



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:40 AM GMT

PDB ID : 2BE2
Title : Crystal structure of HIV-1 reverse transcriptase (RT) in complex with R221239
Authors : Himmel, D.M.; Das, K.; Clark Jr., A.D.; Hughes, S.H.; Benjahad, A.; Oumouch, S.; Guillemont, J.; Coupa, S.; Poncelet, A.; Csoka, I.; Meyer, C.; Andries, K.; Nguyen, C.H.; Grierson, D.S.; Arnold, E.
Deposited on : 2005-10-21
Resolution : 2.43 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

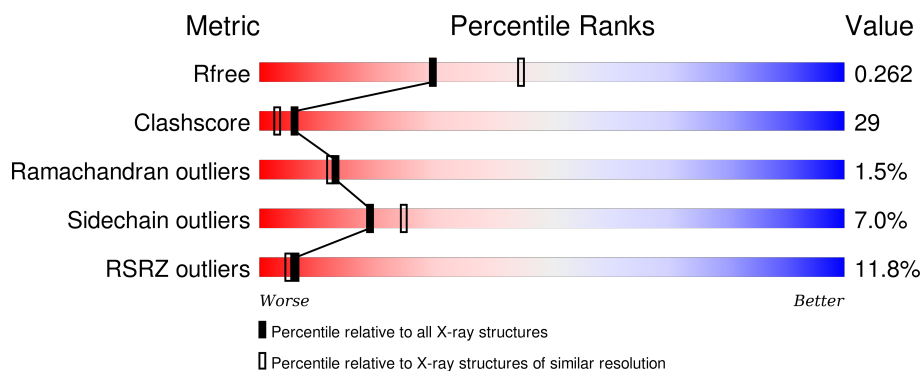
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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	
2	B	430	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SUC	A	2000	-	-	-	X
6	GOL	A	3001	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8262 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 P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4498	2913	748	830	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	ENGINEERED	UNP P03366

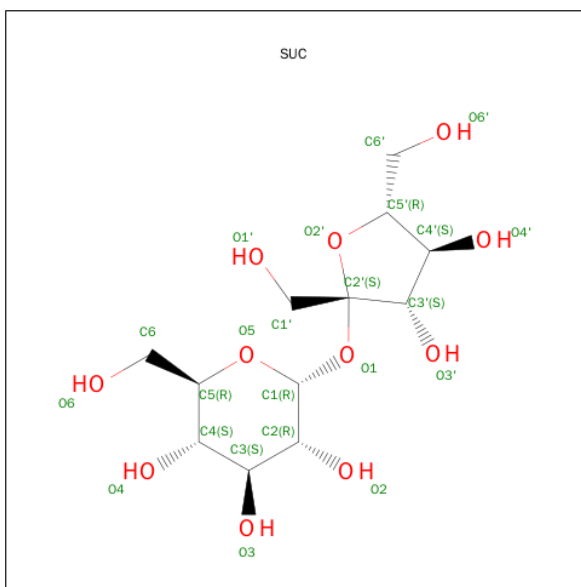
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	0	0
			3525	2297	584	637	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).

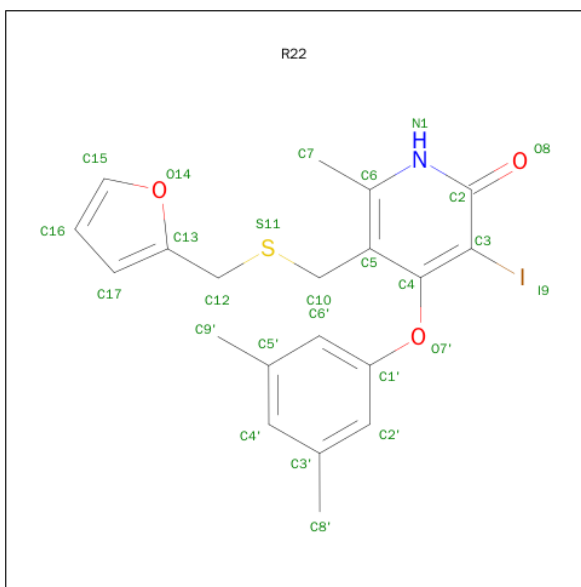


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		
3	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is 4-(3,5-DIMETHYLPHENOXY)-5-(FURAN-2-YLMETHYLSULFANYLM ETHYL)-3-iodo-6-METHYLPYRIDIN-2(1H)-ONE (three-letter code: R22) (formula: C₂₀H₂₀INO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	I	N	O	S	
			26	20	1	1	3	1	

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

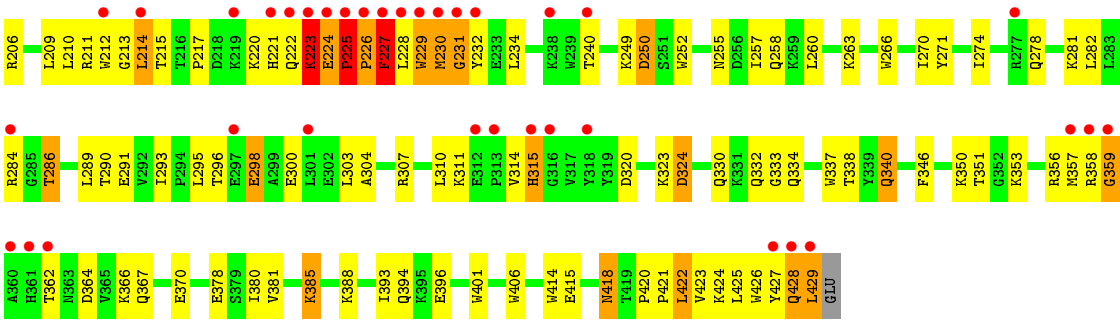


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O		
			6	3 3	0	0

6	A	1	Total	C O		
			6	3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	94	Total 94	O 94	0	0
7	B	60	Total 60	O 60	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.85Å 68.80Å 104.43Å 90.00° 107.22° 90.00°	Depositor
Resolution (Å)	22.95 – 2.43 22.94 – 2.43	Depositor EDS
% Data completeness (in resolution range)	88.4 (22.95-2.43) 88.4 (22.94-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.265 0.233 , 0.262	Depositor DCC
R_{free} test set	2554 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 69.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53398 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8262	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, MN, SUC, R22

