



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:12 AM GMT

PDB ID : 3DOK
Title : Crystal structure of K103N mutant HIV-1 reverse transcriptase in complex with GW678248.
Authors : Chamberlain, P.P.; Ren, J.; Stammers, D.K.
Deposited on : 2008-07-04
Resolution : 2.90 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

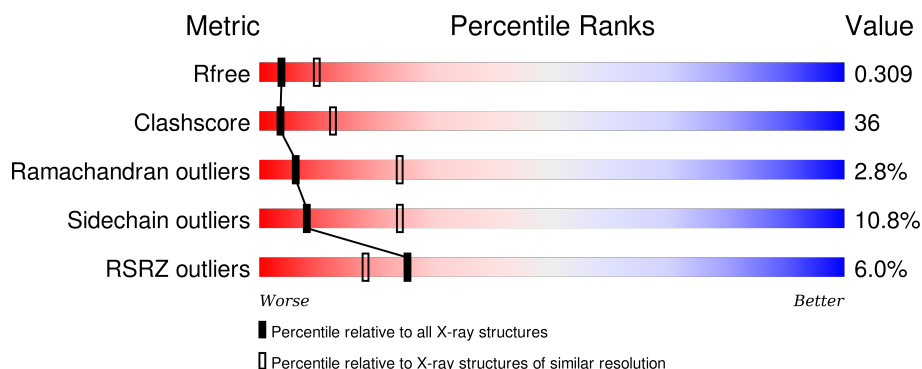
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

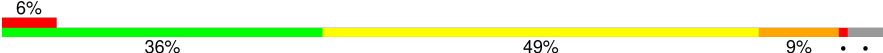
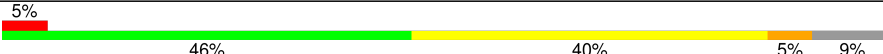
The reported resolution of this entry is 2.90 Å.

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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	560	 6% 36% 49% 9% . .
2	B	440	 5% 46% 40% 5% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7750 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4383	2835	729	811	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	ENGINEERED	UNP P04585

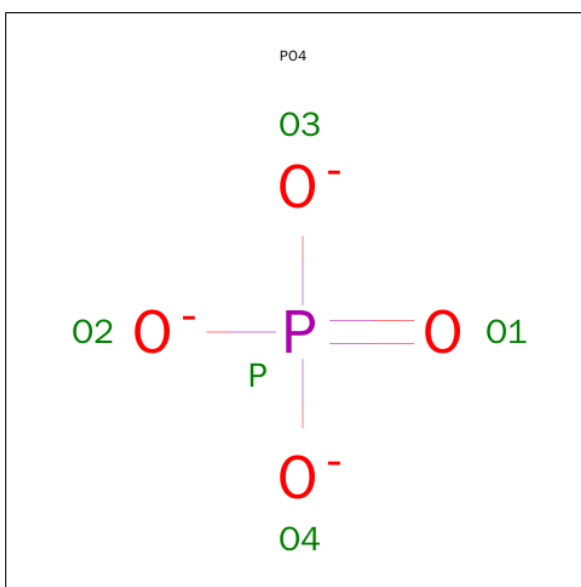
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3320	2158	553	602	7			

There is a discrepancy between the modelled and reference sequences:

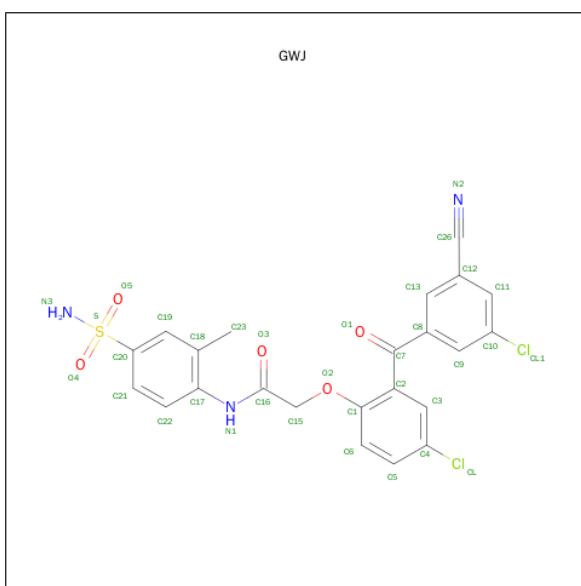
Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LYS	ENGINEERED	UNP P04585

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 2-{4-CHLORO-2-[(3-CHLORO-5-CYANOPHENYL)CARBONYL]PHENOXY}-N-(2-METHYL-4-SULFAMOYLPHENYL)ACETAMIDE (three-letter code: GWJ) (formula: $C_{23}H_{17}Cl_2N_3O_5S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			34	23	2	3	5	1		

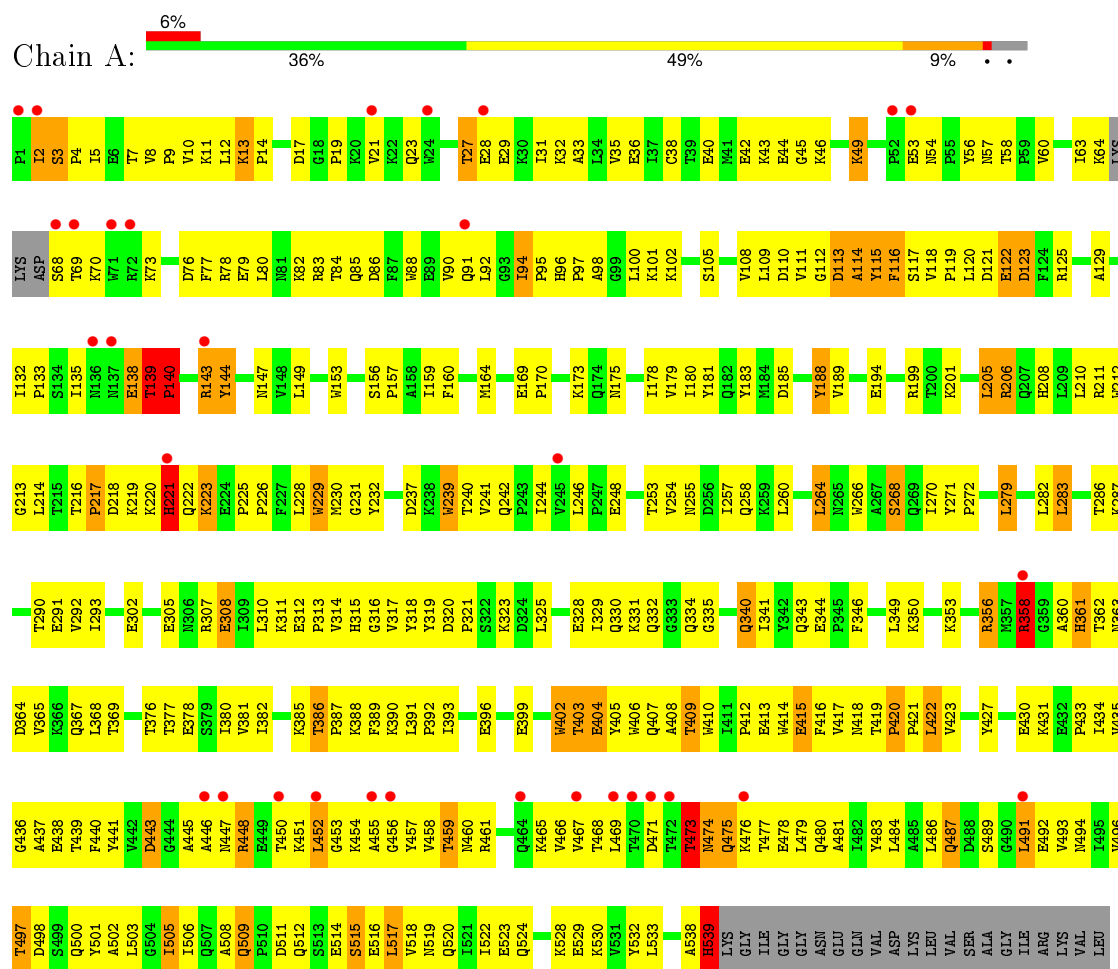
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	2	Total 2	O 2	0	0

