



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:46 PM GMT

PDB ID : 1LW2  
Title : CRYSTAL STRUCTURE OF T215Y MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH 1051U91  
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Deposited on : 2002-05-30  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

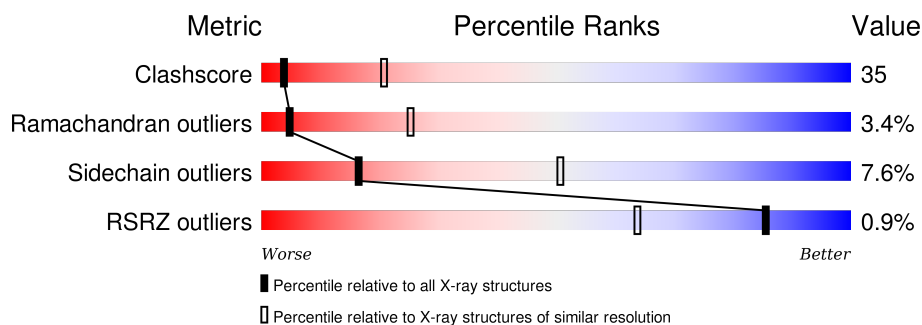
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	440	

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	PO4	A	1301	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7662 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 HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4257	2759	703	787	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	TYR	THR	ENGINEERED	UNP P04585
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	0	0
			3373	2203	555	608	7			

There is a discrepancy between the modelled and reference sequences:

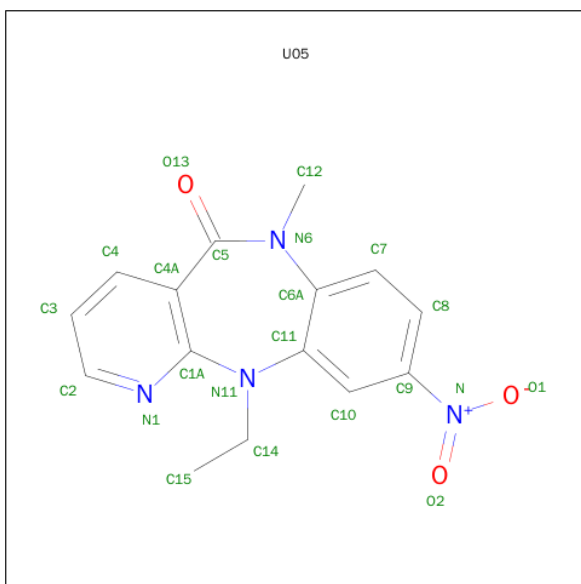
Chain	Residue	Modelled	Actual	Comment	Reference
B	215	TYR	THR	ENGINEERED	UNP P04585

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is 6,11-DIHYDRO-11-ETHYL-6-METHYL-9-NITRO-5H-PYRIDO[2,3-B][1,5]BENZODIAZEPIN-5-ONE (three-letter code: U05) (formula: C<sub>15</sub>H<sub>14</sub>N<sub>4</sub>O<sub>3</sub>).

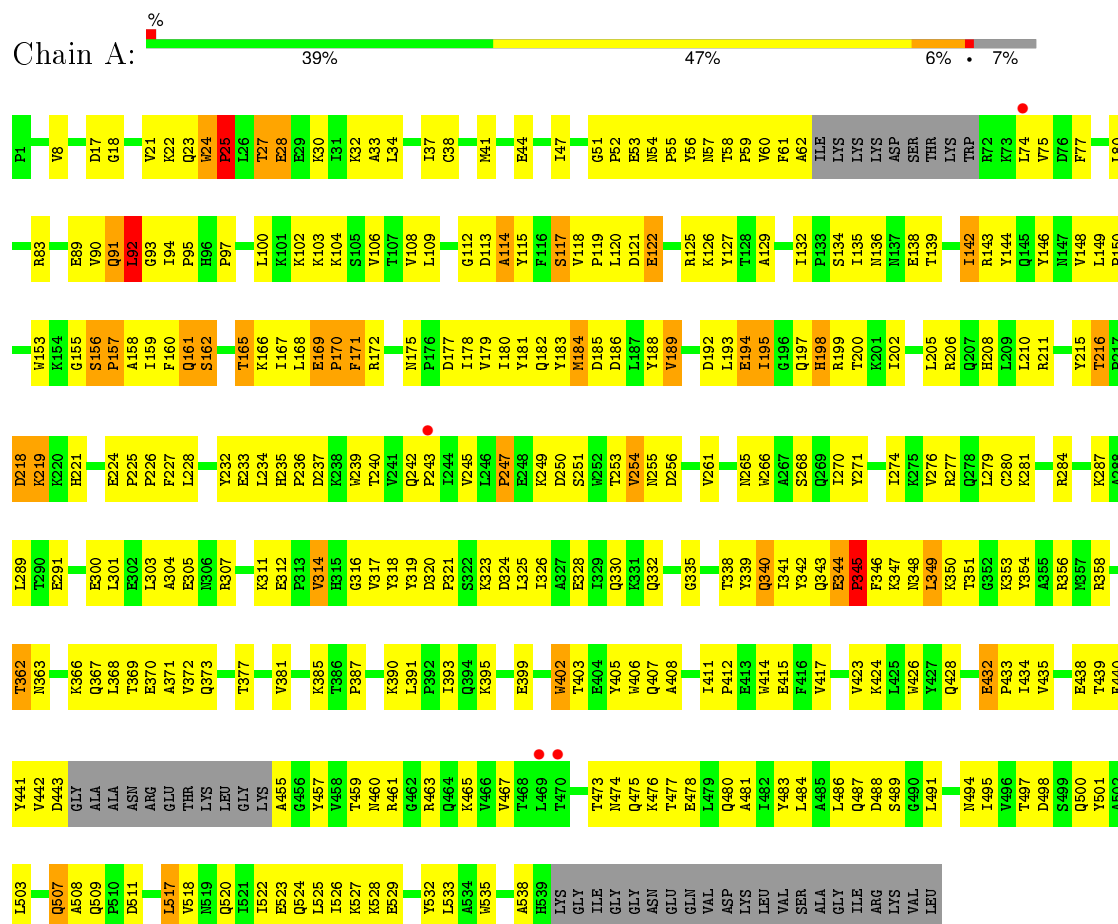


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	15	4	3		

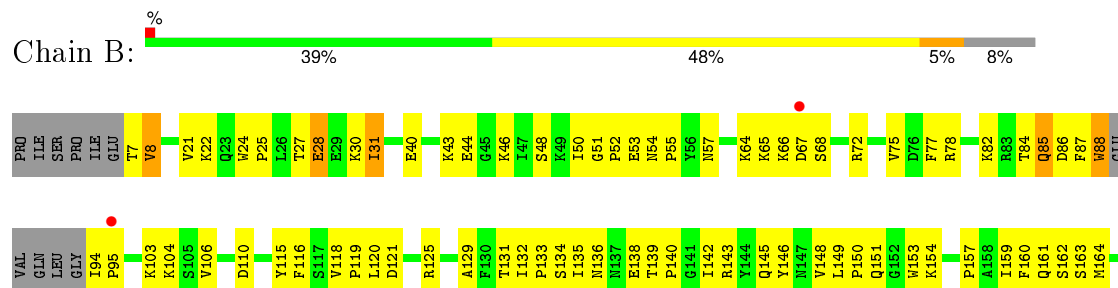
### 3 Residue-property plots

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: HIV-1 REVERSE TRANSCRIPTASE



#### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE



I167	L168	E169	P170	F171	R172	K173	Q174	N175	P176	D177	I178	V179	Y183	M184	D185	V189	G190	S191	D192	L193	E194	I195	G196	Q197	H198	R199	T200	K201	T202	E203	E204	L205	R206	Q207	H208	L209	L210	R211	W212	G213	L214	Y215	T216	PRO	ASP	LYS	LYS	HIS	GLN	K223	E224	P225	P226	F227	L228	W229	M230
G231	Y232	E233	L234	H235	P236	D237	K238	W239	Q242	P243	I244	P247	E248	K249	W252	T253	V254	I257	I258	K259	L260	L264	N265	W266	Q269	I270	Y271	P272	G273	I274	R277	Q278	L279	K281	L282	L283	R284	G285	T286	L289	T290	E291	V292	I293	P294	L295	T296	E297	E300								
L301	E302	E305	N306	I309	V314	H315	G316	V317	Y318	K323	I326	A327	E328	I329	Q330	K331	Q332	G333	Q334	G335	Q336	W337	T338	Y339	Q340	T341	Y342	Q343	E344	N348	L349	G352	K353	K356	MET	ARG	GLY	ALA	HIS	T362	N363	D364	V365	K366	Q367	L368	T369	V372	Q373	K374							
T377	E378	S379	I380	Y381	I382	W383	G384	P387	K388	F389	K390	T393	Q394	H398	W401	F404	Y405	W406	Q407	A408	T409	W410	I411	W414	W418	T419	P420	P421	L422	V423	K424	L425	Q428	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE												

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.30 Å 115.20 Å 64.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 3.00 29.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.78-3.00) 98.7 (29.78-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 3.00 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.205 , 0.267 0.187 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	61.2	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 74.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 20973 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7662	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, U05

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	0.57	0/4363	0.75	0/5934
2	B	0.59	0/3471	0.77	0/4716
All	All	0.58	0/7834	0.76	0/10650

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4257	0	4280	320	0
2	B	3373	0	3399	224	0
3	A	10	0	0	2	0
4	A	22	0	14	1	0
All	All	7662	0	7693	536	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 35.