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	0.44	0/4616	0.75	5/6271 (0.1%)
2	B	0.48	0/3629	0.89	21/4932 (0.4%)
All	All	0.46	0/8245	0.81	26/11203 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	67	ASP	N-CA-C	9.43	136.46	111.00
2	B	359	GLY	N-CA-C	-8.98	90.64	113.10
2	B	89	GLU	N-CA-C	-8.94	86.86	111.00
2	B	214	LEU	CB-CA-C	8.07	125.53	110.20
1	A	285	GLY	N-CA-C	-7.93	93.28	113.10
2	B	89	GLU	CB-CA-C	6.69	123.78	110.40
2	B	214	LEU	N-CA-C	-6.63	93.09	111.00
1	A	222	GLN	N-CA-C	-6.53	93.36	111.00
2	B	226	PRO	N-CA-C	6.49	128.98	112.10
2	B	85	GLN	N-CA-C	6.49	128.51	111.00
2	B	67	ASP	CB-CA-C	-6.27	97.85	110.40
2	B	86	ASP	N-CA-C	-6.17	94.33	111.00
2	B	86	ASP	CB-CA-C	6.14	122.67	110.40
2	B	87	PHE	C-N-CA	-5.89	106.97	121.70
2	B	231	GLY	N-CA-C	-5.63	99.02	113.10
2	B	93	GLY	N-CA-C	-5.61	99.06	113.10
2	B	88	TRP	N-CA-C	-5.57	95.96	111.00
2	B	223	LYS	N-CA-C	5.49	125.83	111.00
2	B	401	TRP	N-CA-C	5.44	125.69	111.00
2	B	229	TRP	N-CA-C	5.22	125.10	111.00
2	B	227	PHE	N-CA-C	5.13	124.85	111.00
2	B	68	SER	CB-CA-C	5.11	119.81	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	SER	N-CA-C	5.09	124.75	111.00
2	B	225	PRO	N-CA-C	-5.05	98.98	112.10
1	A	68	SER	C-N-CA	-5.04	109.09	121.70
1	A	67	ASP	N-CA-C	-5.01	97.47	111.00