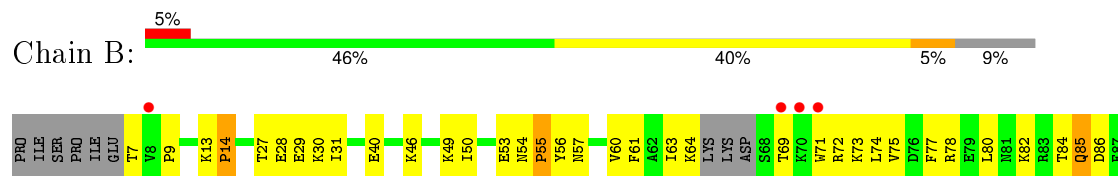
3 Residue-property plots

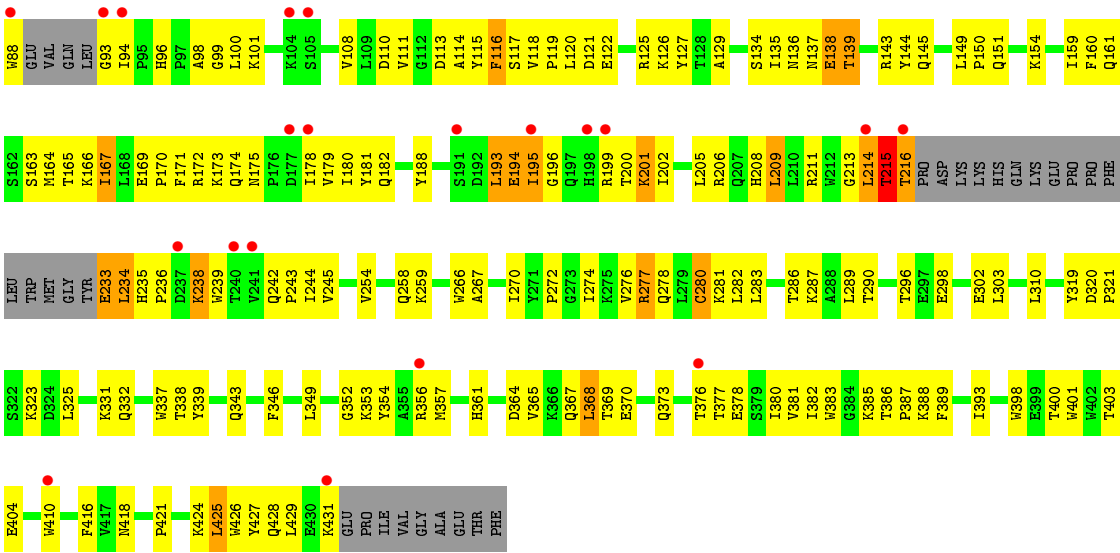
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



• Molecule 2: p51 RT





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.94Å 109.77Å 72.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.90 29.79 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.79-2.90) 99.6 (29.79-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.312 0.215 , 0.309	Depositor DCC
R_{free} test set	1203 reflections (4.86%)	DCC
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 24771 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7750	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: CSD, PO4, GWJ

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	0/4491	0.85	7/6107 (0.1%)
2	B	0.57	0/3412	0.81	3/4635 (0.1%)
All	All	0.58	0/7903	0.83	10/10742 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	215	THR	N-CA-C	8.64	134.32	111.00
1	A	539	HIS	N-CA-C	-7.76	90.03	111.00
1	A	505	ILE	CB-CA-C	-6.26	99.07	111.60
1	A	140	PRO	N-CA-C	6.13	128.04	112.10
2	B	214	LEU	CA-CB-CG	-6.06	101.36	115.30
2	B	216	THR	N-CA-C	5.97	127.12	111.00
1	A	3	SER	N-CA-C	5.51	125.88	111.00
1	A	139	THR	N-CA-C	5.38	125.52	111.00
1	A	239	TRP	N-CA-C	-5.33	96.61	111.00
1	A	473	THR	N-CA-C	-5.15	97.09	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	TYR	Sidechain
1	A	188	TYR	Sidechain

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	4383	0	4416	367	0
2	B	3320	0	3346	207	0
3	A	5	0	0	0	0
4	A	34	0	17	5	0
5	A	6	0	0	1	0
5	B	2	0	0	0	0
All	All	7750	0	7779	559	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 36.