All (536) 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)
2:B:167:ILE:HG21	2:B:214:LEU:HD11	1.30	1.11
1:A:362:THR:HG22	1:A:366:LYS:HD3	1.43	1.00
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.43	0.99
2:B:94:ILE:HD12	2:B:95:PRO:HD2	1.46	0.96
1:A:356:ARG:HE	1:A:358:ARG:HH11	1.14	0.96
1:A:136:ASN:HD22	1:A:139:THR:HG22	1.31	0.95
1:A:206:ARG:HH12	1:A:218:ASP:HB3	1.31	0.95
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.49	0.95
1:A:194:GLU:HG2	1:A:197:GLN:HE21	1.30	0.94
1:A:142:ILE:H	1:A:142:ILE:HD12	1.34	0.91
1:A:476:LYS:HG2	1:A:480:GLN:HE21	1.37	0.89
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.53	0.89
2:B:282:LEU:HG	2:B:293:ILE:HG21	1.55	0.89
1:A:480:GLN:HG3	1:A:517:LEU:HD11	1.57	0.87
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.11	0.85
2:B:270:ILE:O	2:B:272:PRO:HD3	1.76	0.85
1:A:113:ASP:HB3	1:A:117:SER:OG	1.76	0.85
1:A:92:LEU:HD12	1:A:92:LEU:N	1.92	0.85
2:B:142:ILE:HD12	2:B:142:ILE:H	1.41	0.84
1:A:92:LEU:HD12	1:A:92:LEU:H	1.42	0.83
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.61	0.82
1:A:136:ASN:ND2	1:A:139:THR:HG22	1.93	0.82
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.62	0.81
1:A:136:ASN:HD21	1:A:138:GLU:HB2	1.46	0.81
1:A:132:ILE:HG13	1:A:142:ILE:HD13	1.63	0.81
2:B:422:LEU:HA	2:B:425:LEU:HD23	1.62	0.80
1:A:372:VAL:HG11	1:A:411:ILE:HD12	1.63	0.79
2:B:164:MET:SD	2:B:167:ILE:HD11	2.21	0.79
2:B:277:ARG:HB2	2:B:277:ARG:HH11	1.48	0.79
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.65	0.78
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.50	0.77
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.66	0.76
1:A:33:ALA:O	1:A:37:ILE:HG13	1.85	0.76
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.67	0.76
1:A:473:THR:O	1:A:477:THR:HG23	1.85	0.76
1:A:161:GLN:HA	1:A:182:GLN:HE22	1.51	0.76
1:A:142:ILE:HD12	1:A:142:ILE:N	2.01	0.75
1:A:432:GLU:HG3	1:A:433:PRO:HD2	1.69	0.75
2:B:72:ARG:HH12	2:B:110:ASP:CG	1.90	0.75
1:A:399:GLU:HG2	1:A:402:TRP:CE3	2.22	0.74
2:B:195:ILE:O	2:B:199:ARG:HG3	1.87	0.74
1:A:253:THR:HG22	1:A:256:ASP:CG	2.07	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.23	0.73
1:A:518:VAL:O	1:A:522:ILE:HG13	1.89	0.72
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.23	0.72
1:A:23:GLN:O	1:A:25:PRO:HD3	1.89	0.72
2:B:282:LEU:HG	2:B:293:ILE:CG2	2.20	0.72
1:A:22:LYS:HE2	1:A:24:TRP:HD1	1.55	0.72
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.71	0.72
1:A:455:ALA:HB3	1:A:467:VAL:O	1.90	0.71
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.70	0.71
1:A:92:LEU:HD13	1:A:93:GLY:H	1.55	0.71
1:A:524:GLN:HA	1:A:524:GLN:OE1	1.90	0.71
1:A:136:ASN:HD22	1:A:139:THR:CG2	2.02	0.71
1:A:277:ARG:HH11	1:A:277:ARG:HG3	1.55	0.71
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.72	0.71
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.20	0.71
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.21	0.70
1:A:22:LYS:HE2	1:A:24:TRP:CD1	2.26	0.70
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.74	0.70
2:B:175:ASN:ND2	2:B:201:LYS:HD3	2.07	0.70
2:B:88:TRP:C	2:B:88:TRP:CD1	2.65	0.70
1:A:134:SER:OG	1:A:139:THR:HG23	1.92	0.69
2:B:207:GLN:HB3	2:B:211:ARG:HD2	1.73	0.69
2:B:170:PRO:HG3	2:B:212:TRP:CZ3	2.28	0.69
1:A:304:ALA:O	1:A:307:ARG:HB2	1.93	0.69
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.74	0.69
1:A:95:PRO:HB3	2:B:136:ASN:O	1.92	0.69
1:A:162:SER:O	1:A:165:THR:HG23	1.92	0.69
2:B:72:ARG:NH1	2:B:110:ASP:OD1	2.26	0.69
2:B:154:LYS:O	2:B:157:PRO:HD2	1.93	0.69
2:B:393:ILE:HG12	2:B:394:GLN:N	2.06	0.69
1:A:194:GLU:CG	1:A:197:GLN:HE21	2.03	0.68
2:B:393:ILE:HG12	2:B:394:GLN:H	1.58	0.68
2:B:167:ILE:CG2	2:B:214:LEU:HD11	2.16	0.68
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.75	0.68
1:A:172:ARG:NH1	1:A:180:ILE:HB	2.08	0.67
2:B:110:ASP:HB3	2:B:226:PRO:HG2	1.76	0.67
2:B:31:ILE:HD11	2:B:133:PRO:HG2	1.77	0.67
1:A:354:TYR:CZ	1:A:356:ARG:HB3	2.30	0.67
1:A:28:GLU:HG3	1:A:135:ILE:HG12	1.74	0.67
1:A:399:GLU:O	1:A:402:TRP:HB3	1.95	0.66
2:B:64:LYS:NZ	2:B:66:LYS:HA	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:PRO:HG2	1:A:171:PHE:H	1.61	0.66
2:B:139:THR:HB	2:B:140:PRO:HD2	1.77	0.66
1:A:195:ILE:O	1:A:198:HIS:HB3	1.96	0.66
2:B:362:THR:HG22	2:B:363:ASN:N	2.10	0.65
1:A:350:LYS:HG2	1:A:351:THR:N	2.10	0.65
2:B:148:VAL:HG23	2:B:149:LEU:O	1.95	0.65
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.32	0.65
1:A:356:ARG:HE	1:A:358:ARG:NH1	1.90	0.65
1:A:183:TYR:CE1	1:A:184:MET:HG3	2.31	0.65
2:B:27:THR:OG1	2:B:30:LYS:HG2	1.97	0.65
2:B:230:MET:C	2:B:232:TYR:H	2.00	0.65
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.62	0.65
2:B:277:ARG:O	2:B:281:LYS:HG3	1.97	0.65
1:A:319:TYR:OH	1:A:385:LYS:HE2	1.97	0.65
2:B:167:ILE:CD1	2:B:168:LEU:HG	2.27	0.64
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.32	0.64
1:A:148:VAL:O	1:A:150:PRO:HD3	1.97	0.64
1:A:206:ARG:HH12	1:A:218:ASP:CB	2.07	0.64
2:B:362:THR:CG2	2:B:367:GLN:HE21	2.09	0.64
1:A:112:GLY:O	1:A:113:ASP:HB2	1.97	0.64
2:B:78:ARG:HD3	2:B:411:ILE:O	1.98	0.64
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.33	0.64
1:A:89:GLU:OE2	1:A:92:LEU:HA	1.98	0.63
1:A:136:ASN:ND2	1:A:139:THR:H	1.96	0.63
1:A:197:GLN:O	1:A:200:THR:HB	1.98	0.63
2:B:326:ILE:HG22	2:B:327:ALA:N	2.12	0.63
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.29	0.63
2:B:53:GLU:OE1	2:B:53:GLU:N	2.28	0.63
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.18	0.63
1:A:476:LYS:HG2	1:A:480:GLN:NE2	2.13	0.63
1:A:114:ALA:HB2	1:A:185:ASP:OD2	1.98	0.63
2:B:131:THR:OG1	2:B:143:ARG:HG2	1.99	0.63
2:B:167:ILE:HD12	2:B:168:LEU:N	2.13	0.62
1:A:344:GLU:HB3	1:A:347:LYS:HE3	1.81	0.62
2:B:202:ILE:HG22	2:B:203:GLU:N	2.15	0.62
2:B:362:THR:HG21	2:B:367:GLN:HE21	1.64	0.62
1:A:438:GLU:OE1	1:A:463:ARG:HD3	1.99	0.62
1:A:178:ILE:HG22	1:A:179:VAL:N	2.15	0.62
2:B:167:ILE:HD12	2:B:168:LEU:HG	1.81	0.62
2:B:203:GLU:O	2:B:207:GLN:HG3	1.99	0.62
1:A:104:LYS:CB	1:A:192:ASP:HA	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.48	0.61
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.34	0.61
1:A:210:LEU:HD23	1:A:210:LEU:O	2.00	0.61
2:B:31:ILE:CD1	2:B:133:PRO:HG2	2.30	0.61
1:A:171:PHE:HE1	1:A:205:LEU:HA	1.65	0.61
1:A:27:THR:HG23	1:A:30:LYS:CG	2.31	0.61