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	4498	0	4560	277	0
2	B	3525	0	3562	198	0
3	A	23	0	22	2	0
3	B	23	0	22	0	0
4	A	1	0	0	0	0
5	A	26	0	20	3	0
6	A	12	0	16	5	0
7	A	94	0	0	5	0
7	B	60	0	0	3	0
All	All	8262	0	8202	465	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 29.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLY:O	1:A:334:GLN:HG2	1.20	1.31
2:B:88:TRP:H	2:B:90:VAL:HG23	1.08	1.13
1:A:296:THR:HG23	1:A:299:ALA:H	1.09	1.10
1:A:255:ASN:OD1	1:A:259:LYS:HE3	1.52	1.09
1:A:26:LEU:HG	1:A:27:THR:H	1.10	1.08
1:A:330:GLN:HE21	1:A:338:THR:HG23	1.17	1.08
2:B:224:GLU:HB3	2:B:225:PRO:HD3	1.20	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:OG	1:A:139:THR:HG22	1.53	1.05
1:A:134:SER:HB2	1:A:139:THR:O	1.55	1.05
2:B:11:LYS:H	2:B:11:LYS:HE2	1.12	1.05
2:B:257:ILE:HD12	2:B:293:ILE:HD11	1.41	1.01
1:A:296:THR:HG22	1:A:299:ALA:CB	1.90	1.01
2:B:90:VAL:O	2:B:90:VAL:HG12	1.58	1.01
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.41	0.99
1:A:253:THR:HG23	1:A:256:ASP:H	1.28	0.98
1:A:333:GLY:O	1:A:334:GLN:CG	2.11	0.97
2:B:63:ILE:HG21	2:B:406:TRP:O	1.64	0.97
2:B:68:SER:HB3	2:B:70:LYS:HE2	1.46	0.96
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.46	0.95
1:A:195:ILE:H	1:A:195:ILE:HD12	1.29	0.95
2:B:224:GLU:CB	2:B:225:PRO:HD3	1.96	0.93
2:B:65:LYS:HE3	2:B:70:LYS:HD2	1.49	0.93
1:A:50:ILE:HD12	1:A:55:PRO:HG2	1.49	0.92
2:B:85:GLN:CD	2:B:85:GLN:O	2.09	0.92
2:B:418:ASN:HD22	2:B:418:ASN:H	1.14	0.91
1:A:139:THR:OG1	1:A:140:PRO:HD2	1.69	0.91
1:A:258:GLN:HG2	1:A:283:LEU:HD21	1.50	0.91
2:B:206:ARG:HE	2:B:217:PRO:HG2	1.36	0.90
1:A:131:THR:CG2	1:A:143:ARG:HE	1.86	0.89
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.08	0.89
2:B:63:ILE:HG22	2:B:64:LYS:N	1.86	0.89
1:A:56:TYR:HD1	1:A:56:TYR:H	1.20	0.88
1:A:333:GLY:C	1:A:334:GLN:HG2	1.93	0.88
1:A:362:THR:HG22	1:A:363:ASN:H	1.39	0.87
2:B:11:LYS:N	2:B:11:LYS:HE2	1.90	0.86
2:B:84:THR:O	2:B:87:PHE:HE2	1.59	0.85
1:A:500:GLN:H	6:A:3001:GOL:H12	1.39	0.85
1:A:296:THR:HG22	1:A:299:ALA:HB2	1.54	0.85
1:A:296:THR:CG2	1:A:299:ALA:H	1.89	0.85
2:B:429:LEU:HD23	2:B:429:LEU:H	1.41	0.85
1:A:362:THR:HG22	1:A:363:ASN:N	1.92	0.85
2:B:270:ILE:HG22	2:B:314:VAL:HG21	1.58	0.85
2:B:63:ILE:HG22	2:B:64:LYS:H	1.42	0.85
2:B:13:LYS:NZ	2:B:86:ASP:HB2	1.92	0.85
1:A:54:ASN:ND2	1:A:54:ASN:O	2.09	0.84
1:A:296:THR:HG22	1:A:299:ALA:HB3	1.59	0.84
1:A:109:LEU:HB3	1:A:216:THR:CG2	2.06	0.84
1:A:296:THR:HG23	1:A:299:ALA:N	1.91	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:CG	1:A:27:THR:H	1.91	0.84
1:A:131:THR:HG23	1:A:143:ARG:HE	1.42	0.83
1:A:296:THR:CG2	1:A:299:ALA:CB	2.56	0.83
2:B:87:PHE:CG	2:B:87:PHE:O	2.31	0.82
1:A:26:LEU:HG	1:A:27:THR:N	1.92	0.82
1:A:282:LEU:HG	1:A:282:LEU:O	1.77	0.82
1:A:240:THR:HG22	1:A:241:VAL:H	1.44	0.82
1:A:478:GLU:HG2	1:A:499:SER:CB	2.09	0.82
1:A:500:GLN:N	6:A:3001:GOL:H12	1.93	0.82
1:A:134:SER:CB	1:A:139:THR:O	2.28	0.81
1:A:478:GLU:CG	1:A:499:SER:HB2	2.10	0.80
1:A:22:LYS:HE3	1:A:23:GLN:O	1.81	0.80
1:A:109:LEU:HB3	1:A:216:THR:HG22	1.64	0.79
2:B:252:TRP:NE1	2:B:295:LEU:HD11	1.96	0.79
1:A:56:TYR:N	1:A:56:TYR:CD1	2.47	0.79
2:B:27:THR:HG22	2:B:29:GLU:H	1.46	0.78
2:B:66:LYS:HD3	2:B:66:LYS:O	1.83	0.78
1:A:19:PRO:O	1:A:56:TYR:HB3	1.84	0.78
1:A:343:GLN:HG3	1:A:349:LEU:HD21	1.63	0.78
2:B:88:TRP:N	2:B:90:VAL:HG23	1.94	0.78
2:B:257:ILE:CD1	2:B:293:ILE:HD11	2.13	0.78
1:A:308:GLU:OE1	1:A:311:LYS:HD2	1.83	0.78
1:A:342:TYR:HA	1:A:349:LEU:HD23	1.65	0.78
2:B:68:SER:O	2:B:69:THR:OG1	2.02	0.77
1:A:253:THR:HG22	1:A:256:ASP:OD2	1.84	0.77
1:A:218:ASP:C	1:A:220:LYS:H	1.87	0.77
1:A:296:THR:CG2	1:A:299:ALA:HB2	2.14	0.76
1:A:330:GLN:NE2	1:A:338:THR:HG23	1.97	0.76
2:B:90:VAL:O	2:B:90:VAL:CG1	2.30	0.76
2:B:67:ASP:C	2:B:69:THR:H	1.85	0.75
1:A:195:ILE:O	1:A:199:ARG:HG3	1.87	0.75
1:A:63:ILE:HG23	1:A:64:LYS:HE2	1.68	0.75
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.67	0.75
2:B:63:ILE:CG2	2:B:64:LYS:H	2.00	0.74
1:A:88:TRP:HD1	7:A:1154:HOH:O	1.69	0.74
1:A:240:THR:HG22	1:A:241:VAL:N	2.01	0.73
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.23	0.73
1:A:257:ILE:CG2	1:A:283:LEU:HD13	2.18	0.73
2:B:227:PHE:HD2	2:B:228:LEU:HG	1.52	0.73
1:A:344:GLU:OE1	1:A:347:LYS:HD2	1.88	0.73
1:A:50:ILE:HD12	1:A:55:PRO:CG	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.54	0.72
1:A:217:PRO:HB3	1:A:222:GLN:HG2	1.72	0.72
1:A:369:THR:HG1	1:A:398:TRP:HZ3	1.37	0.72
2:B:63:ILE:CG2	2:B:64:LYS:N	2.53	0.71
2:B:388:LYS:HE2	2:B:415:GLU:OE1	1.92	0.70
2:B:12:LEU:CD2	2:B:84:THR:HG22	2.22	0.70
1:A:547:GLN:HG3	2:B:286:THR:HG22	1.74	0.70
1:A:348:ASN:OD1	3:A:2000:SUC:H61	1.91	0.70
2:B:250:ASP:OD2	2:B:250:ASP:N	2.25	0.70
2:B:91:GLN:O	2:B:92:LEU:HG	1.92	0.69
2:B:85:GLN:CG	2:B:85:GLN:O	2.38	0.69
1:A:254:VAL:HB	1:A:288:ALA:O	1.91	0.69
1:A:366:LYS:O	1:A:370:GLU:HG3	1.91	0.69
2:B:282:LEU:HB3	2:B:293:ILE:HD12	1.73	0.69
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.20	0.69
1:A:132:ILE:HG12	1:A:142:ILE:HG12	1.75	0.69
1:A:197:GLN:O	1:A:200:THR:HB	1.93	0.69
1:A:253:THR:HG22	1:A:256:ASP:CG	2.14	0.68
1:A:362:THR:CG2	1:A:363:ASN:H	2.06	0.68
2:B:84:THR:O	2:B:87:PHE:CE2	2.45	0.68
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.76	0.68
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.76	0.68
2:B:65:LYS:HE3	2:B:70:LYS:CD	2.23	0.67
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.29	0.67