All (559) 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:139:THR:HB	1:A:140:PRO:HD2	1.28	1.14
1:A:448:ARG:HD3	1:A:448:ARG:H	0.93	1.09
1:A:49:LYS:H	1:A:49:LYS:HD3	0.97	1.05
1:A:49:LYS:H	1:A:49:LYS:CD	1.64	1.03
1:A:448:ARG:HD3	1:A:448:ARG:N	1.75	0.99
1:A:448:ARG:CD	1:A:448:ARG:H	1.77	0.96
2:B:278:GLN:HE21	2:B:298:GLU:CB	1.77	0.96
1:A:312:GLU:HG2	1:A:313:PRO:HD2	1.48	0.96
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.45	0.95
2:B:84:THR:HG22	2:B:154:LYS:HE2	1.49	0.94
1:A:49:LYS:N	1:A:49:LYS:HD3	1.77	0.93
1:A:139:THR:CB	1:A:140:PRO:HD2	1.95	0.92
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.04	0.92
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.52	0.90
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.08	0.88
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.39	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:GLU:HG3	2:B:139:THR:HG22	1.56	0.86
1:A:94:ILE:HG22	1:A:183:TYR:HE2	1.37	0.86
1:A:149:LEU:HD11	1:A:159:ILE:HG21	1.58	0.85
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.12	0.85
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.57	0.85
1:A:335:GLY:HA2	1:A:367:GLN:OE1	1.76	0.84
1:A:489:SER:OG	1:A:493:VAL:HG21	1.77	0.84
1:A:206:ARG:HG2	1:A:206:ARG:HH11	1.43	0.84
1:A:206:ARG:CG	1:A:206:ARG:HH11	1.90	0.84
1:A:149:LEU:HD21	1:A:159:ILE:HG22	1.60	0.84
2:B:163:SER:O	2:B:167:ILE:HG23	1.78	0.83
1:A:518:VAL:O	1:A:522:ILE:HG13	1.79	0.83
1:A:491:LEU:CD1	1:A:492:GLU:HG3	2.10	0.82
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.60	0.81
1:A:465:LYS:O	1:A:466:VAL:HG23	1.79	0.81
2:B:135:ILE:H	2:B:135:ILE:HD12	1.46	0.80
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.61	0.80
1:A:308:GLU:HA	1:A:308:GLU:OE2	1.82	0.80
2:B:214:LEU:O	2:B:215:THR:HG23	1.83	0.78
1:A:399:GLU:O	1:A:403:THR:HB	1.84	0.77
1:A:418:ASN:O	1:A:420:PRO:HD3	1.84	0.77
1:A:23:GLN:OE1	1:A:60:VAL:HG12	1.84	0.76
2:B:376:THR:O	2:B:380:ILE:HG13	1.85	0.76
1:A:248:GLU:HG3	1:A:307:ARG:NH2	1.99	0.76
1:A:9:PRO:HG2	2:B:53:GLU:HG3	1.66	0.76
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.86	0.76
1:A:8:VAL:HG13	2:B:53:GLU:OE1	1.87	0.76
1:A:2:ILE:HG22	1:A:3:SER:N	2.02	0.75
1:A:79:GLU:CD	1:A:83:ARG:HH12	1.91	0.74
1:A:109:LEU:HD23	1:A:216:THR:HG21	1.66	0.74
1:A:122:GLU:CD	1:A:122:GLU:H	1.89	0.74
1:A:358:ARG:HD3	1:A:358:ARG:H	1.53	0.73
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.68	0.73
2:B:173:LYS:N	2:B:173:LYS:HD2	2.02	0.73
1:A:129:ALA:HB1	1:A:143:ARG:HH12	1.52	0.73
1:A:403:THR:HG23	1:A:404:GLU:OE1	1.89	0.73
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.70	0.73
1:A:220:LYS:O	1:A:220:LYS:HD3	1.88	0.72
1:A:220:LYS:O	1:A:221:HIS:HB2	1.88	0.72
2:B:373:GLN:O	2:B:377:THR:HG23	1.89	0.72
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.06	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.70	0.72
1:A:27:THR:O	1:A:31:ILE:HG13	1.88	0.72
1:A:206:ARG:CB	1:A:206:ARG:HH11	2.04	0.71
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.23	0.71
1:A:474:ASN:O	1:A:477:THR:OG1	2.07	0.71
1:A:17:ASP:O	1:A:83:ARG:HD3	1.89	0.71
1:A:218:ASP:C	1:A:220:LYS:H	1.94	0.71
1:A:100:LEU:HD23	1:A:181:TYR:HE1	1.57	0.70
1:A:334:GLN:O	1:A:356:ARG:HD2	1.91	0.70
1:A:474:ASN:O	1:A:478:GLU:HG3	1.91	0.70
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.56	0.70
1:A:102:LYS:HE2	1:A:237:ASP:HA	1.72	0.70
2:B:98:ALA:O	2:B:101:LYS:HG2	1.91	0.70
1:A:478:GLU:O	1:A:481:ALA:HB3	1.93	0.69
1:A:248:GLU:HG3	1:A:307:ARG:CZ	2.23	0.69
2:B:94:ILE:HD11	2:B:181:TYR:HD2	1.56	0.69
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.28	0.68
2:B:170:PRO:O	2:B:174:GLN:HG3	1.94	0.68
1:A:317:VAL:HG12	1:A:318:TYR:N	2.08	0.68
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.28	0.68
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.74	0.68
1:A:219:LYS:HD2	1:A:222:GLN:NE2	2.08	0.68
1:A:350:LYS:HE3	1:A:378:GLU:OE1	1.93	0.68
2:B:278:GLN:HE21	2:B:298:GLU:HB3	1.58	0.68
2:B:134:SER:CB	2:B:139:THR:HG23	2.24	0.68
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.58	0.68
1:A:94:ILE:HG22	1:A:183:TYR:CE2	2.26	0.68
1:A:139:THR:HB	1:A:140:PRO:CD	2.16	0.67
1:A:454:LYS:HA	1:A:467:VAL:O	1.95	0.67
1:A:112:GLY:O	1:A:114:ALA:N	2.24	0.67
2:B:424:LYS:HD2	2:B:425:LEU:HD13	1.75	0.67
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.29	0.67
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.83	0.67
1:A:111:VAL:HG22	1:A:185:ASP:HB3	1.77	0.67
1:A:439:THR:HG22	1:A:439:THR:O	1.95	0.67
1:A:206:ARG:HB3	1:A:206:ARG:NH1	2.10	0.66
2:B:376:THR:CG2	2:B:386:THR:HG22	2.25	0.66
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.24	0.66
1:A:122:GLU:HB3	1:A:125:ARG:NH1	2.10	0.66
1:A:122:GLU:N	1:A:122:GLU:OE1	2.27	0.66
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASP:OD2	1:A:123:ASP:HB2	1.96	0.65
2:B:245:VAL:HG13	2:B:431:LYS:HB2	1.79	0.65
1:A:49:LYS:N	1:A:49:LYS:CD	2.46	0.65
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.78	0.65
1:A:438:GLU:OE1	1:A:459:THR:OG1	2.08	0.65
1:A:491:LEU:HD13	1:A:492:GLU:HG3	1.77	0.65
2:B:161:GLN:HE22	2:B:182:GLN:HE22	1.45	0.65
1:A:493:VAL:HG12	1:A:494:ASN:N	2.11	0.64
1:A:516:GLU:O	1:A:519:ASN:HB2	1.97	0.64
1:A:486:LEU:O	1:A:528:LYS:NZ	2.31	0.64
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.78	0.64
1:A:388:LYS:NZ	1:A:415:GLU:HB3	2.12	0.64
2:B:13:LYS:HE3	2:B:84:THR:O	1.97	0.63
1:A:317:VAL:HG12	1:A:318:TYR:H	1.63	0.63
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.80	0.63
2:B:169:GLU:O	2:B:173:LYS:HD3	1.98	0.63
1:A:79:GLU:OE1	1:A:82:LYS:HD3	1.98	0.63
2:B:196:GLY:O	2:B:200:THR:HG23	1.98	0.63
1:A:178:ILE:HD11	1:A:201:LYS:HG2	1.79	0.63
1:A:149:LEU:HD21	1:A:159:ILE:CG2	2.28	0.63
1:A:402:TRP:CD1	1:A:402:TRP:C	2.71	0.63
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.80	0.62
1:A:225:PRO:HA	1:A:226:PRO:C	2.20	0.62
2:B:56:TYR:HE2	2:B:126:LYS:HE3	1.63	0.62
1:A:445:ALA:HA	5:A:1306:HOH:O	1.99	0.62
1:A:408:ALA:HB3	2:B:393:ILE:CG1	2.28	0.62
1:A:358:ARG:O	1:A:358:ARG:HG2	1.98	0.62
1:A:218:ASP:C	1:A:220:LYS:N	2.54	0.62
1:A:101:LYS:HA	1:A:319:TYR:O	2.00	0.61
1:A:210:LEU:HD22	1:A:214:LEU:O	2.00	0.61
1:A:3:SER:HB3	1:A:5:ILE:CG1	2.29	0.61
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.35	0.61
1:A:68:SER:C	1:A:70:LYS:H	2.04	0.61
2:B:169:GLU:HG2	2:B:173:LYS:HZ3	1.66	0.61
1:A:100:LEU:HD23	1:A:181:TYR:CE1	2.35	0.61
2:B:88:TRP:HZ3	2:B:93:GLY:N	1.99	0.61
2:B:84:THR:CG2	2:B:154:LYS:HE2	2.26	0.61
1:A:241:VAL:CG2	1:A:270:ILE:HD13	2.31	0.61
1:A:491:LEU:HD22	1:A:529:GLU:CD	2.20	0.61