1:A:487:GLN:HA	1:A:524:GLN:NE2	2.16	0.61
1:A:277:ARG:NH1	1:A:277:ARG:HG3	2.15	0.60
2:B:340:GLN:HB3	2:B:348:ASN:HD22	1.66	0.60
1:A:28:GLU:O	1:A:32:LYS:HG3	2.01	0.60
2:B:210:LEU:HG	2:B:223:LYS:O	2.01	0.60
1:A:34:LEU:HD13	1:A:132:ILE:HG22	1.83	0.60
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.15	0.60
1:A:399:GLU:HG2	1:A:402:TRP:HE3	1.63	0.60
1:A:90:VAL:HG22	1:A:91:GLN:HG2	1.83	0.60
1:A:391:LEU:HD12	1:A:414:TRP:CE3	2.36	0.60
1:A:61:PHE:CE1	1:A:74:LEU:HD23	2.37	0.60
2:B:88:TRP:C	2:B:88:TRP:HD1	2.06	0.59
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.83	0.59
1:A:108:VAL:C	1:A:109:LEU:HD12	2.22	0.59
1:A:161:GLN:HG2	1:A:182:GLN:NE2	2.17	0.59
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.16	0.59
1:A:228:LEU:HA	1:A:232:TYR:O	2.02	0.59
1:A:60:VAL:HG22	1:A:75:VAL:HG13	1.82	0.59
1:A:30:LYS:CD	1:A:62:ALA:HB3	2.32	0.59
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.38	0.59
2:B:64:LYS:HZ1	2:B:66:LYS:HA	1.66	0.59
1:A:120:LEU:HD23	1:A:125:ARG:HG2	1.86	0.58
1:A:102:LYS:O	1:A:103:LYS:HD3	2.04	0.58
2:B:333:GLY:O	2:B:336:GLN:HG2	2.03	0.58
2:B:215:TYR:HE2	2:B:225:PRO:HG3	1.68	0.58
1:A:115:TYR:N	1:A:115:TYR:CD2	2.70	0.58
1:A:56:TYR:O	1:A:143:ARG:NH2	2.36	0.58
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.39	0.58
1:A:92:LEU:H	1:A:92:LEU:CD1	2.07	0.58
2:B:197:GLN:O	2:B:200:THR:HB	2.03	0.58
1:A:253:THR:O	1:A:256:ASP:N	2.36	0.58
1:A:95:PRO:HG3	4:A:999:U05:O2	2.04	0.58
2:B:317:VAL:HG11	2:B:348:ASN:O	2.03	0.57
2:B:365:VAL:O	2:B:369:THR:HG23	2.04	0.57
1:A:442:VAL:CG1	1:A:481:ALA:CB	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.85	0.57
1:A:311:LYS:HD2	1:A:312:GLU:HG3	1.85	0.57
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.04	0.57
1:A:142:ILE:H	1:A:142:ILE:CD1	2.12	0.57
1:A:473:THR:HG22	1:A:475:GLN:H	1.70	0.57
2:B:167:ILE:HG12	2:B:214:LEU:HD21	1.85	0.57
2:B:8:VAL:HG13	2:B:159:ILE:HD13	1.87	0.57
2:B:229:TRP:CE3	2:B:229:TRP:HA	2.40	0.57
1:A:342:TYR:CA	1:A:349:LEU:HD12	2.35	0.57
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.86	0.57
2:B:40:GLU:O	2:B:44:GLU:HG3	2.05	0.56
2:B:215:TYR:OH	2:B:225:PRO:HA	2.05	0.56
1:A:161:GLN:HG2	1:A:182:GLN:HE22	1.70	0.56
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.39	0.56
2:B:277:ARG:NH1	2:B:277:ARG:HB2	2.19	0.56
1:A:307:ARG:CG	1:A:307:ARG:HH11	2.19	0.56
2:B:175:ASN:HB2	2:B:177:ASP:OD1	2.05	0.56
2:B:202:ILE:CG2	2:B:203:GLU:N	2.68	0.56
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.38	0.56
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.40	0.56
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.06	0.56
1:A:390:LYS:HE2	1:A:415:GLU:OE2	2.05	0.56
1:A:332:GLN:HE21	1:A:338:THR:CG2	2.19	0.56
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.06	0.56
1:A:28:GLU:HB3	1:A:32:LYS:NZ	2.20	0.55
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.87	0.55
2:B:65:LYS:HB2	2:B:68:SER:HB3	1.87	0.55
2:B:178:ILE:CD1	2:B:201:LYS:HG2	2.36	0.55
2:B:85:GLN:O	2:B:85:GLN:HG3	2.07	0.55
2:B:247:PRO:HB2	2:B:249:LYS:HD3	1.88	0.55
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.42	0.55
2:B:332:GLN:CG	2:B:338:THR:HG23	2.37	0.55
1:A:172:ARG:HH12	1:A:180:ILE:HB	1.72	0.55
1:A:90:VAL:O	1:A:91:GLN:HG2	2.06	0.54
1:A:303:LEU:C	1:A:303:LEU:HD23	2.27	0.54
1:A:328:GLU:O	1:A:339:TYR:HA	2.08	0.54
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.89	0.54
2:B:104:LYS:HD2	2:B:192:ASP:O	2.07	0.54
2:B:131:THR:HG22	2:B:132:ILE:N	2.22	0.54
2:B:317:VAL:CG1	2:B:349:LEU:HD23	2.37	0.54
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:SER:O	2:B:167:ILE:HG13	2.08	0.54
1:A:356:ARG:HH21	1:A:358:ARG:NH1	2.05	0.54
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.90	0.54
2:B:284:ARG:O	2:B:284:ARG:HG3	2.07	0.54
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.42	0.54
2:B:103:LYS:CE	2:B:179:VAL:HG23	2.38	0.54
1:A:276:VAL:O	1:A:276:VAL:HG12	2.07	0.54
2:B:282:LEU:HD11	2:B:296:THR:HG23	1.90	0.54
1:A:155:GLY:O	1:A:156:SER:C	2.46	0.53
1:A:473:THR:HG22	1:A:474:ASN:N	2.23	0.53
1:A:432:GLU:OE1	1:A:432:GLU:HA	2.08	0.53
1:A:225:PRO:HG3	1:A:227:PHE:HE2	1.72	0.53
2:B:362:THR:CG2	2:B:363:ASN:N	2.70	0.53
2:B:150:PRO:HG2	2:B:153:TRP:HB2	1.90	0.53
1:A:28:GLU:CG	1:A:135:ILE:HG23	2.39	0.53
1:A:279:LEU:O	1:A:280:CSD:C	2.56	0.53
1:A:177:ASP:N	1:A:177:ASP:OD2	2.42	0.53
1:A:480:GLN:O	1:A:483:TYR:HB3	2.08	0.53
2:B:31:ILE:HD13	2:B:133:PRO:O	2.08	0.53
2:B:171:PHE:HB2	2:B:208:HIS:ND1	2.24	0.52
1:A:245:VAL:HG13	1:A:245:VAL:O	2.09	0.52
2:B:344:GLU:OE1	2:B:344:GLU:HA	2.08	0.52
1:A:103:LYS:O	1:A:236:PRO:HB3	2.09	0.52
1:A:22:LYS:CE	1:A:24:TRP:HD1	2.20	0.52
2:B:229:TRP:CZ3	2:B:407:GLN:HG3	2.45	0.52
2:B:295:LEU:HB3	2:B:300:GLU:HG2	1.91	0.52
1:A:393:ILE:HG23	1:A:414:TRP:CH2	2.43	0.52
2:B:380:ILE:O	2:B:384:GLY:N	2.43	0.52
1:A:183:TYR:CD1	1:A:184:MET:HG3	2.45	0.52
2:B:420:PRO:C	2:B:422:LEU:H	2.14	0.52
1:A:368:LEU:HD22	1:A:423:VAL:HG11	1.92	0.52
1:A:159:ILE:O	1:A:162:SER:HB3	2.10	0.52
1:A:106:VAL:HG13	1:A:236:PRO:HG3	1.92	0.52
1:A:523:GLU:O	1:A:527:LYS:HG2	2.09	0.52
2:B:142:ILE:CD1	2:B:142:ILE:H	2.16	0.52
2:B:199:ARG:O	2:B:202:ILE:HG22	2.09	0.52
1:A:51:GLY:C	1:A:53:GLU:H	2.14	0.52
2:B:296:THR:O	2:B:297:GLU:C	2.49	0.51
1:A:41:MET:HB2	1:A:47:ILE:HD11	1.91	0.51
1:A:90:VAL:C	1:A:91:GLN:HG2	2.31	0.51
1:A:487:GLN:HA	1:A:524:GLN:HE21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.46	0.51
1:A:460:ASN:ND2	3:A:1301:PO4:O4	2.32	0.51
1:A:225:PRO:HA	1:A:226:PRO:C	2.30	0.51
1:A:255:ASN:HD22	1:A:289:LEU:HB3	1.74	0.51
2:B:420:PRO:O	2:B:422:LEU:N	2.42	0.51
2:B:420:PRO:HG2	2:B:423:VAL:HG23	1.92	0.51
1:A:432:GLU:CG	1:A:433:PRO:HD2	2.39	0.51
1:A:136:ASN:HB3	1:A:139:THR:HG22	1.92	0.51
2:B:171:PHE:HB2	2:B:208:HIS:CE1	2.45	0.51
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.26	0.51
1:A:253:THR:O	1:A:254:VAL:C	2.49	0.51
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.38	0.51
1:A:113:ASP:O	1:A:114:ALA:C	2.49	0.51
1:A:372:VAL:CG1	1:A:411:ILE:HD12	2.38	0.51
1:A:215:TYR:CD1	1:A:216:THR:N	2.80	0.50
1:A:206:ARG:NH1	1:A:218:ASP:HB3	2.12	0.50
1:A:193:LEU:O	1:A:194:GLU:C	2.48	0.50
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.41	0.50
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.46	0.50
2:B:215:TYR:CE2	2:B:225:PRO:HG3	2.46	0.50