1:A:139:THR:CB	1:A:140:PRO:HD2	2.25	0.67
1:A:92:LEU:HD12	1:A:93:GLY:N	2.09	0.67
2:B:232:TYR:CE2	2:B:234:LEU:HD21	2.31	0.66
2:B:223:LYS:N	2:B:229:TRP:O	2.29	0.66
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.11	0.66
2:B:420:PRO:HD2	2:B:422:LEU:HD23	1.77	0.66
2:B:13:LYS:HZ2	2:B:86:ASP:HB2	1.56	0.66
2:B:249:LYS:HB2	2:B:252:TRP:NE1	2.11	0.65
2:B:314:VAL:HG12	2:B:315:HIS:N	2.12	0.65
1:A:109:LEU:HB3	1:A:216:THR:HG21	1.78	0.65
2:B:223:LYS:HA	2:B:229:TRP:HB2	1.77	0.65
1:A:501:TYR:HB2	6:A:3001:GOL:O2	1.95	0.65
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.61	0.65
2:B:96:HIS:HE1	2:B:381:VAL:O	1.80	0.65
2:B:87:PHE:O	2:B:87:PHE:CD2	2.49	0.65
1:A:22:LYS:HD2	1:A:23:GLN:H	1.62	0.64
2:B:222:GLN:HA	2:B:229:TRP:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:THR:HG21	2:B:124:PHE:HZ	1.62	0.64
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.32	0.64
2:B:418:ASN:N	2:B:418:ASN:HD22	1.85	0.64
1:A:362:THR:CG2	1:A:363:ASN:N	2.61	0.64
1:A:65:LYS:HE2	1:A:67:ASP:HB3	1.78	0.64
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.27	0.64
2:B:281:LYS:HA	2:B:284:ARG:NH1	2.13	0.64
2:B:6:GLU:O	2:B:6:GLU:HG3	1.98	0.64
1:A:503:LEU:HD12	1:A:533:LEU:CD1	2.28	0.64
1:A:19:PRO:O	1:A:56:TYR:CB	2.47	0.63
1:A:88:TRP:CD1	7:A:1154:HOH:O	2.46	0.63
1:A:317:VAL:HG12	1:A:348:ASN:O	1.99	0.63
1:A:265:ASN:O	1:A:268:SER:HB3	1.98	0.63
1:A:348:ASN:OD1	3:A:2000:SUC:C6	2.47	0.63
1:A:17:ASP:O	1:A:83:ARG:HD3	1.99	0.63
1:A:134:SER:OG	1:A:135:ILE:N	2.32	0.63
1:A:257:ILE:HD12	1:A:293:ILE:HD12	1.81	0.62
2:B:296:THR:HB	2:B:298:GLU:OE2	1.99	0.62
1:A:330:GLN:HE21	1:A:338:THR:CG2	2.04	0.62
2:B:314:VAL:HG12	2:B:315:HIS:H	1.64	0.62
1:A:63:ILE:HG22	1:A:64:LYS:N	2.15	0.62
2:B:13:LYS:HE3	2:B:86:ASP:H	1.64	0.61
2:B:227:PHE:O	2:B:228:LEU:HD23	2.01	0.61
2:B:63:ILE:CG2	2:B:406:TRP:O	2.46	0.61
2:B:85:GLN:O	2:B:85:GLN:NE2	2.32	0.61
1:A:317:VAL:HG22	1:A:318:TYR:N	2.15	0.61
1:A:54:ASN:O	1:A:55:PRO:C	2.36	0.61
1:A:109:LEU:HD13	1:A:216:THR:HG21	1.82	0.61
1:A:342:TYR:HA	1:A:349:LEU:CD2	2.30	0.61
1:A:73:LYS:NZ	1:A:130:PHE:CE2	2.67	0.61
2:B:67:ASP:C	2:B:69:THR:N	2.51	0.61
1:A:51:GLY:HA3	1:A:53:GLU:OE1	2.01	0.61
2:B:126:LYS:HG2	2:B:127:TYR:N	2.15	0.61
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.35	0.61
1:A:460:ASN:H	1:A:460:ASN:HD22	1.49	0.60
1:A:255:ASN:OD1	1:A:259:LYS:CE	2.40	0.60
1:A:54:ASN:H	1:A:55:PRO:HD3	1.65	0.60
1:A:112:GLY:O	1:A:113:ASP:HB2	1.99	0.60
2:B:220:LYS:HD2	2:B:231:GLY:O	2.02	0.60
2:B:324:ASP:OD1	2:B:324:ASP:N	2.26	0.60
1:A:253:THR:OG1	1:A:290:THR:HA	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:ILE:HG23	2:B:119:PRO:HG3	1.82	0.60
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.16	0.60
1:A:547:GLN:HG3	2:B:286:THR:CG2	2.31	0.60
1:A:55:PRO:HB3	1:A:129:ALA:HB2	1.82	0.60
2:B:13:LYS:HZ1	2:B:86:ASP:HB2	1.64	0.60
1:A:439:THR:H	1:A:460:ASN:ND2	2.00	0.59
2:B:5:ILE:HG22	2:B:7:THR:HG23	1.84	0.59
2:B:63:ILE:HD13	2:B:406:TRP:HB3	1.84	0.59
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.83	0.59
2:B:210:LEU:HD13	2:B:217:PRO:HD2	1.83	0.59
2:B:224:GLU:HB3	2:B:225:PRO:CD	2.14	0.59
2:B:68:SER:CB	2:B:70:LYS:HE2	2.28	0.59
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.85	0.59
1:A:134:SER:CB	1:A:139:THR:HG22	2.33	0.59
1:A:518:VAL:O	1:A:522:ILE:HG13	2.02	0.59
1:A:50:ILE:CD1	1:A:55:PRO:HG2	2.27	0.59
1:A:63:ILE:CG2	1:A:64:LYS:N	2.66	0.59
1:A:181:TYR:CZ	2:B:138:GLU:HG3	2.38	0.59
1:A:253:THR:HG23	1:A:256:ASP:N	2.10	0.58
2:B:249:LYS:CB	2:B:252:TRP:CE2	2.84	0.58
2:B:266:TRP:CG	2:B:425:LEU:HD13	2.38	0.58
2:B:88:TRP:CH2	2:B:159:ILE:CG1	2.86	0.58
1:A:132:ILE:CG1	1:A:142:ILE:HG12	2.34	0.57
1:A:454:LYS:HB2	1:A:552:VAL:HG13	1.85	0.57
2:B:266:TRP:CE3	2:B:425:LEU:HB3	2.39	0.57
1:A:411:ILE:HG22	1:A:412:PRO:O	2.04	0.57
1:A:478:GLU:CG	1:A:499:SER:CB	2.79	0.57
1:A:253:THR:CG2	1:A:256:ASP:H	2.09	0.57
1:A:240:THR:CG2	1:A:241:VAL:H	2.15	0.57
1:A:376:THR:HG23	1:A:386:THR:HG22	1.85	0.57
2:B:263:LYS:HA	2:B:425:LEU:HD22	1.86	0.56
2:B:12:LEU:HD22	2:B:84:THR:HG22	1.87	0.56
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.87	0.56
2:B:88:TRP:CH2	2:B:159:ILE:HG13	2.40	0.56
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.87	0.56
2:B:249:LYS:HB2	2:B:252:TRP:CZ2	2.41	0.56
1:A:132:ILE:HD11	1:A:142:ILE:CD1	2.36	0.56
1:A:34:LEU:HD13	1:A:132:ILE:HG22	1.87	0.56
1:A:65:LYS:HB3	1:A:70:LYS:O	2.06	0.56
2:B:307:ARG:O	2:B:311:LYS:HG3	2.05	0.55
2:B:258:GLN:NE2	7:B:1061:HOH:O	2.30	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:LEU:CD1	2:B:217:PRO:HD2	2.37	0.55
1:A:288:ALA:CB	1:A:291:GLU:HB2	2.37	0.55
2:B:11:LYS:HE3	2:B:87:PHE:CZ	2.42	0.55
1:A:223:LYS:HD2	1:A:225:PRO:HD3	1.88	0.55
2:B:284:ARG:NH1	2:B:284:ARG:HG3	2.22	0.54
1:A:139:THR:OG1	1:A:140:PRO:CD	2.49	0.54
1:A:195:ILE:H	1:A:195:ILE:CD1	2.06	0.54
1:A:194:GLU:OE1	1:A:197:GLN:NE2	2.40	0.54
2:B:420:PRO:HD2	2:B:422:LEU:CD2	2.37	0.54
1:A:3:SER:HB2	1:A:117:SER:O	2.06	0.54
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.89	0.54
1:A:5:ILE:HD13	1:A:163:SER:HB3	1.89	0.54
1:A:139:THR:HG1	1:A:140:PRO:HD2	1.73	0.54
2:B:65:LYS:HB3	2:B:72:ARG:HH11	1.73	0.54
1:A:279:LEU:HD21	1:A:299:ALA:O	2.07	0.53
1:A:257:ILE:HG21	1:A:283:LEU:HD13	1.89	0.53
1:A:317:VAL:CG2	1:A:318:TYR:N	2.72	0.53
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.55	0.53
1:A:364:ASP:CB	1:A:423:VAL:HG13	2.39	0.53
1:A:221:HIS:HB2	1:A:223:LYS:CG	2.38	0.53