1:A:2:ILE:HG22	1:A:3:SER:H	1.64	0.61
2:B:161:GLN:HE22	2:B:182:GLN:NE2	1.97	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG13	1:A:119:PRO:HD2	1.82	0.60
1:A:241:VAL:HG21	1:A:270:ILE:HD13	1.82	0.60
1:A:31:ILE:O	1:A:35:VAL:HG23	2.02	0.60
1:A:538:ALA:O	1:A:539:HIS:HB3	2.01	0.60
1:A:312:GLU:HG2	1:A:313:PRO:CD	2.28	0.60
2:B:266:TRP:CZ3	2:B:426:TRP:CG	2.89	0.60
1:A:508:ALA:O	1:A:509:GLN:C	2.39	0.60
1:A:346:PHE:N	1:A:346:PHE:CD2	2.66	0.60
2:B:278:GLN:HB2	2:B:302:GLU:OE1	2.01	0.60
1:A:139:THR:CB	1:A:140:PRO:CD	2.76	0.60
1:A:231:GLY:C	1:A:242:GLN:HG2	2.21	0.60
1:A:318:TYR:CD1	4:A:999:GWJ:H15A	2.38	0.59
2:B:27:THR:O	2:B:31:ILE:HG13	2.03	0.59
1:A:115:TYR:O	1:A:117:SER:N	2.35	0.59
1:A:515:SER:OG	1:A:518:VAL:HG23	2.03	0.59
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.84	0.59
1:A:206:ARG:HG2	1:A:206:ARG:NH1	2.15	0.59
2:B:120:LEU:O	2:B:121:ASP:C	2.40	0.59
1:A:102:LYS:CE	1:A:237:ASP:HA	2.32	0.59
1:A:358:ARG:HD3	1:A:358:ARG:N	2.18	0.58
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.37	0.58
1:A:489:SER:CB	1:A:493:VAL:HG21	2.34	0.58
1:A:219:LYS:HA	1:A:222:GLN:HG2	1.86	0.58
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.15	0.58
2:B:61:PHE:CD1	2:B:403:THR:HG22	2.39	0.58
1:A:219:LYS:HD2	1:A:222:GLN:HE21	1.68	0.58
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.38	0.58
1:A:376:THR:O	1:A:380:ILE:HG12	2.02	0.58
2:B:194:GLU:OE2	2:B:195:ILE:HG22	2.04	0.58
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.85	0.58
1:A:320:ASP:OD1	1:A:323:LYS:HG3	2.04	0.58
1:A:232:TYR:N	1:A:242:GLN:HE21	2.00	0.58
2:B:113:ASP:O	2:B:116:PHE:HD2	1.86	0.57
1:A:43:LYS:C	1:A:45:GLY:H	2.07	0.57
1:A:291:GLU:HG2	1:A:293:ILE:CD1	2.34	0.57
1:A:98:ALA:HB2	1:A:349:LEU:O	2.04	0.57
2:B:175:ASN:HB3	2:B:178:ILE:HD12	1.86	0.57
2:B:114:ALA:HB2	2:B:214:LEU:HD11	1.87	0.57
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.86	0.57
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.18	0.57
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:O	1:A:403:THR:CB	2.53	0.57
2:B:331:LYS:NZ	2:B:364:ASP:OD1	2.34	0.57
1:A:43:LYS:C	1:A:45:GLY:N	2.55	0.57
1:A:257:ILE:HD13	1:A:282:LEU:HD23	1.85	0.57
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.87	0.57
2:B:235:HIS:O	2:B:238:LYS:HG2	2.05	0.57
2:B:339:TYR:CE1	2:B:352:GLY:HA3	2.39	0.57
1:A:308:GLU:OE2	1:A:311:LYS:HE2	2.05	0.56
2:B:254:VAL:O	2:B:258:GLN:HG3	2.05	0.56
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.87	0.56
1:A:109:LEU:HB3	1:A:216:THR:HG23	1.86	0.56
2:B:365:VAL:O	2:B:369:THR:HG23	2.04	0.56
2:B:161:GLN:O	2:B:165:THR:HG23	2.06	0.56
1:A:439:THR:HG22	1:A:441:TYR:HE1	1.70	0.56
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.34	0.56
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.87	0.56
1:A:503:LEU:O	1:A:506:ILE:HB	2.06	0.56
1:A:268:SER:HB3	1:A:353:LYS:HE2	1.86	0.56
2:B:163:SER:O	2:B:167:ILE:CG2	2.50	0.56
2:B:242:GLN:NE2	2:B:243:PRO:HD2	2.21	0.56
2:B:111:VAL:HA	2:B:214:LEU:HD22	1.87	0.56
2:B:56:TYR:O	2:B:57:ASN:HB2	2.06	0.55
1:A:334:GLN:NE2	1:A:512:GLN:HB3	2.20	0.55
2:B:29:GLU:CG	2:B:30:LYS:N	2.70	0.55
1:A:506:ILE:HG13	1:A:533:LEU:HD23	1.89	0.55
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.88	0.55
2:B:376:THR:HG23	2:B:386:THR:HG22	1.87	0.55
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.36	0.55
1:A:220:LYS:O	1:A:221:HIS:CB	2.52	0.55
1:A:43:LYS:O	1:A:45:GLY:N	2.40	0.55
1:A:388:LYS:HZ1	1:A:415:GLU:HB3	1.72	0.55
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.88	0.55
2:B:278:GLN:OE1	2:B:278:GLN:HA	2.06	0.55
1:A:111:VAL:HG21	1:A:160:PHE:CZ	2.42	0.55
2:B:195:ILE:HG23	2:B:196:GLY:H	1.72	0.55
2:B:27:THR:HB	2:B:29:GLU:HG2	1.89	0.55
1:A:448:ARG:HG2	1:A:448:ARG:NH1	2.22	0.55
2:B:169:GLU:HB2	2:B:170:PRO:CD	2.31	0.55
1:A:28:GLU:HG3	1:A:29:GLU:N	2.22	0.55
1:A:308:GLU:OE2	1:A:308:GLU:CA	2.53	0.54
1:A:109:LEU:HD23	1:A:216:THR:CG2	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:HD2	1:A:98:ALA:H	1.55	0.54
1:A:331:LYS:NZ	1:A:364:ASP:OD1	2.37	0.54
1:A:254:VAL:O	1:A:258:GLN:HG3	2.07	0.54
1:A:170:PRO:HA	1:A:173:LYS:NZ	2.21	0.54
1:A:440:PHE:HZ	1:A:489:SER:HB3	1.67	0.54
1:A:505:ILE:O	1:A:509:GLN:N	2.39	0.54
1:A:205:LEU:O	1:A:208:HIS:N	2.40	0.54
2:B:254:VAL:HG21	2:B:287:LYS:HG3	1.89	0.54
1:A:493:VAL:CG1	1:A:494:ASN:N	2.70	0.54
1:A:491:LEU:HD12	1:A:492:GLU:HG3	1.90	0.54
1:A:220:LYS:C	1:A:220:LYS:HD3	2.27	0.54
2:B:193:LEU:HD23	2:B:193:LEU:N	2.23	0.54
1:A:206:ARG:HB3	1:A:206:ARG:HH11	1.66	0.54
1:A:332:GLN:HG2	1:A:332:GLN:O	2.07	0.54
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.72	0.54
1:A:302:GLU:HA	1:A:305:GLU:OE1	2.07	0.54
1:A:268:SER:CB	1:A:353:LYS:HE2	2.37	0.54
2:B:7:THR:HG22	2:B:119:PRO:CG	2.34	0.54
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.43	0.53
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.22	0.53
2:B:337:TRP:O	2:B:353:LYS:HA	2.09	0.53
1:A:84:THR:HG22	1:A:85:GLN:N	2.22	0.53
1:A:419:THR:HG22	1:A:419:THR:O	2.06	0.53
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.90	0.53
1:A:455:ALA:O	1:A:484:LEU:HD12	2.08	0.53
1:A:434:ILE:HB	1:A:437:ALA:HB3	1.89	0.53
1:A:179:VAL:HG13	1:A:181:TYR:CE2	2.43	0.53
1:A:451:LYS:O	1:A:471:ASP:N	2.41	0.53
1:A:95:PRO:HA	2:B:136:ASN:OD1	2.09	0.53
1:A:206:ARG:CB	1:A:206:ARG:NH1	2.71	0.52
2:B:424:LYS:NZ	2:B:428:GLN:NE2	2.57	0.52
1:A:420:PRO:HA	1:A:421:PRO:C	2.29	0.52
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.90	0.52
1:A:388:LYS:HD3	1:A:413:GLU:OE2	2.10	0.52
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.74	0.52
1:A:42:GLU:OE2	1:A:49:LYS:HG2	2.10	0.52
1:A:199:ARG:HG3	1:A:219:LYS:NZ	2.24	0.52
1:A:416:PHE:HZ	1:A:422:LEU:HD11	1.73	0.52
2:B:245:VAL:CG1	2:B:431:LYS:HB2	2.39	0.52
1:A:49:LYS:HG3	1:A:144:TYR:CE2	2.44	0.52
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:THR:O	1:A:475:GLN:N	2.42	0.52
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.92	0.52
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.44	0.52
1:A:58:THR:HG23	1:A:76:ASP:O	2.10	0.52
1:A:42:GLU:OE2	1:A:49:LYS:CG	2.57	0.52
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.91	0.52
1:A:246:LEU:O	1:A:307:ARG:NH1	2.29	0.52
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.91	0.52
1:A:335:GLY:CA	1:A:367:GLN:OE1	2.56	0.52
1:A:491:LEU:HD22	1:A:529:GLU:OE2	2.10	0.52
2:B:426:TRP:O	2:B:429:LEU:HB2	2.10	0.52
1:A:170:PRO:O	1:A:173:LYS:HB2	2.10	0.52
1:A:69:THR:HG22	1:A:69:THR:O	2.10	0.52
1:A:63:ILE:C	1:A:63:ILE:HD12	2.30	0.51
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.38	0.51