1:A:253:THR:CG2	1:A:256:ASP:H	2.25	0.50
2:B:201:LYS:NZ	2:B:204:GLU:OE2	2.38	0.50
2:B:333:GLY:O	2:B:334:GLN:HB2	2.11	0.50
2:B:168:LEU:O	2:B:172:ARG:HB2	2.10	0.50
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.46	0.50
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.41	0.50
1:A:270:ILE:HG23	1:A:271:TYR:N	2.27	0.50
2:B:205:LEU:O	2:B:209:LEU:HG	2.12	0.50
1:A:249:LYS:HD2	1:A:251:SER:O	2.11	0.50
2:B:167:ILE:HG21	2:B:214:LEU:CD1	2.21	0.50
1:A:480:GLN:CG	1:A:517:LEU:HD11	2.34	0.50
1:A:136:ASN:HB3	1:A:139:THR:CG2	2.42	0.49
1:A:198:HIS:O	1:A:202:ILE:HG12	2.12	0.49
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.47	0.49
2:B:131:THR:CG2	2:B:132:ILE:N	2.75	0.49
1:A:54:ASN:HB3	1:A:143:ARG:NH1	2.27	0.49
1:A:115:TYR:N	1:A:115:TYR:HD2	2.11	0.49
2:B:334:GLN:HB3	2:B:336:GLN:OE1	2.12	0.49
1:A:108:VAL:HG13	1:A:108:VAL:O	2.11	0.49
1:A:324:ASP:O	1:A:343:GLN:HG2	2.13	0.49
2:B:326:ILE:CG2	2:B:327:ALA:N	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:MET:C	2:B:232:TYR:N	2.66	0.49
1:A:148:VAL:O	1:A:150:PRO:CD	2.61	0.49
1:A:233:GLU:O	1:A:234:LEU:HD23	2.13	0.49
1:A:274:ILE:O	1:A:353:LYS:NZ	2.45	0.49
1:A:433:PRO:HA	1:A:532:TYR:CG	2.47	0.49
2:B:139:THR:CB	2:B:140:PRO:HD2	2.40	0.49
1:A:57:ASN:HA	1:A:129:ALA:O	2.13	0.49
2:B:195:ILE:HG23	2:B:196:GLY:N	2.26	0.49
1:A:281:LYS:O	1:A:284:ARG:HG3	2.13	0.49
1:A:344:GLU:HG3	1:A:345:PRO:HD2	1.95	0.48
2:B:234:LEU:HD11	2:B:377:THR:HG21	1.94	0.48
1:A:326:ILE:O	1:A:341:ILE:HA	2.13	0.48
1:A:24:TRP:O	1:A:25:PRO:O	2.31	0.48
1:A:457:TYR:C	1:A:457:TYR:CD1	2.86	0.48
2:B:206:ARG:HB3	2:B:224:GLU:CG	2.43	0.48
1:A:399:GLU:HG2	1:A:402:TRP:CZ3	2.48	0.48
1:A:320:ASP:OD1	1:A:323:LYS:HG3	2.13	0.48
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.94	0.48
1:A:356:ARG:NE	1:A:358:ARG:HG2	2.29	0.48
1:A:474:ASN:O	1:A:478:GLU:HG3	2.14	0.48
1:A:363:ASN:HA	1:A:511:ASP:CG	2.34	0.48
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.49	0.48
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.95	0.48
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.49	0.47
1:A:476:LYS:HG3	1:A:517:LEU:HD12	1.96	0.47
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.50	0.47
1:A:24:TRP:HZ3	1:A:61:PHE:CD2	2.32	0.47
1:A:118:VAL:HB	1:A:149:LEU:HG	1.97	0.47
1:A:149:LEU:HD11	1:A:159:ILE:HG22	1.96	0.47
2:B:106:VAL:HA	2:B:189:VAL:O	2.14	0.47
1:A:346:PHE:N	1:A:346:PHE:CD1	2.80	0.47
2:B:282:LEU:CD1	2:B:296:THR:HG23	2.45	0.47
1:A:167:ILE:O	1:A:170:PRO:HD2	2.15	0.47
2:B:167:ILE:HD12	2:B:167:ILE:C	2.35	0.47
2:B:227:PHE:CB	2:B:231:GLY:HA2	2.42	0.47
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.96	0.47
1:A:354:TYR:CE1	1:A:356:ARG:HB3	2.49	0.47
1:A:60:VAL:HG12	1:A:61:PHE:N	2.30	0.47
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.11	0.47
1:A:507:GLN:O	1:A:509:GLN:HG3	2.15	0.47
1:A:160:PHE:O	1:A:161:GLN:C	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ILE:O	1:A:526:ILE:HG13	2.14	0.47
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.30	0.47
2:B:207:GLN:HG2	2:B:224:GLU:OE2	2.15	0.46
1:A:27:THR:HG23	1:A:30:LYS:HG2	1.96	0.46
2:B:21:VAL:HG12	2:B:22:LYS:N	2.29	0.46
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.51	0.46
1:A:100:LEU:HD23	2:B:138:GLU:OE2	2.15	0.46
1:A:24:TRP:CH2	1:A:59:PRO:HB2	2.50	0.46
2:B:330:GLN:OE1	2:B:338:THR:OG1	2.24	0.46
2:B:242:GLN:HE21	2:B:353:LYS:HG2	1.80	0.46
1:A:276:VAL:O	1:A:277:ARG:C	2.52	0.46
2:B:297:GLU:O	2:B:301:LEU:HG	2.16	0.46
1:A:113:ASP:O	1:A:114:ALA:O	2.33	0.46
1:A:319:TYR:CE1	1:A:321:PRO:HG3	2.51	0.46
1:A:332:GLN:HE21	1:A:338:THR:HG21	1.80	0.46
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.50	0.46
1:A:178:ILE:CG2	1:A:179:VAL:N	2.77	0.46
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.16	0.46
2:B:378:GLU:O	2:B:381:VAL:N	2.49	0.46
1:A:317:VAL:HG22	1:A:318:TYR:H	1.80	0.46
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.96	0.46
2:B:86:ASP:HA	2:B:154:LYS:HZ1	1.81	0.46
1:A:503:LEU:O	1:A:507:GLN:HB2	2.16	0.46
2:B:57:ASN:HA	2:B:129:ALA:O	2.16	0.46
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.98	0.46
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.98	0.45
1:A:461:ARG:NH1	3:A:1300:PO4:O2	2.42	0.45
2:B:225:PRO:HA	2:B:226:PRO:HD2	1.78	0.45
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.51	0.45
2:B:228:LEU:HA	2:B:228:LEU:HD23	1.79	0.45
2:B:229:TRP:HE3	2:B:229:TRP:HA	1.82	0.45
1:A:503:LEU:HD12	1:A:533:LEU:HD23	1.98	0.45
1:A:377:THR:O	1:A:381:VAL:HG23	2.16	0.45
2:B:329:ILE:HG22	2:B:330:GLN:N	2.31	0.45
1:A:303:LEU:HD23	1:A:303:LEU:O	2.16	0.45
1:A:206:ARG:NH2	1:A:216:THR:O	2.48	0.45
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.98	0.45
2:B:67:ASP:HB2	2:B:230:MET:CE	2.46	0.45
2:B:78:ARG:O	2:B:82:LYS:HG3	2.17	0.45
2:B:228:LEU:O	2:B:229:TRP:HB2	2.17	0.45
1:A:157:PRO:HB2	1:A:158:ALA:H	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:O	1:A:372:VAL:HB	2.17	0.45
2:B:378:GLU:O	2:B:379:SER:C	2.55	0.45
1:A:126:LYS:HE3	1:A:127:TYR:CE2	2.51	0.45
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.98	0.45
2:B:178:ILE:HG23	2:B:190:GLY:O	2.17	0.45
1:A:491:LEU:HD13	1:A:529:GLU:HG2	1.97	0.45
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.80	0.45
2:B:374:LYS:O	2:B:378:GLU:HG3	2.16	0.45
1:A:181:TYR:OH	1:A:183:TYR:HD2	2.00	0.45
1:A:300:GLU:HA	1:A:300:GLU:OE2	2.17	0.45
1:A:428:GLN:O	1:A:428:GLN:HG3	2.17	0.45
1:A:340:GLN:HA	1:A:351:THR:HA	1.98	0.45
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.31	0.45
1:A:344:GLU:CB	1:A:347:LYS:HE3	2.45	0.45
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.52	0.45
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.52	0.44
2:B:170:PRO:O	2:B:174:GLN:HG2	2.17	0.44
1:A:270:ILE:HG13	1:A:314:VAL:CG1	2.48	0.44
1:A:166:LYS:O	1:A:169:GLU:HB3	2.17	0.44
1:A:199:ARG:O	1:A:202:ILE:HB	2.18	0.44
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.99	0.44
2:B:342:TYR:CB	2:B:348:ASN:HA	2.45	0.44
1:A:332:GLN:HG2	1:A:338:THR:HG23	1.99	0.44
1:A:89:GLU:CD	1:A:92:LEU:HA	2.38	0.44
2:B:362:THR:CG2	2:B:363:ASN:H	2.29	0.44
1:A:381:VAL:HG12	1:A:381:VAL:O	2.17	0.44
2:B:278:GLN:HB2	2:B:302:GLU:CD	2.38	0.44
1:A:27:THR:HG23	1:A:30:LYS:HG3	2.00	0.44
2:B:208:HIS:O	2:B:212:TRP:HB2	2.18	0.44
