.40
1:A:342:GLU:O	1:A:343:VAL:C	2.64	0.40
1:A:56:SER:HB3	1:A:119:ASN:HB3	2.03	0.40
1:A:121:GLY:N	1:A:123:PRO:HD2	2.37	0.40
1:A:327:PRO:C	1:A:329:LEU:H	2.30	0.40
1:A:351:LEU:HD23	1:A:351:LEU:O	2.21	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	415/417 (100%)	276 (66%)	95 (23%)	44 (11%)	0 0

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	75	TYR
1	A	243	PHE
1	A	252	ALA
1	A	279	ALA
1	A	288	GLY
1	A	325	GLU
1	A	346	SER
1	A	379	GLN
1	A	61	PRO
1	A	62	LEU
1	A	67	SER
1	A	88	ALA
1	A	181	ALA
1	A	186	PHE
1	A	201	VAL
1	A	234	CYS
1	A	270	LEU
1	A	281	LEU
1	A	378	PHE
1	A	402	GLY
1	A	99	LEU
1	A	102	ASN
1	A	134	ARG
1	A	140	PHE
1	A	175	GLY
1	A	204	ASN
1	A	233	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	250	PHE
1	A	280	PRO
1	A	326	VAL
1	A	407	SER
1	A	26	TYR
1	A	111	GLY
1	A	118	PHE
1	A	168	PHE
1	A	191	ALA
1	A	277	PHE
1	A	156	SER
1	A	328	PHE
1	A	89	PRO
1	A	179	ILE
1	A	220	PRO
1	A	94	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	345/345 (100%)	271 (79%)	74 (21%)	1 2

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	PHE
1	A	54	LEU
1	A	57	LEU
1	A	62	LEU
1	A	65	LEU
1	A	69	LYS
1	A	70	LEU
1	A	72	LEU
1	A	74	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	76	LEU
1	A	77	LEU
1	A	78	TRP
1	A	92	ILE
1	A	100	GLN
1	A	103	ILE
1	A	104	LEU
1	A	108	ILE
1	A	114	LEU
1	A	116	PHE
1	A	129	ILE
1	A	130	GLU
1	A	133	SER
1	A	136	SER
1	A	138	PHE
1	A	151	TRP
1	A	166	ASN
1	A	167	GLN
1	A	170	PHE
1	A	174	SER
1	A	176	CYS
1	A	183	LEU
1	A	186	PHE
1	A	189	THR
1	A	196	THR
1	A	199	ASN
1	A	208	PHE
1	A	209	SER
1	A	216	LEU
1	A	222	LEU
1	A	226	SER
1	A	227	LEU
1	A	237	ASP
1	A	240	ASP
1	A	242	GLN
1	A	256	GLN
1	A	264	VAL
1	A	265	THR
1	A	277	PHE
1	A	278	PHE
1	A	281	LEU
1	A	298	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	300	SER
1	A	310	THR
1	A	315	VAL
1	A	320	THR
1	A	323	MET
1	A	326	VAL
1	A	330	LEU
1	A	339	SER
1	A	340	GLN
1	A	349	ILE
1	A	352	VAL
1	A	359	GLN
1	A	360	LEU
1	A	368	LEU
1	A	376	ILE
1	A	383	LEU
1	A	388	VAL
1	A	390	LEU
1	A	397	VAL
1	A	406	LEU
1	A	409	LEU
1	A	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	38	ASN
1	A	39	HIS
1	A	60	GLN
1	A	100	GLN
1	A	102	ASN
1	A	166	ASN
1	A	241	GLN
1	A	256	GLN
1	A	340	GLN
1	A	371	ASN
1	A	379	GLN
1	A	414	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	408/417 (97%)	-0.04	21 (5%) 33 28	44, 77, 138, 186	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	VAL	9.4
1	A	404	GLY	6.2
1	A	191	ALA	5.1
1	A	416	VAL	4.7
1	A	405	PRO	4.5
1	A	192	PRO	4.4
1	A	285	ARG	4.3
1	A	194	SER	4.0
1	A	407	SER	3.7
1	A	237	ASP	3.3
1	A	176	CYS	3.3
1	A	177	ALA	3.2
1	A	103	ILE	3.1
1	A	101	TYR	3.1
1	A	107	SER	2.9
1	A	408	LEU	2.7
1	A	231	GLY	2.4
1	A	406	LEU	2.4
1	A	145	MET	2.4
1	A	275	ILE	2.3
1	A	3	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HG	A	504	1/1	0.94	0.11	127,127,127,127	1
2	HG	A	501	1/1	0.95	0.08	200,200,200,200	1
2	HG	A	503	1/1	0.99	0.09	67,67,67,67	1
2	HG	A	502	1/1	0.99	0.08	73,73,73,73	1
2	HG	A	505	1/1	1.00	0.05	44,44,44,44	1

6.5 Other polymers [i](#)

There are no such residues in this entry.