1:A:465:LYS:O	1:A:466:VAL:CG2	2.56	0.51
1:A:439:THR:CG2	1:A:441:TYR:HE1	2.23	0.51
1:A:129:ALA:HA	1:A:144:TYR:O	2.11	0.51
1:A:408:ALA:HB3	2:B:393:ILE:CB	2.41	0.51
1:A:454:LYS:NZ	1:A:468:THR:HG23	2.26	0.51
2:B:27:THR:CG2	2:B:29:GLU:HG2	2.40	0.51
1:A:292:VAL:C	1:A:293:ILE:HD12	2.30	0.51
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.45	0.51
1:A:476:LYS:O	1:A:480:GLN:HB2	2.10	0.51
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.93	0.51
1:A:53:GLU:HG3	1:A:53:GLU:O	2.09	0.51
2:B:173:LYS:CD	2:B:173:LYS:N	2.71	0.51
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.41	0.51
2:B:72:ARG:NH2	2:B:151:GLN:OE1	2.44	0.51
1:A:68:SER:C	1:A:70:LYS:N	2.64	0.51
1:A:377:THR:O	1:A:381:VAL:HG23	2.11	0.51
1:A:112:GLY:C	1:A:114:ALA:H	2.11	0.51
1:A:254:VAL:HG22	1:A:286:THR:HG21	1.92	0.51
1:A:502:ALA:O	1:A:503:LEU:C	2.50	0.50
1:A:435:VAL:HA	2:B:290:THR:HG21	1.92	0.50
1:A:484:LEU:O	1:A:487:GLN:HG3	2.12	0.50
2:B:277:ARG:O	2:B:281:LYS:HG3	2.12	0.50
1:A:170:PRO:HA	1:A:173:LYS:HZ1	1.76	0.50
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.10	0.50
2:B:356:ARG:NH1	2:B:357:MET:O	2.44	0.50
1:A:389:PHE:HB2	1:A:414:TRP:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:LEU:HD13	2:B:205:LEU:C	2.32	0.50
1:A:489:SER:HB2	1:A:493:VAL:CG2	2.42	0.50
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.27	0.50
1:A:109:LEU:HB3	1:A:216:THR:CG2	2.42	0.50
1:A:110:ASP:OD1	1:A:217:PRO:HG2	2.11	0.50
1:A:439:THR:CG2	1:A:441:TYR:CE1	2.95	0.50
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.46	0.50
1:A:253:THR:O	1:A:257:ILE:HG13	2.11	0.50
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.46	0.50
1:A:84:THR:CG2	1:A:85:GLN:N	2.75	0.50
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.12	0.49
2:B:173:LYS:HD2	2:B:173:LYS:H	1.76	0.49
1:A:447:ASN:CG	1:A:450:THR:HG23	2.32	0.49
2:B:195:ILE:HG23	2:B:196:GLY:N	2.27	0.49
2:B:277:ARG:HG2	2:B:278:GLN:H	1.77	0.49
1:A:465:LYS:CG	1:A:466:VAL:N	2.76	0.49
1:A:291:GLU:HG2	1:A:293:ILE:HD12	1.94	0.49
2:B:110:ASP:HB3	2:B:216:THR:CG2	2.43	0.49
2:B:233:GLU:N	2:B:233:GLU:CD	2.65	0.49
2:B:159:ILE:CG2	2:B:159:ILE:O	2.60	0.49
2:B:343:GLN:HG3	2:B:349:LEU:HD11	1.95	0.49
2:B:320:ASP:C	2:B:320:ASP:OD1	2.51	0.49
1:A:179:VAL:CG1	1:A:181:TYR:CE2	2.95	0.49
2:B:129:ALA:HA	2:B:144:TYR:O	2.13	0.49
2:B:175:ASN:CB	2:B:178:ILE:HD12	2.43	0.49
2:B:368:LEU:HD13	2:B:398:TRP:CZ3	2.47	0.49
2:B:270:ILE:O	2:B:272:PRO:HD3	2.12	0.49
1:A:418:ASN:C	1:A:420:PRO:HD3	2.33	0.48
2:B:98:ALA:O	2:B:101:LYS:CG	2.61	0.48
2:B:424:LYS:HZ3	2:B:428:GLN:NE2	2.11	0.48
1:A:96:HIS:O	1:A:97:PRO:C	2.48	0.48
1:A:113:ASP:O	1:A:117:SER:HB2	2.12	0.48
1:A:399:GLU:O	1:A:403:THR:CG2	2.61	0.48
1:A:105:SER:HA	4:A:999:GWJ:H21	1.94	0.48
2:B:53:GLU:O	2:B:55:PRO:HD3	2.13	0.48
1:A:12:LEU:O	1:A:13:LYS:O	2.31	0.48
2:B:172:ARG:O	2:B:175:ASN:C	2.52	0.48
1:A:308:GLU:OE2	1:A:311:LYS:CE	2.62	0.48
1:A:216:THR:HG22	1:A:217:PRO:N	2.29	0.48
2:B:276:VAL:O	2:B:280:CYS:HB2	2.14	0.48
1:A:100:LEU:O	1:A:318:TYR:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.49	0.48
2:B:46:LYS:HE2	2:B:116:PHE:HD1	1.78	0.48
1:A:457:TYR:C	1:A:457:TYR:CD1	2.87	0.48
1:A:229:TRP:O	1:A:232:TYR:HB2	2.14	0.48
1:A:287:LYS:N	1:A:291:GLU:OE2	2.39	0.48
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.53	0.48
1:A:402:TRP:CG	1:A:403:THR:N	2.80	0.48
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.28	0.48
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.49	0.47
1:A:317:VAL:CG1	1:A:318:TYR:N	2.76	0.47
2:B:54:ASN:O	2:B:143:ARG:NH2	2.47	0.47
1:A:453:GLY:O	1:A:469:LEU:N	2.28	0.47
1:A:108:VAL:HG21	1:A:223:LYS:HG3	1.96	0.47
1:A:122:GLU:HB3	1:A:125:ARG:HH12	1.77	0.47
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.45	0.47
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.34	0.47
1:A:408:ALA:HB3	2:B:393:ILE:HB	1.96	0.47
1:A:427:TYR:CE2	1:A:509:GLN:HB3	2.49	0.47
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.46	0.47
1:A:279:LEU:O	1:A:282:LEU:HB2	2.15	0.47
1:A:443:ASP:O	1:A:455:ALA:HA	2.15	0.47
1:A:49:LYS:HG3	1:A:144:TYR:HE2	1.80	0.47
1:A:489:SER:CB	1:A:493:VAL:CG2	2.93	0.47
2:B:214:LEU:O	2:B:215:THR:CG2	2.59	0.47
1:A:237:ASP:N	1:A:237:ASP:OD2	2.48	0.47
2:B:421:PRO:O	2:B:425:LEU:HD22	2.14	0.47
1:A:473:THR:HG22	1:A:475:GLN:H	1.78	0.47
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.71	0.47
2:B:61:PHE:CE1	2:B:74:LEU:CD2	2.94	0.47
2:B:161:GLN:NE2	2:B:161:GLN:HA	2.29	0.47
2:B:239:TRP:CZ3	2:B:378:GLU:HG2	2.50	0.47
2:B:173:LYS:CD	2:B:173:LYS:H	2.29	0.46
1:A:291:GLU:HG2	1:A:293:ILE:HD11	1.96	0.46
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.98	0.46
2:B:108:VAL:HG22	2:B:188:TYR:CE2	2.50	0.46
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.50	0.46
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.63	0.46
1:A:460:ASN:HA	2:B:286:THR:O	2.15	0.46
1:A:97:PRO:HA	1:A:100:LEU:CD1	2.45	0.46
1:A:199:ARG:HH11	1:A:199:ARG:HG2	1.80	0.46
1:A:497:THR:OG1	1:A:498:ASP:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:O	1:A:85:GLN:HB3	2.16	0.46
1:A:483:TYR:CE2	1:A:487:GLN:NE2	2.83	0.46
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.51	0.46
1:A:477:THR:O	1:A:481:ALA:N	2.31	0.46
1:A:477:THR:HG1	1:A:478:GLU:H	1.64	0.46
1:A:436:GLY:O	1:A:461:ARG:NH2	2.43	0.46
1:A:57:ASN:HD22	1:A:143:ARG:NH2	2.13	0.46
1:A:341:ILE:O	1:A:349:LEU:HB2	2.16	0.46
2:B:361:HIS:CD2	2:B:361:HIS:C	2.88	0.46
2:B:118:VAL:HB	2:B:149:LEU:HG	1.98	0.46
1:A:418:ASN:OD1	1:A:420:PRO:HD3	2.15	0.46
1:A:418:ASN:OD1	1:A:418:ASN:O	2.34	0.46
2:B:425:LEU:HD12	2:B:425:LEU:HA	1.61	0.46
1:A:489:SER:HB2	1:A:493:VAL:HG22	1.96	0.45
1:A:514:GLU:HG3	1:A:515:SER:N	2.31	0.45
2:B:114:ALA:N	2:B:214:LEU:HD21	2.31	0.45
2:B:61:PHE:CZ	2:B:74:LEU:HG	2.52	0.45
2:B:235:HIS:O	2:B:238:LYS:CG	2.64	0.45
1:A:218:ASP:O	1:A:220:LYS:N	2.49	0.45
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.52	0.45
2:B:369:THR:O	2:B:373:GLN:HG3	2.16	0.45
1:A:427:TYR:CD2	1:A:427:TYR:C	2.89	0.45
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.58	0.45
1:A:57:ASN:HA	1:A:129:ALA:O	2.17	0.45
2:B:118:VAL:CG1	2:B:119:PRO:HD2	2.47	0.45
1:A:479:LEU:HB2	1:A:517:LEU:HD13	1.98	0.45
1:A:517:LEU:HA	1:A:517:LEU:HD23	1.56	0.45
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.52	0.45
1:A:3:SER:OG	1:A:212:TRP:O	2.30	0.45
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.98	0.45
1:A:405:TYR:O	2:B:331:LYS:HE2	2.17	0.45
1:A:77:PHE:O	1:A:78:ARG:C	2.54	0.44
2:B:205:LEU:CD1	2:B:209:LEU:HD22	2.47	0.44
2:B:235:HIS:HB2	2:B:238:LYS:HG2	1.99	0.44