2:B:118:VAL:HA	2:B:119:PRO:HD3	1.78	0.44
2:B:51:GLY:C	2:B:53:GLU:OE1	2.56	0.44
2:B:293:ILE:HG23	2:B:294:PRO:HD2	2.00	0.44
1:A:183:TYR:O	1:A:184:MET:HB2	2.17	0.44
1:A:92:LEU:CD1	1:A:93:GLY:H	2.28	0.43
1:A:402:TRP:CG	1:A:403:THR:N	2.85	0.43
2:B:86:ASP:HA	2:B:154:LYS:NZ	2.33	0.43
1:A:488:ASP:N	1:A:488:ASP:OD2	2.49	0.43
1:A:80:LEU:O	1:A:83:ARG:N	2.45	0.43
1:A:183:TYR:HE1	1:A:184:MET:HE3	1.83	0.43
1:A:28:GLU:HG3	1:A:135:ILE:CG1	2.45	0.43
2:B:64:LYS:HG2	2:B:65:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PHE:CE1	1:A:150:PRO:HB2	2.54	0.43
1:A:8:VAL:HG12	2:B:53:GLU:HB3	2.00	0.43
1:A:122:GLU:HG3	1:A:125:ARG:NH1	2.33	0.43
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.35	0.43
2:B:210:LEU:CG	2:B:223:LYS:O	2.66	0.43
1:A:465:LYS:HD2	1:A:484:LEU:HD22	2.00	0.43
2:B:72:ARG:CZ	2:B:409:THR:HG22	2.48	0.43
1:A:253:THR:HG23	1:A:256:ASP:H	1.84	0.43
1:A:307:ARG:CG	1:A:307:ARG:NH1	2.76	0.43
2:B:173:LYS:O	2:B:176:PRO:HD3	2.18	0.43
1:A:439:THR:HG21	2:B:289:LEU:HD13	2.01	0.43
1:A:434:ILE:HG13	1:A:434:ILE:H	1.61	0.43
1:A:180:ILE:HG22	1:A:181:TYR:N	2.34	0.43
1:A:118:VAL:HG13	1:A:119:PRO:HD2	2.00	0.43
1:A:219:LYS:NZ	1:A:224:GLU:OE2	2.52	0.43
1:A:89:GLU:OE1	1:A:92:LEU:HB3	2.19	0.43
1:A:92:LEU:CD1	1:A:92:LEU:N	2.62	0.43
2:B:120:LEU:O	2:B:121:ASP:C	2.57	0.43
1:A:435:VAL:HG22	2:B:290:THR:HG21	2.00	0.43
2:B:339:TYR:C	2:B:339:TYR:CD2	2.91	0.43
1:A:247:PRO:O	1:A:307:ARG:NH2	2.39	0.43
1:A:198:HIS:O	1:A:199:ARG:C	2.57	0.43
2:B:281:LYS:C	2:B:283:LEU:N	2.72	0.43
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.54	0.43
2:B:242:GLN:NE2	2:B:352:GLY:HA2	2.34	0.43
2:B:305:GLU:O	2:B:309:ILE:HG13	2.18	0.43
1:A:265:ASN:O	1:A:266:TRP:C	2.56	0.43
2:B:281:LYS:O	2:B:283:LEU:N	2.51	0.42
1:A:486:LEU:O	1:A:528:LYS:NZ	2.52	0.42
1:A:393:ILE:CB	1:A:423:VAL:HG13	2.49	0.42
2:B:266:TRP:O	2:B:269:GLN:HG3	2.18	0.42
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.49	0.42
1:A:183:TYR:CE1	1:A:184:MET:HE3	2.54	0.42
1:A:54:ASN:HA	1:A:55:PRO:HD2	1.89	0.42
1:A:242:GLN:HG3	1:A:243:PRO:HD2	2.02	0.42
2:B:21:VAL:CG1	2:B:22:LYS:N	2.82	0.42
2:B:46:LYS:HE2	2:B:116:PHE:HB3	2.01	0.42
2:B:160:PHE:O	2:B:161:GLN:C	2.57	0.42
1:A:171:PHE:CD2	1:A:171:PHE:C	2.93	0.42
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.01	0.42
2:B:422:LEU:O	2:B:425:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:HG3	1:A:237:ASP:HA	2.01	0.42
1:A:54:ASN:HB3	1:A:143:ARG:HH12	1.82	0.42
2:B:24:TRP:HA	2:B:25:PRO:HD3	1.91	0.42
1:A:108:VAL:HG23	1:A:188:TYR:CE1	2.55	0.42
1:A:311:LYS:HE3	1:A:311:LYS:HB3	1.81	0.42
1:A:370:GLU:O	1:A:371:ALA:C	2.57	0.42
1:A:393:ILE:HG23	1:A:414:TRP:CZ3	2.55	0.42
1:A:169:GLU:OE1	1:A:169:GLU:HA	2.20	0.42
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.55	0.42
2:B:316:GLY:HA2	2:B:318:TYR:CE2	2.55	0.42
1:A:194:GLU:O	1:A:194:GLU:HG3	2.18	0.42
2:B:327:ALA:HA	2:B:340:GLN:O	2.19	0.42
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.20	0.42
1:A:28:GLU:HG3	1:A:135:ILE:HG23	1.99	0.42
1:A:195:ILE:O	1:A:198:HIS:CB	2.66	0.42
1:A:266:TRP:HA	1:A:266:TRP:CE3	2.55	0.42
1:A:287:LYS:N	1:A:291:GLU:OE2	2.43	0.42
1:A:170:PRO:CG	1:A:171:PHE:H	2.31	0.41
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.50	0.41
2:B:43:LYS:HB2	2:B:43:LYS:HE3	1.86	0.41
2:B:254:VAL:O	2:B:258:GLN:HG3	2.20	0.41
1:A:103:LYS:O	1:A:236:PRO:CB	2.68	0.41
2:B:214:LEU:C	2:B:216:THR:H	2.21	0.41
1:A:232:TYR:HB3	1:A:240:THR:O	2.20	0.41
1:A:53:GLU:O	1:A:55:PRO:HD3	2.20	0.41
2:B:185:ASP:N	2:B:185:ASP:OD2	2.51	0.41
2:B:327:ALA:O	2:B:389:PHE:HA	2.20	0.41
2:B:27:THR:O	2:B:28:GLU:C	2.58	0.41
1:A:108:VAL:O	1:A:109:LEU:HD12	2.20	0.41
2:B:264:LEU:O	2:B:265:ASN:C	2.58	0.41
2:B:200:THR:C	2:B:202:ILE:N	2.73	0.41
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.55	0.41
2:B:306:ASN:HA	2:B:309:ILE:HD12	2.02	0.41
2:B:254:VAL:HG23	2:B:291:GLU:O	2.20	0.41
1:A:211:ARG:HB2	1:A:211:ARG:HE	1.71	0.41
1:A:94:ILE:O	1:A:94:ILE:HG13	2.18	0.41
1:A:208:HIS:C	1:A:208:HIS:CD2	2.94	0.41
1:A:136:ASN:CB	1:A:139:THR:HG22	2.50	0.41
2:B:87:PHE:CE1	2:B:154:LYS:HE2	2.55	0.41
2:B:87:PHE:O	2:B:88:TRP:C	2.59	0.41
2:B:57:ASN:HD21	2:B:131:THR:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ALA:O	1:A:509:GLN:HB2	2.21	0.41
1:A:194:GLU:HG2	1:A:197:GLN:NE2	2.14	0.41
1:A:233:GLU:HB3	1:A:240:THR:HG22	2.02	0.41
2:B:260:LEU:O	2:B:264:LEU:HG	2.21	0.41
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.81	0.41
1:A:171:PHE:CE2	1:A:175:ASN:ND2	2.89	0.41
1:A:210:LEU:C	1:A:210:LEU:HD23	2.41	0.41
1:A:17:ASP:O	1:A:83:ARG:NH1	2.52	0.41
1:A:426:TRP:N	1:A:426:TRP:CD1	2.87	0.41
1:A:356:ARG:HG2	1:A:358:ARG:HG3	2.03	0.41
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.85	0.41
2:B:84:THR:O	2:B:154:LYS:NZ	2.52	0.41
2:B:401:TRP:O	2:B:404:GLU:HB2	2.20	0.41
1:A:38:CYS:O	1:A:47:ILE:HD11	2.21	0.41
1:A:362:THR:HG22	1:A:366:LYS:CD	2.31	0.41
1:A:206:ARG:NH1	1:A:218:ASP:CA	2.82	0.41
1:A:153:TRP:CZ3	1:A:155:GLY:HA3	2.56	0.41
2:B:195:ILE:CG2	2:B:196:GLY:N	2.84	0.41
2:B:230:MET:O	2:B:232:TYR:N	2.54	0.41
1:A:221:HIS:CD2	1:A:221:HIS:N	2.89	0.41
1:A:497:THR:O	1:A:535:TRP:HA	2.21	0.41
1:A:368:LEU:O	1:A:372:VAL:HG23	2.21	0.40
2:B:198:HIS:O	2:B:200:THR:N	2.54	0.40
2:B:364:ASP:O	2:B:367:GLN:HB2	2.21	0.40
1:A:495:ILE:HB	1:A:533:LEU:HD12	2.02	0.40
1:A:169:GLU:OE1	1:A:169:GLU:CA	2.69	0.40
2:B:52:PRO:C	2:B:54:ASN:N	2.75	0.40
1:A:525:LEU:HA	1:A:525:LEU:HD23	1.91	0.40
1:A:89:GLU:HG2	1:A:89:GLU:O	2.21	0.40
2:B:169:GLU:N	2:B:170:PRO:HD2	2.36	0.40
2:B:253:THR:O	2:B:254:VAL:C	2.59	0.40
1:A:183:TYR:O	1:A:183:TYR:CD1	2.74	0.40
2:B:372:VAL:HA	2:B:389:PHE:CE2	2.56	0.40
2:B:230:MET:HA	2:B:230:MET:CE	2.51	0.40
2:B:257:ILE:O	2:B:260:LEU:HB3	2.22	0.40
1:A:473:THR:CG2	1:A:474:ASN:N	2.84	0.40
1:A:24:TRP:O	1:A:25:PRO:C	2.58	0.40
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.56	0.40
1:A:343:GLN:HG3	1:A:349:LEU:CD1	2.32	0.40
2:B:198:HIS:C	2:B:200:THR:N	2.75	0.40
2:B:203:GLU:O	2:B:206:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:THR:O	2:B:85:GLN:C	2.59	0.40
1:A:239:TRP:CD1	1:A:316:GLY:C	2.95	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	512/560 (91%)	447 (87%)	44 (9%)	21 (4%)	3	20
2	B	398/440 (90%)	334 (84%)	54 (14%)	10 (2%)	7	34
All	All	910/1000 (91%)	781 (86%)	98 (11%)	31 (3%)	5	25