1:A:94:ILE:HD11	1:A:183:TYR:CZ	2.44	0.53
1:A:201:LYS:O	1:A:204:GLU:HB2	2.09	0.52
1:A:254:VAL:CB	1:A:288:ALA:O	2.56	0.52
1:A:368:LEU:HD22	1:A:423:VAL:HG21	1.91	0.52
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.91	0.52
2:B:420:PRO:O	2:B:422:LEU:N	2.40	0.52
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.09	0.52
1:A:22:LYS:HD2	1:A:23:GLN:N	2.23	0.52
1:A:503:LEU:HD11	1:A:507:GLN:OE1	2.09	0.52
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.43	0.52
2:B:394:GLN:HE21	2:B:396:GLU:HB2	1.74	0.52
1:A:102:LYS:O	1:A:103:LYS:HD2	2.10	0.52
2:B:10:VAL:HG22	2:B:88:TRP:CZ2	2.45	0.52
2:B:68:SER:C	2:B:69:THR:HG1	2.10	0.52
2:B:230:MET:O	2:B:232:TYR:N	2.43	0.52
1:A:177:ASP:OD1	1:A:178:ILE:HG12	2.10	0.51
2:B:298:GLU:CD	2:B:298:GLU:H	2.14	0.51
2:B:333:GLY:O	2:B:334:GLN:HB2	2.10	0.51
2:B:206:ARG:HE	2:B:217:PRO:CG	2.17	0.51
2:B:88:TRP:CZ3	2:B:159:ILE:HG13	2.46	0.51
2:B:249:LYS:HG3	2:B:252:TRP:CD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:TRP:HH2	2:B:159:ILE:HD11	1.75	0.51
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.93	0.51
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.46	0.51
2:B:393:ILE:HG12	2:B:394:GLN:N	2.26	0.51
1:A:369:THR:OG1	1:A:398:TRP:HZ3	1.92	0.50
1:A:151:GLN:NE2	7:A:1066:HOH:O	2.44	0.50
2:B:23:GLN:OE1	2:B:60:VAL:HG22	2.11	0.50
1:A:50:ILE:HG21	1:A:145:GLN:HB3	1.93	0.50
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.93	0.50
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.11	0.50
1:A:55:PRO:CB	1:A:129:ALA:HB2	2.41	0.50
1:A:295:LEU:HD23	1:A:300:GLU:HG2	1.93	0.50
1:A:257:ILE:HD12	1:A:293:ILE:CD1	2.41	0.49
1:A:288:ALA:HB3	1:A:291:GLU:CB	2.42	0.49
1:A:544:GLY:HA2	2:B:286:THR:HB	1.94	0.49
2:B:220:LYS:HB2	2:B:231:GLY:H	1.77	0.49
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.48	0.49
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.42	0.49
2:B:80:LEU:HD11	2:B:84:THR:HG21	1.94	0.49
2:B:252:TRP:CG	2:B:295:LEU:HD21	2.48	0.49
1:A:296:THR:CG2	1:A:299:ALA:HB3	2.31	0.49
1:A:378:GLU:HG2	1:A:382:ILE:HD12	1.93	0.49
2:B:212:TRP:HA	2:B:212:TRP:CE3	2.47	0.49
2:B:6:GLU:O	2:B:6:GLU:CG	2.61	0.49
1:A:218:ASP:C	1:A:220:LYS:N	2.56	0.49
2:B:393:ILE:HG12	2:B:394:GLN:H	1.76	0.49
2:B:175:ASN:OD1	2:B:201:LYS:HD2	2.13	0.49
1:A:447:ASN:O	1:A:451:LYS:HA	2.12	0.49
1:A:55:PRO:CB	1:A:129:ALA:CB	2.90	0.48
2:B:88:TRP:CH2	2:B:159:ILE:HD11	2.48	0.48
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.94	0.48
2:B:350:LYS:NZ	2:B:378:GLU:OE1	2.46	0.48
2:B:65:LYS:CE	2:B:70:LYS:HD2	2.33	0.48
1:A:516:GLU:H	1:A:516:GLU:CD	2.15	0.48
1:A:194:GLU:H	1:A:194:GLU:CD	2.16	0.48
1:A:142:ILE:HD11	1:A:144:TYR:HE1	1.78	0.48
1:A:129:ALA:HA	1:A:144:TYR:O	2.14	0.48
1:A:103:LYS:HE2	1:A:179:VAL:HG21	1.94	0.48
1:A:516:GLU:O	1:A:520:GLN:HG3	2.12	0.48
1:A:324:ASP:HA	7:A:1014:HOH:O	2.13	0.48
1:A:142:ILE:HD11	1:A:144:TYR:CE1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HD11	1:A:183:TYR:CE1	2.48	0.48
1:A:516:GLU:HG2	1:A:517:LEU:N	2.29	0.48
1:A:126:LYS:HE2	1:A:127:TYR:CZ	2.48	0.48
1:A:542:ILE:HD12	1:A:542:ILE:N	2.29	0.48
1:A:418:ASN:HD22	1:A:418:ASN:C	2.17	0.48
1:A:139:THR:HG23	1:A:141:GLY:H	1.78	0.47
1:A:55:PRO:HB3	1:A:129:ALA:CB	2.45	0.47
1:A:131:THR:HG21	1:A:143:ARG:HE	1.73	0.47
2:B:97:PRO:HD2	2:B:181:TYR:CD1	2.50	0.47
2:B:346:PHE:CD2	2:B:346:PHE:N	2.79	0.47
2:B:418:ASN:N	2:B:418:ASN:ND2	2.57	0.47
2:B:230:MET:O	2:B:231:GLY:C	2.50	0.47
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.97	0.47
2:B:252:TRP:HE1	2:B:295:LEU:HD11	1.76	0.47
1:A:63:ILE:HG22	1:A:64:LYS:O	2.15	0.47
1:A:194:GLU:O	1:A:197:GLN:N	2.47	0.47
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.49	0.47
1:A:255:ASN:HB2	1:A:289:LEU:O	2.15	0.47
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.12	0.47
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.96	0.47
2:B:366:LYS:O	2:B:370:GLU:HG3	2.15	0.47
2:B:252:TRP:CD1	2:B:295:LEU:HD21	2.50	0.47
1:A:66:LYS:O	1:A:66:LYS:HG2	2.15	0.47
1:A:134:SER:O	1:A:135:ILE:C	2.53	0.47
1:A:537:PRO:HB2	1:A:540:LYS:HG3	1.96	0.47
1:A:3:SER:HA	1:A:4:PRO:HD3	1.67	0.47
2:B:358:ARG:C	2:B:359:GLY:O	2.49	0.47
2:B:85:GLN:NE2	2:B:154:LYS:HD3	2.30	0.46
2:B:92:LEU:HD23	2:B:92:LEU:HA	1.80	0.46
1:A:254:VAL:HA	1:A:293:ILE:CD1	2.45	0.46
1:A:282:LEU:CG	1:A:282:LEU:O	2.54	0.46
2:B:271:TYR:HB2	2:B:274:ILE:CD1	2.45	0.46
2:B:11:LYS:H	2:B:11:LYS:CE	2.04	0.46
1:A:132:ILE:HD11	1:A:142:ILE:HD11	1.97	0.46
1:A:216:THR:HG22	1:A:217:PRO:HD3	1.97	0.46
1:A:23:GLN:OE1	1:A:60:VAL:HG23	2.14	0.46
1:A:320:ASP:O	1:A:343:GLN:NE2	2.48	0.46
2:B:91:GLN:HG3	2:B:91:GLN:O	2.15	0.46
2:B:224:GLU:CB	2:B:225:PRO:CD	2.82	0.46
1:A:72:ARG:HD2	1:A:72:ARG:HA	1.74	0.46
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LYS:O	2:B:67:ASP:HB2	2.16	0.46
1:A:54:ASN:CG	1:A:54:ASN:O	2.53	0.46
1:A:454:LYS:HD2	1:A:552:VAL:O	2.16	0.46
1:A:50:ILE:CG2	1:A:145:GLN:HB3	2.46	0.45
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.97	0.45
2:B:175:ASN:HB3	2:B:178:ILE:HD12	1.98	0.45
1:A:546:GLU:OE1	1:A:546:GLU:HA	2.15	0.45
1:A:407:GLN:NE2	7:A:1033:HOH:O	2.49	0.45
2:B:427:TYR:CD1	2:B:428:GLN:O	2.68	0.45
2:B:337:TRP:O	2:B:353:LYS:HA	2.15	0.45
1:A:169:GLU:N	1:A:170:PRO:HD2	2.31	0.45
1:A:500:GLN:H	6:A:3001:GOL:C1	2.21	0.45
1:A:308:GLU:O	1:A:311:LYS:HB2	2.16	0.45
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.96	0.45
1:A:36:GLU:O	1:A:39:THR:HG22	2.15	0.45