2:B:325:LEU:HA	2:B:325:LEU:HD12	1.72	0.44
2:B:49:LYS:HA	2:B:143:ARG:O	2.17	0.44
1:A:532:TYR:CE2	2:B:289:LEU:HD23	2.53	0.44
1:A:54:ASN:OD1	1:A:56:TYR:HB2	2.18	0.44
1:A:475:GLN:O	1:A:479:LEU:HG	2.18	0.44
1:A:456:GLY:HA3	1:A:466:VAL:HG22	1.98	0.44
1:A:317:VAL:CG1	1:A:318:TYR:H	2.29	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:HD13	1:A:264:LEU:HA	1.87	0.44
1:A:94:ILE:HA	1:A:95:PRO:HD3	1.85	0.44
1:A:257:ILE:CD1	1:A:282:LEU:HD23	2.48	0.44
1:A:149:LEU:HG	1:A:156:SER:HA	1.99	0.44
1:A:439:THR:CG2	1:A:439:THR:O	2.64	0.44
2:B:27:THR:HG22	2:B:29:GLU:H	1.82	0.44
2:B:208:HIS:CD2	2:B:208:HIS:C	2.89	0.44
1:A:19:PRO:O	1:A:56:TYR:HA	2.18	0.44
1:A:175:ASN:OD1	1:A:201:LYS:HE2	2.18	0.44
2:B:258:GLN:O	2:B:259:LYS:C	2.55	0.44
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.53	0.43
1:A:516:GLU:O	1:A:520:GLN:HG3	2.18	0.43
1:A:253:THR:HA	1:A:291:GLU:O	2.18	0.43
2:B:181:TYR:CD2	2:B:182:GLN:N	2.86	0.43
2:B:179:VAL:HG12	2:B:180:ILE:N	2.33	0.43
1:A:56:TYR:O	1:A:143:ARG:NH2	2.37	0.43
2:B:202:ILE:O	2:B:205:LEU:HB3	2.18	0.43
1:A:246:LEU:HD22	1:A:260:LEU:HD11	2.00	0.43
1:A:454:LYS:HG3	1:A:468:THR:HA	2.00	0.43
1:A:68:SER:O	1:A:70:LYS:N	2.52	0.43
1:A:483:TYR:O	1:A:487:GLN:HG2	2.17	0.43
1:A:283:LEU:HA	1:A:283:LEU:HD12	1.80	0.43
1:A:382:ILE:O	2:B:135:ILE:HG22	2.19	0.43
2:B:172:ARG:HH21	2:B:180:ILE:HB	1.83	0.43
1:A:319:TYR:OH	1:A:385:LYS:HD3	2.18	0.43
2:B:27:THR:HG22	2:B:28:GLU:N	2.34	0.43
1:A:43:LYS:HA	1:A:43:LYS:HD3	1.85	0.43
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.48	0.43
2:B:115:TYR:C	2:B:117:SER:N	2.71	0.43
2:B:113:ASP:O	2:B:116:PHE:CD2	2.70	0.43
1:A:318:TYR:CE1	4:A:999:GWJ:H15A	2.53	0.43
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.54	0.43
2:B:332:GLN:NE2	2:B:428:GLN:HB2	2.33	0.43
2:B:29:GLU:HG3	2:B:30:LYS:N	2.34	0.43
1:A:328:GLU:HG3	1:A:390:LYS:CB	2.49	0.43
2:B:78:ARG:O	2:B:82:LYS:HG3	2.19	0.43
1:A:42:GLU:HG3	1:A:49:LYS:HD2	2.00	0.42
2:B:46:LYS:HE2	2:B:116:PHE:CD1	2.53	0.42
1:A:417:VAL:O	1:A:417:VAL:HG13	2.20	0.42
1:A:409:THR:O	1:A:410:TRP:HB2	2.19	0.42
1:A:205:LEU:O	1:A:206:ARG:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.53	0.42
1:A:109:LEU:N	1:A:109:LEU:HD12	2.34	0.42
1:A:122:GLU:CB	1:A:125:ARG:NH1	2.80	0.42
2:B:94:ILE:HD11	2:B:182:GLN:H	1.84	0.42
1:A:88:TRP:HE3	1:A:88:TRP:HA	1.84	0.42
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.54	0.42
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.00	0.42
2:B:400:THR:HG22	2:B:401:TRP:CD2	2.54	0.42
1:A:239:TRP:CE2	1:A:316:GLY:CA	2.96	0.42
2:B:61:PHE:HE1	2:B:74:LEU:HD23	1.79	0.42
2:B:169:GLU:CB	2:B:170:PRO:CD	2.95	0.42
1:A:122:GLU:CD	1:A:122:GLU:N	2.67	0.42
2:B:167:ILE:HD11	2:B:209:LEU:CD1	2.50	0.42
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.55	0.42
2:B:169:GLU:HA	2:B:173:LYS:NZ	2.35	0.42
2:B:115:TYR:O	2:B:117:SER:N	2.52	0.42
2:B:208:HIS:O	2:B:208:HIS:HD2	2.03	0.42
1:A:109:LEU:CD2	1:A:216:THR:HG21	2.43	0.42
2:B:427:TYR:C	2:B:429:LEU:H	2.22	0.42
1:A:100:LEU:CD2	4:A:999:GWJ:H9	2.49	0.42
1:A:415:GLU:HG3	1:A:416:PHE:O	2.20	0.42
2:B:113:ASP:HB2	2:B:214:LEU:HD23	2.01	0.42
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.54	0.42
1:A:175:ASN:OD1	1:A:201:LYS:CE	2.68	0.42
2:B:99:GLY:O	2:B:100:LEU:C	2.58	0.42
1:A:97:PRO:HA	1:A:100:LEU:HD12	2.02	0.41
2:B:206:ARG:O	2:B:209:LEU:N	2.54	0.41
1:A:416:PHE:CZ	1:A:422:LEU:HD11	2.54	0.41
1:A:117:SER:OG	1:A:213:GLY:O	2.38	0.41
2:B:235:HIS:N	2:B:236:PRO:HD3	2.35	0.41
2:B:270:ILE:HG12	2:B:346:PHE:HB3	2.03	0.41
1:A:33:ALA:O	1:A:36:GLU:HB3	2.20	0.41
2:B:134:SER:HB2	2:B:139:THR:HG23	2.02	0.41
1:A:491:LEU:HD13	1:A:492:GLU:CG	2.48	0.41
1:A:12:LEU:CD2	1:A:83:ARG:O	2.68	0.41
2:B:416:PHE:N	2:B:416:PHE:CD1	2.88	0.41
1:A:194:GLU:HA	1:A:194:GLU:OE1	2.20	0.41
1:A:135:ILE:O	1:A:138:GLU:HG3	2.20	0.41
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.79	0.41
2:B:214:LEU:HD23	2:B:214:LEU:HA	1.73	0.41
1:A:216:THR:CG2	1:A:217:PRO:N	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TYR:HE1	1:A:524:GLN:HG3	1.84	0.41
2:B:343:GLN:HG3	2:B:349:LEU:CD1	2.49	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.21	0.41
2:B:137:ASN:C	2:B:139:THR:H	2.22	0.41
2:B:138:GLU:C	2:B:139:THR:HG22	2.40	0.41
2:B:126:LYS:HE2	2:B:127:TYR:CE1	2.56	0.41
1:A:115:TYR:C	1:A:117:SER:N	2.74	0.41
1:A:469:LEU:HD11	1:A:480:GLN:HG2	2.03	0.41
2:B:64:LYS:NZ	2:B:69:THR:O	2.52	0.41
2:B:234:LEU:HD12	2:B:234:LEU:N	2.34	0.41
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.54	0.41
2:B:377:THR:HG22	2:B:410:TRP:HZ2	1.86	0.41
1:A:483:TYR:CE1	1:A:524:GLN:HG3	2.56	0.41
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.56	0.41
1:A:135:ILE:O	1:A:138:GLU:CG	2.69	0.41
2:B:167:ILE:CD1	2:B:209:LEU:HD12	2.50	0.41
2:B:428:GLN:O	2:B:428:GLN:HG2	2.20	0.41
1:A:452:LEU:HA	1:A:469:LEU:O	2.21	0.41
1:A:246:LEU:HD11	1:A:310:LEU:HD12	2.03	0.41
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.81	0.41
2:B:208:HIS:CD2	2:B:208:HIS:O	2.73	0.41
1:A:3:SER:HA	1:A:4:PRO:HD3	1.71	0.41
1:A:96:HIS:CD2	1:A:98:ALA:H	2.37	0.41
1:A:188:TYR:O	4:A:999:GWJ:CL	2.76	0.41
1:A:164:MET:CE	1:A:214:LEU:HD13	2.51	0.41
1:A:169:GLU:OE2	1:A:173:LYS:HE3	2.21	0.41
1:A:476:LYS:O	1:A:480:GLN:N	2.39	0.41
2:B:50:ILE:HD12	2:B:54:ASN:HB3	2.03	0.41
1:A:430:GLU:HB2	1:A:532:TYR:HB2	2.03	0.41
1:A:135:ILE:N	1:A:135:ILE:HD12	2.35	0.41
1:A:386:THR:HA	1:A:387:PRO:HD3	1.87	0.41
2:B:96:HIS:CE1	2:B:381:VAL:O	2.74	0.41
1:A:360:ALA:O	1:A:361:HIS:HB3	2.21	0.41
1:A:8:VAL:O	1:A:121:ASP:HB2	2.21	0.41
1:A:125:ARG:NE	1:A:147:ASN:HA	2.36	0.41
1:A:329:ILE:O	1:A:392:PRO:HD3	2.21	0.41
2:B:85:GLN:HG3	2:B:86:ASP:O	2.21	0.41
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.89	0.40
1:A:3:SER:HB3	1:A:5:ILE:CD1	2.51	0.40
1:A:474:ASN:HA	1:A:477:THR:OG1	2.21	0.40
1:A:240:THR:HG22	1:A:315:HIS:CB	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HG23	1:A:189:VAL:HG22	2.03	0.40
1:A:447:ASN:O	1:A:451:LYS:N	2.38	0.40
1:A:522:ILE:O	1:A:523:GLU:C	2.59	0.40
1:A:270:ILE:HG22	1:A:314:VAL:HG21	2.02	0.40
2:B:238:LYS:NZ	2:B:239:TRP:HD1	2.19	0.40
2:B:134:SER:OG	2:B:139:THR:HG23	2.22	0.40
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.57	0.40
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.52	0.40
1:A:132:ILE:HA	1:A:133:PRO:HD2	1.90	0.40
1:A:363:ASN:OD1	1:A:365:VAL:N	2.54	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	531/560 (95%)	441 (83%)	72 (14%)	18 (3%)	5	19
2	B	394/440 (90%)	347 (88%)	39 (10%)	8 (2%)	9	33
All	All	925/1000 (92%)	788 (85%)	111 (12%)	26 (3%)	6	24