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	114	ALA
1	A	157	PRO
1	A	195	ILE
1	A	219	LYS
1	A	402	TRP
2	B	193	LEU
1	A	25	PRO
1	A	268	SER
2	B	85	GLN
2	B	213	GLY
1	A	156	SER
1	A	198	HIS
1	A	345	PRO
1	A	412	PRO
2	B	162	SER

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Mol	Chain	Res	Type
2	B	232	TYR
2	B	282	LEU
2	B	421	PRO
1	A	92	LEU
1	A	117	SER
1	A	121	ASP
1	A	162	SER
2	B	170	PRO
1	A	254	VAL
2	B	225	PRO
1	A	170	PRO
1	A	169	GLU
1	A	52	PRO
1	A	247	PRO
2	B	176	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	467/499 (94%)	430 (92%)	37 (8%)	15	48
2	B	371/400 (93%)	344 (93%)	27 (7%)	17	52
All	All	838/899 (93%)	774 (92%)	64 (8%)	16	51

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	25	PRO
1	A	27	THR
1	A	28	GLU
1	A	44	GLU
1	A	58	THR
1	A	92	LEU
1	A	97	PRO

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Mol	Chain	Res	Type
1	A	122	GLU
1	A	142	ILE
1	A	161	GLN
1	A	165	THR
1	A	168	LEU
1	A	171	PHE
1	A	184	MET
1	A	186	ASP
1	A	189	VAL
1	A	194	GLU
1	A	216	THR
1	A	218	ASP
1	A	250	ASP
1	A	305	GLU
1	A	314	VAL
1	A	340	GLN
1	A	344	GLU
1	A	345	PRO
1	A	349	LEU
1	A	362	THR
1	A	373	GLN
1	A	405	TYR
1	A	424	LYS
1	A	432	GLU
1	A	443	ASP
1	A	459	THR
1	A	500	GLN
1	A	507	GLN
1	A	517	LEU
2	B	8	VAL
2	B	28	GLU
2	B	31	ILE
2	B	48	SER
2	B	55	PRO
2	B	88	TRP
2	B	134	SER
2	B	172	ARG
2	B	201	LYS
2	B	210	LEU
2	B	230	MET
2	B	242	GLN
2	B	277	ARG