1:A:229:TRP:O	1:A:232:TYR:HB2	2.16	0.45
2:B:63:ILE:HD12	2:B:74:LEU:HD22	1.99	0.45
1:A:65:LYS:C	1:A:67:ASP:H	2.20	0.45
1:A:103:LYS:HE2	1:A:179:VAL:CG2	2.46	0.45
2:B:332:GLN:HE22	2:B:423:VAL:HB	1.81	0.45
1:A:1:PRO:C	1:A:2:ILE:HG12	2.36	0.45
2:B:206:ARG:NE	2:B:217:PRO:HG2	2.17	0.45
1:A:236:PRO:HA	5:A:4002:R22:C15	2.47	0.45
1:A:49:LYS:HG3	1:A:144:TYR:CE2	2.52	0.45
1:A:408:ALA:O	2:B:393:ILE:HG13	2.16	0.45
2:B:12:LEU:HD23	2:B:84:THR:HG22	1.97	0.45
1:A:55:PRO:HB2	1:A:129:ALA:CB	2.46	0.45
1:A:65:LYS:HG2	1:A:67:ASP:HB3	1.99	0.45
1:A:301:LEU:O	1:A:305:GLU:HG3	2.17	0.45
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.98	0.45
2:B:314:VAL:CG1	2:B:315:HIS:N	2.80	0.45
2:B:300:GLU:OE1	2:B:304:ALA:HB2	2.17	0.45
1:A:94:ILE:HG23	1:A:229:TRP:HH2	1.81	0.44
2:B:388:LYS:NZ	7:B:1132:HOH:O	2.50	0.44
1:A:447:ASN:O	1:A:451:LYS:N	2.51	0.44
1:A:470:THR:O	1:A:471:ASN:C	2.55	0.44
1:A:438:GLU:OE2	1:A:461:LYS:HB2	2.17	0.44
1:A:457:TYR:CD2	1:A:457:TYR:C	2.91	0.44
1:A:255:ASN:O	1:A:259:LYS:HG3	2.18	0.44
1:A:35:VAL:HG22	1:A:132:ILE:HD12	2.00	0.44
1:A:454:LYS:CB	1:A:552:VAL:HG13	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:N	2:B:282:LEU:HD12	2.33	0.44
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.53	0.44
1:A:183:TYR:OH	1:A:230:MET:HE1	2.17	0.44
2:B:271:TYR:HB2	2:B:274:ILE:HD11	1.99	0.44
1:A:206:ARG:NH1	1:A:217:PRO:O	2.50	0.44
1:A:368:LEU:O	1:A:372:VAL:HG23	2.18	0.44
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.99	0.44
1:A:77:PHE:O	1:A:80:LEU:N	2.51	0.44
1:A:298:GLU:H	1:A:298:GLU:CD	2.21	0.43
1:A:357:MET:O	1:A:358:ARG:HB2	2.17	0.43
2:B:65:LYS:HE3	2:B:70:LYS:CE	2.48	0.43
2:B:340:GLN:NE2	7:B:1043:HOH:O	2.51	0.43
2:B:12:LEU:HD23	2:B:124:PHE:HE1	1.84	0.43
2:B:80:LEU:CD1	2:B:84:THR:CG2	2.97	0.43
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.53	0.43
1:A:497:THR:O	1:A:535:TRP:HA	2.19	0.43
2:B:156:SER:N	2:B:157:PRO:HD2	2.32	0.43
2:B:163:SER:O	2:B:167:ILE:HG13	2.18	0.43
2:B:213:GLY:CA	2:B:215:THR:HG23	2.49	0.43
2:B:252:TRP:CE2	2:B:295:LEU:HD11	2.53	0.43
2:B:220:LYS:O	2:B:230:MET:HA	2.19	0.43
1:A:503:LEU:HD12	1:A:533:LEU:HD12	2.00	0.43
1:A:325:LEU:HB3	1:A:387:PRO:HB3	2.00	0.43
2:B:214:LEU:HD23	2:B:214:LEU:HA	1.54	0.43
1:A:314:VAL:HG12	1:A:315:HIS:N	2.34	0.43
1:A:148:VAL:O	1:A:150:PRO:HD3	2.18	0.43
1:A:500:GLN:HB2	6:A:3001:GOL:C1	2.49	0.43
2:B:212:TRP:HE3	2:B:212:TRP:HA	1.84	0.43
2:B:206:ARG:CZ	2:B:206:ARG:HB3	2.46	0.42
1:A:547:GLN:HG2	1:A:547:GLN:H	1.60	0.42
1:A:31:ILE:O	1:A:35:VAL:HG23	2.19	0.42
2:B:87:PHE:CD2	2:B:87:PHE:C	2.93	0.42
1:A:227:PHE:CD2	5:A:4002:R22:H122	2.54	0.42
1:A:451:LYS:HB3	1:A:451:LYS:HE2	1.82	0.42
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.50	0.42
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.54	0.42
1:A:317:VAL:CG2	1:A:318:TYR:H	2.31	0.42
2:B:220:LYS:HB2	2:B:231:GLY:N	2.34	0.42
2:B:105:SER:O	2:B:190:GLY:HA2	2.20	0.42
2:B:323:LYS:O	2:B:385:LYS:NZ	2.53	0.42
2:B:11:LYS:N	2:B:11:LYS:CE	2.71	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:HA	2:B:87:PHE:HD2	1.84	0.42
1:A:406:TRP:CH2	1:A:407:GLN:OE1	2.73	0.42
1:A:364:ASP:OD2	1:A:512:LYS:NZ	2.45	0.42
1:A:65:LYS:CE	1:A:67:ASP:HB3	2.47	0.42
1:A:503:LEU:HD12	1:A:533:LEU:HD11	2.01	0.42
2:B:257:ILE:HD12	2:B:293:ILE:CD1	2.30	0.42
1:A:257:ILE:HB	1:A:283:LEU:CD1	2.50	0.42
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.84	0.42
2:B:213:GLY:HA3	2:B:215:THR:HG23	2.02	0.42
2:B:96:HIS:CE1	2:B:381:VAL:O	2.68	0.41
2:B:350:LYS:HG2	2:B:351:THR:N	2.34	0.41
2:B:300:GLU:HA	2:B:303:LEU:HB3	2.00	0.41
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.50	0.41
2:B:320:ASP:C	2:B:320:ASP:OD1	2.57	0.41
2:B:84:THR:CG2	2:B:124:PHE:HZ	2.32	0.41
2:B:222:GLN:C	2:B:229:TRP:O	2.58	0.41
2:B:422:LEU:HD12	2:B:426:TRP:CD1	2.56	0.41
2:B:423:VAL:HG23	2:B:424:LYS:N	2.36	0.41
1:A:142:ILE:CD1	1:A:144:TYR:CE1	3.03	0.41
2:B:424:LYS:HA	2:B:427:TYR:HD2	1.85	0.41
2:B:290:THR:O	2:B:291:GLU:C	2.58	0.41
1:A:470:THR:CG2	1:A:471:ASN:N	2.83	0.41
2:B:80:LEU:HD12	2:B:84:THR:HG23	2.02	0.41
1:A:131:THR:HG22	1:A:143:ARG:HG2	2.03	0.41
1:A:113:ASP:O	1:A:114:ALA:C	2.58	0.41
1:A:223:LYS:C	1:A:223:LYS:HD2	2.40	0.41
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.01	0.41
2:B:209:LEU:HB3	2:B:215:THR:OG1	2.21	0.41
1:A:291:GLU:OE1	1:A:292:VAL:O	2.39	0.41
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.77	0.41
2:B:13:LYS:O	2:B:16:MET:HB2	2.21	0.41
1:A:254:VAL:HA	1:A:293:ILE:HD12	2.03	0.41
1:A:439:THR:H	1:A:460:ASN:HD21	1.66	0.41
1:A:416:PHE:CE2	1:A:418:ASN:HB2	2.56	0.41
1:A:115:TYR:CD2	1:A:156:SER:HB3	2.56	0.40
1:A:10:VAL:HG12	1:A:11:LYS:N	2.36	0.40
1:A:360:ALA:HB3	1:A:361:HIS:NE2	2.36	0.40
1:A:406:TRP:CH2	2:B:418:ASN:CA	3.01	0.40
1:A:100:LEU:HD21	5:A:4002:R22:H9'1	2.02	0.40
2:B:330:GLN:NE2	2:B:340:GLN:OE1	2.55	0.40
1:A:240:THR:CG2	1:A:241:VAL:N	2.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:HIS:C	1:A:223:LYS:H	2.24	0.40
1:A:1:PRO:HB2	1:A:46:LYS:CE	2.52	0.40
2:B:278:GLN:OE1	2:B:278:GLN:HA	2.21	0.40
2:B:195:ILE:HG13	2:B:195:ILE:H	1.58	0.40
1:A:35:VAL:O	1:A:39:THR:HG22	2.22	0.40
1:A:194:GLU:O	1:A:196:GLY:N	2.55	0.40
2:B:30:LYS:HB3	2:B:62:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/560 (98%)	497 (90%)	45 (8%)	8 (2%)	13	12
2	B	424/430 (99%)	371 (88%)	46 (11%)	7 (2%)	11	10
All	All	974/990 (98%)	868 (89%)	91 (9%)	15 (2%)	13	12