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	114	ALA
1	A	116	PHE
1	A	140	PRO
1	A	223	LYS
1	A	474	ASN
1	A	113	ASP
1	A	221	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	358	ARG
1	A	361	HIS
2	B	215	THR
1	A	115	TYR
1	A	139	THR
2	B	14	PRO
2	B	85	GLN
2	B	213	GLY
1	A	230	MET
2	B	116	PHE
2	B	404	GLU
1	A	13	LYS
2	B	166	LYS
1	A	44	GLU
1	A	91	GLN
1	A	14	PRO
1	A	420	PRO
2	B	195	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	480/499 (96%)	414 (86%)	66 (14%)	4	13
2	B	365/400 (91%)	340 (93%)	25 (7%)	20	49
All	All	845/899 (94%)	754 (89%)	91 (11%)	8	24

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	27	THR
1	A	32	LYS
1	A	40	GLU
1	A	49	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	64	LYS
1	A	73	LYS
1	A	86	ASP
1	A	90	VAL
1	A	92	LEU
1	A	94	ILE
1	A	120	LEU
1	A	122	GLU
1	A	123	ASP
1	A	138	GLU
1	A	140	PRO
1	A	143	ARG
1	A	205	LEU
1	A	206	ARG
1	A	211	ARG
1	A	217	PRO
1	A	221	HIS
1	A	228	LEU
1	A	229	TRP
1	A	244	ILE
1	A	255	ASN
1	A	264	LEU
1	A	266	TRP
1	A	268	SER
1	A	279	LEU
1	A	283	LEU
1	A	290	THR
1	A	308	GLU
1	A	340	GLN
1	A	344	GLU
1	A	356	ARG
1	A	358	ARG
1	A	362	THR
1	A	368	LEU
1	A	369	THR
1	A	386	THR
1	A	396	GLU
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	409	THR
1	A	415	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	422	LEU
1	A	431	LYS
1	A	443	ASP
1	A	448	ARG
1	A	452	LEU
1	A	458	VAL
1	A	459	THR
1	A	473	THR
1	A	475	GLN
1	A	487	GLN
1	A	491	LEU
1	A	496	VAL
1	A	497	THR
1	A	500	GLN
1	A	501	TYR
1	A	509	GLN
1	A	515	SER
1	A	517	LEU
1	A	539	HIS
2	B	14	PRO
2	B	40	GLU
2	B	55	PRO
2	B	73	LYS
2	B	138	GLU
2	B	139	THR
2	B	164	MET
2	B	167	ILE
2	B	193	LEU
2	B	194	GLU
2	B	201	LYS
2	B	209	LEU
2	B	211	ARG
2	B	215	THR
2	B	233	GLU
2	B	234	LEU
2	B	238	LYS
2	B	277	ARG
2	B	280	CYS
2	B	283	LEU
2	B	303	LEU
2	B	323	LYS
2	B	368	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	388	LYS
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	96	HIS
1	A	208	HIS
1	A	222	GLN
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	334	GLN
1	A	336	GLN
1	A	361	HIS
1	A	475	GLN
1	A	500	GLN
1	A	512	GLN
2	B	57	ASN
2	B	103	ASN
2	B	175	ASN
2	B	182	GLN
2	B	197	GLN
2	B	208	HIS
2	B	235	HIS
2	B	242	GLN
2	B	278	GLN
2	B	332	GLN
2	B	336	GLN
2	B	361	HIS
2	B	394	GLN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSD	A	280	1	3,7,8	0.67	0	3,8,10	1.26	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
1	CSD	A	280	1	-	0/2/6/8	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.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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
3	PO4	A	1300	-	4,4,4	1.14	0	6,6,6	0.27	0
4	GWJ	A	999	-	36,36,36	2.64	10 (27%)	51,52,52	1.62	8 (15%)