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Mol	Chain	Res	Type
2	B	280	CYS
2	B	283	LEU
2	B	286	THR
2	B	314	VAL
2	B	323	LYS
2	B	334	GLN
2	B	336	GLN
2	B	368	LEU
2	B	379	SER
2	B	394	GLN
2	B	410	TRP
2	B	414	TRP
2	B	418	ASN
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	136	ASN
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	208	HIS
1	A	221	HIS
1	A	222	GLN
1	A	255	ASN
1	A	332	GLN
1	A	373	GLN
1	A	475	GLN
1	A	480	GLN
1	A	509	GLN
1	A	520	GLN
2	B	57	ASN
2	B	147	ASN
2	B	151	GLN
2	B	242	GLN
2	B	278	GLN
2	B	407	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	0.80	0	3,8,10	5.25	1 (33%)

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	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	8.91	120.26	105.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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
3	PO4	A	1301	-	4,4,4	1.14	0	6,6,6	0.27	0
4	U05	A	999	-	16,24,24	1.63	4 (25%)	15,35,35	1.69	2 (13%)

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
3	PO4	A	1301	-	-	0/0/0/0	0/0/0/0
4	U05	A	999	-	-	0/4/6/6	0/2/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	U05	C2-N1	2.18	1.36	1.32
4	A	999	U05	C3-C4	2.52	1.42	1.36
4	A	999	U05	C7-C8	2.75	1.42	1.36
4	A	999	U05	C12-N6	3.43	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	U05	C2-N1-C1A	2.29	119.78	116.93
4	A	999	U05	C15-C14-N11	5.00	122.38	111.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1300	PO4	1	0
3	A	1301	PO4	1	0
4	A	999	U05	1	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	518/560 (92%)	-0.59	4 (0%) 87 67	18, 58, 109, 145	0
2	B	406/440 (92%)	-0.52	4 (0%) 84 60	18, 55, 107, 141	0
All	All	924/1000 (92%)	-0.56	8 (0%) 85 64	18, 57, 108, 145	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	237	ASP	3.0
1	A	74	LEU	2.8
2	B	95	PRO	2.7
1	A	243	PRO	2.3
1	A	470	THR	2.3
2	B	67	ASP	2.3
1	A	469	LEU	2.1
2	B	223	LYS	2.1

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CSD	A	280	8/9	0.98	0.11	-	30,37,83,85	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	1301	5/5	0.91	0.22	3.19	120,120,124,125	0
3	PO4	A	1300	5/5	0.89	0.19	0.89	125,126,133,133	0
4	U05	A	999	22/22	0.98	0.17	0.69	21,48,69,75	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.