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	54	ASN
1	A	2	ILE
1	A	195	ILE
2	B	221	HIS
1	A	56	TYR
2	B	226	PRO
1	A	27	THR
1	A	243	PRO
1	A	471	ASN
2	B	421	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	223	LYS
2	B	224	GLU
2	B	176	PRO
2	B	225	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	494/500 (99%)	461 (93%)	33 (7%)	20	26
2	B	388/392 (99%)	359 (92%)	29 (8%)	17	22
All	All	882/892 (99%)	820 (93%)	62 (7%)	19	25

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	46	LYS
1	A	56	TYR
1	A	64	LYS
1	A	68	SER
1	A	73	LYS
1	A	94	ILE
1	A	105	SER
1	A	110	ASP
1	A	122	GLU
1	A	137	ASN
1	A	139	THR
1	A	142	ILE
1	A	162	SER
1	A	216	THR
1	A	221	HIS
1	A	223	LYS
1	A	224	GLU
1	A	244	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	277	ARG
1	A	281	LYS
1	A	282	LEU
1	A	287	LYS
1	A	291	GLU
1	A	295	LEU
1	A	357	MET
1	A	361	HIS
1	A	414	TRP
1	A	418	ASN
1	A	460	ASN
1	A	529	GLU
1	A	547	GLN
1	A	551	LEU
2	B	11	LYS
2	B	55	PRO
2	B	69	THR
2	B	86	ASP
2	B	87	PHE
2	B	88	TRP
2	B	89	GLU
2	B	91	GLN
2	B	101	LYS
2	B	109	LEU
2	B	187	LEU
2	B	211	ARG
2	B	227	PHE
2	B	230	MET
2	B	240	THR
2	B	250	ASP
2	B	286	THR
2	B	298	GLU
2	B	315	HIS
2	B	324	ASP
2	B	340	GLN
2	B	356	ARG
2	B	357	MET
2	B	385	LYS
2	B	414	TRP
2	B	418	ASN
2	B	422	LEU
2	B	428	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	429	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	91	GLN
1	A	137	ASN
1	A	182	GLN
1	A	197	GLN
1	A	208	HIS
1	A	258	GLN
1	A	315	HIS
1	A	330	GLN
1	A	340	GLN
1	A	407	GLN
1	A	418	ASN
1	A	428	GLN
1	A	460	ASN
1	A	509	GLN
2	B	85	GLN
2	B	91	GLN
2	B	96	HIS
2	B	182	GLN
2	B	258	GLN
2	B	330	GLN
2	B	332	GLN
2	B	340	GLN
2	B	394	GLN
2	B	418	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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	SUC	A	2000	-	24,24,24	1.42	5 (20%)	36,36,36	0.90	1 (2%)
6	GOL	A	3000	-	5,5,5	0.54	0	5,5,5	0.39	0
6	GOL	A	3001	-	5,5,5	0.54	0	5,5,5	0.39	0
5	R22	A	4002	-	25,28,28	1.99	10 (40%)	29,39,39	2.09	6 (20%)
3	SUC	B	2001	-	24,24,24	1.01	2 (8%)	36,36,36	1.10	1 (2%)