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
3	PO4	A	1300	-	-	0/0/0/0	0/0/0/0
4	GWJ	A	999	-	-	0/25/25/25	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	GWJ	C3-C2	-3.62	1.34	1.39
4	A	999	GWJ	C19-C18	-2.51	1.35	1.39
4	A	999	GWJ	C17-N1	-2.04	1.37	1.41
4	A	999	GWJ	C13-C8	2.09	1.42	1.39
4	A	999	GWJ	C3-C4	4.03	1.45	1.38
4	A	999	GWJ	C22-C21	5.05	1.47	1.38
4	A	999	GWJ	C19-C20	5.25	1.49	1.39
4	A	999	GWJ	C2-C1	6.09	1.52	1.40
4	A	999	GWJ	C5-C6	6.42	1.50	1.38
4	A	999	GWJ	C17-C18	7.09	1.53	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	GWJ	O5-S-O4	-4.98	111.80	118.80
4	A	999	GWJ	C20-S-N3	-3.48	103.84	108.45
4	A	999	GWJ	C22-C17-C18	-2.89	117.37	120.67
4	A	999	GWJ	C3-C4-CL	-2.05	116.60	119.14
4	A	999	GWJ	C2-C7-C8	2.21	123.24	119.47
4	A	999	GWJ	C15-O2-C1	2.37	122.99	117.58
4	A	999	GWJ	C15-C16-N1	2.53	120.29	115.77
4	A	999	GWJ	O5-S-N3	4.43	113.02	107.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	GWJ	5	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	535/560 (95%)	0.03	32 (5%) 25 18	37, 72, 116, 174	0
2	B	402/440 (91%)	0.04	24 (5%) 25 18	32, 69, 120, 148	0
All	All	937/1000 (93%)	0.03	56 (5%) 25 18	32, 71, 119, 174	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	SER	5.9
1	A	471	ASP	5.8
2	B	431	LYS	5.7
1	A	470	THR	5.4
1	A	2	ILE	5.4
1	A	137	ASN	5.3
1	A	52	PRO	4.7
1	A	136	ASN	4.6
1	A	455	ALA	4.0
2	B	104	LYS	4.0
2	B	214	LEU	3.8
1	A	452	LEU	3.8
1	A	472	THR	3.7
1	A	446	ALA	3.7
2	B	198	HIS	3.6
2	B	69	THR	3.6
1	A	1	PRO	3.5
1	A	469	LEU	3.5
1	A	447	ASN	3.4
2	B	356	ARG	3.4
1	A	450	THR	3.3
1	A	456	GLY	3.1
2	B	177	ASP	3.1
2	B	94	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	195	ILE	3.0
2	B	241	VAL	3.0
2	B	71	TRP	2.9
1	A	53	GLU	2.9
2	B	376	THR	2.9
1	A	358	ARG	2.9
1	A	464	GLN	2.8
2	B	8	VAL	2.8
1	A	71	TRP	2.8
2	B	105	SER	2.8
2	B	88	TRP	2.7
1	A	21	VAL	2.6
1	A	476	LYS	2.6
2	B	410	TRP	2.6
2	B	216	THR	2.6
2	B	70	LYS	2.6
1	A	245	VAL	2.5
1	A	221	HIS	2.5
1	A	491	LEU	2.5
1	A	91	GLN	2.4
1	A	28	GLU	2.4
2	B	240	THR	2.4
2	B	93	GLY	2.3
1	A	72	ARG	2.2
2	B	191	SER	2.2
1	A	24	TRP	2.2
1	A	467	VAL	2.1
1	A	69	THR	2.1
2	B	199	ARG	2.1
2	B	237	ASP	2.1
1	A	143	ARG	2.0
2	B	178	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	280	8/9	0.95	0.14	-	58,64,81,94	0

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
4	GWJ	A	999	34/34	0.97	0.17	-0.34	35,59,75,78	0
3	PO4	A	1300	5/5	0.85	0.21	-0.37	132,137,152,154	0

6.5 Other polymers [i](#)

There are no such residues in this entry.