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	SUC	A	2000	-	-	0/12/51/51	0/2/2/2
6	GOL	A	3000	-	-	0/4/4/4	0/0/0/0
6	GOL	A	3001	-	-	0/4/4/4	0/0/0/0
5	R22	A	4002	-	-	0/9/10/10	0/2/3/3
3	SUC	B	2001	-	-	0/12/51/51	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4002	R22	C3-I9	-3.45	2.02	2.10
5	A	4002	R22	C12-S11	-2.48	1.78	1.82
5	A	4002	R22	C5-C6	-2.20	1.35	1.38
3	A	2000	SUC	C1-C2	2.11	1.58	1.52
5	A	4002	R22	C2'-C3'	2.13	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4002	R22	C2-N1	2.20	1.37	1.33
3	A	2000	SUC	C4-C5	2.21	1.57	1.53
5	A	4002	R22	C4'-C5'	2.43	1.43	1.38
5	A	4002	R22	C4'-C3'	2.60	1.43	1.38
5	A	4002	R22	C2'-C1'	2.63	1.43	1.38
3	A	2000	SUC	O2'-C5'	2.80	1.50	1.43
3	A	2000	SUC	O5-C5	2.93	1.51	1.44
3	B	2001	SUC	O5-C1	3.05	1.49	1.41
3	B	2001	SUC	O5-C5	3.25	1.52	1.44
5	A	4002	R22	C6'-C1'	3.32	1.44	1.38
3	A	2000	SUC	O5-C1	3.37	1.50	1.41
5	A	4002	R22	C6-N1	4.99	1.41	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4002	R22	C3-C2-N1	-7.54	115.43	123.79
3	B	2001	SUC	C1-O5-C5	-4.61	104.80	113.75
5	A	4002	R22	C7-C6-N1	-2.79	111.92	116.34
3	A	2000	SUC	C2'-O1-C1	2.13	123.15	117.53
5	A	4002	R22	C12-C13-C17	2.30	135.06	129.15
5	A	4002	R22	C7-C6-C5	2.56	127.23	122.41
5	A	4002	R22	C2-N1-C6	2.75	123.53	117.82
5	A	4002	R22	C5-C10-S11	2.95	121.60	112.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	SUC	2	0
6	A	3001	GOL	5	0
5	A	4002	R22	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	552/560 (98%)	0.50	57 (10%) 9 7	28, 58, 106, 141	0
2	B	426/430 (99%)	0.73	58 (13%) 4 3	24, 55, 124, 150	0
All	All	978/990 (98%)	0.60	115 (11%) 6 5	24, 57, 118, 150	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	227	PHE	16.2
2	B	230	MET	12.3
2	B	358	ARG	9.8
2	B	4	PRO	9.8
2	B	229	TRP	9.5
2	B	359	GLY	8.9
2	B	5	ILE	8.5
2	B	224	GLU	7.9
2	B	66	LYS	7.7
2	B	226	PRO	7.4
2	B	92	LEU	7.4
2	B	361	HIS	7.3
2	B	90	VAL	7.1
2	B	357	MET	6.9
2	B	225	PRO	6.8
2	B	221	HIS	6.8
2	B	223	LYS	6.6
1	A	67	ASP	6.4
2	B	228	LEU	6.4
1	A	24	TRP	6.3
2	B	360	ALA	5.8
1	A	1	PRO	5.4
2	B	67	ASP	5.4
1	A	68	SER	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	221	HIS	5.3
2	B	94	ILE	5.2
2	B	222	GLN	5.2
2	B	91	GLN	5.1
2	B	68	SER	5.0
2	B	429	LEU	4.8
1	A	136	ASN	4.7
1	A	135	ILE	4.7
1	A	92	LEU	4.5
2	B	362	THR	4.5
1	A	52	PRO	4.4
1	A	66	LYS	4.4
2	B	87	PHE	4.4
2	B	93	GLY	4.4
2	B	69	THR	4.3
1	A	65	LYS	4.3
1	A	360	ALA	4.1
1	A	25	PRO	4.1
2	B	85	GLN	4.1
1	A	139	THR	4.1
2	B	231	GLY	4.1
1	A	359	GLY	3.8
2	B	6	GLU	3.7
1	A	134	SER	3.7
2	B	301	LEU	3.7
2	B	316	GLY	3.7
2	B	219	LYS	3.6
2	B	86	ASP	3.6
1	A	358	ARG	3.5
1	A	284	ARG	3.5
1	A	495	ILE	3.5
2	B	95	PRO	3.3
2	B	88	TRP	3.3
2	B	232	TYR	3.3
2	B	312	GLU	3.2
2	B	297	GLU	3.2
1	A	69	THR	3.1
2	B	427	TYR	3.1
1	A	286	THR	3.0
2	B	238	LYS	2.9
1	A	496	VAL	2.9
2	B	313	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	15	GLY	2.9
1	A	32	LYS	2.8
1	A	312	GLU	2.8
1	A	435	VAL	2.8
1	A	173	LYS	2.8
2	B	70	LYS	2.8
1	A	2	ILE	2.8
1	A	72	ARG	2.8
1	A	26	LEU	2.8
1	A	357	MET	2.8
1	A	514	GLU	2.7
1	A	355	ALA	2.7
1	A	137	ASN	2.7
2	B	315	HIS	2.7
1	A	368	LEU	2.7
1	A	290	THR	2.7
2	B	284	ARG	2.7
1	A	54	ASN	2.7
2	B	428	GLN	2.6
1	A	356	ARG	2.6
2	B	277	ARG	2.5
2	B	214	LEU	2.5
2	B	173	LYS	2.5
1	A	177	ASP	2.4
1	A	138	GLU	2.4
1	A	194	GLU	2.4
1	A	282	LEU	2.4
1	A	224	GLU	2.4
1	A	334	GLN	2.3
2	B	65	LYS	2.3
1	A	287	LYS	2.3
1	A	448	ARG	2.3
1	A	251	SER	2.3
1	A	369	THR	2.2
1	A	133	PRO	2.2
1	A	482	ILE	2.1
1	A	197	GLN	2.1
1	A	146	TYR	2.1
1	A	140	PRO	2.1
2	B	240	THR	2.1
1	A	410	TRP	2.1
2	B	212	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	245	VAL	2.1
2	B	189	VAL	2.1
1	A	222	GLN	2.0
1	A	396	GLU	2.0
2	B	318	TYR	2.0
1	A	149	LEU	2.0
2	B	128	THR	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(Å ²)	Q<0.9
6	GOL	A	3001	6/6	0.78	0.31	3.67	80,88,96,97	0
3	SUC	A	2000	23/23	0.77	0.28	2.31	92,102,106,114	0
3	SUC	B	2001	23/23	0.94	0.15	-0.23	29,47,53,68	0
5	R22	A	4002	26/26	0.96	0.17	-0.49	33,45,81,88	0
6	GOL	A	3000	6/6	0.64	0.20	-	76,80,88,90	0
4	MN	A	4001	1/1	0.97	0.12	-	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.