



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:26 PM GMT

PDB ID : 1TKZ
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN
COMPLEX WITH GW429576
Authors : Hopkins, A.L.; Ren, J.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2004-06-09
Resolution : 2.81 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

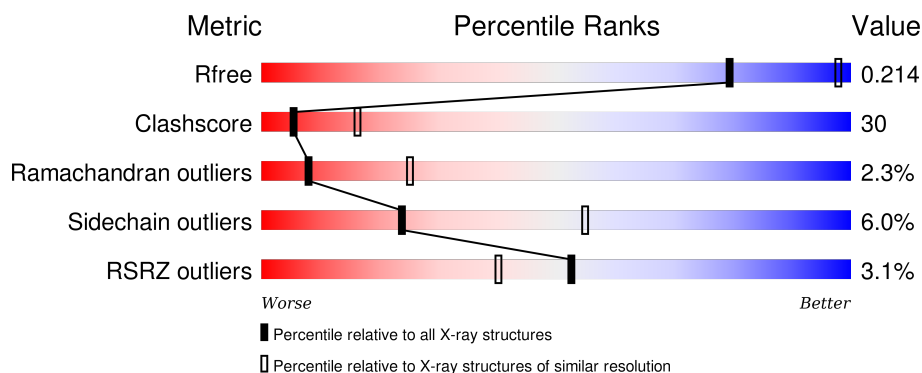
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	 3% 43% 43% 5% • 8%
2	B	440	 3% 42% 47% • 9%

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
3	PO4	A	1302	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7612 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 Pol polyprotein, Reverse transcriptase, Chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4247	2754	701	784	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	OXIDIZED CY	UNP P04585

- Molecule 2 is a protein called Pol polyprotein, Reverse transcriptase, Chain B.

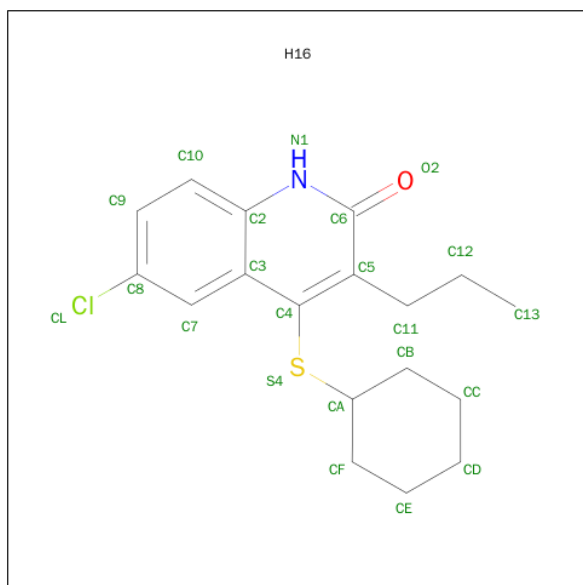
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3328	2173	548	600	7			

- 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		
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-CHLORO-4-(CYCLOHEXYLSULFANYL)-3-PROPYLQUINOLIN-2(1H)-ONE (three-letter code: H16) (formula: C₁₈H₂₂ClNOS).

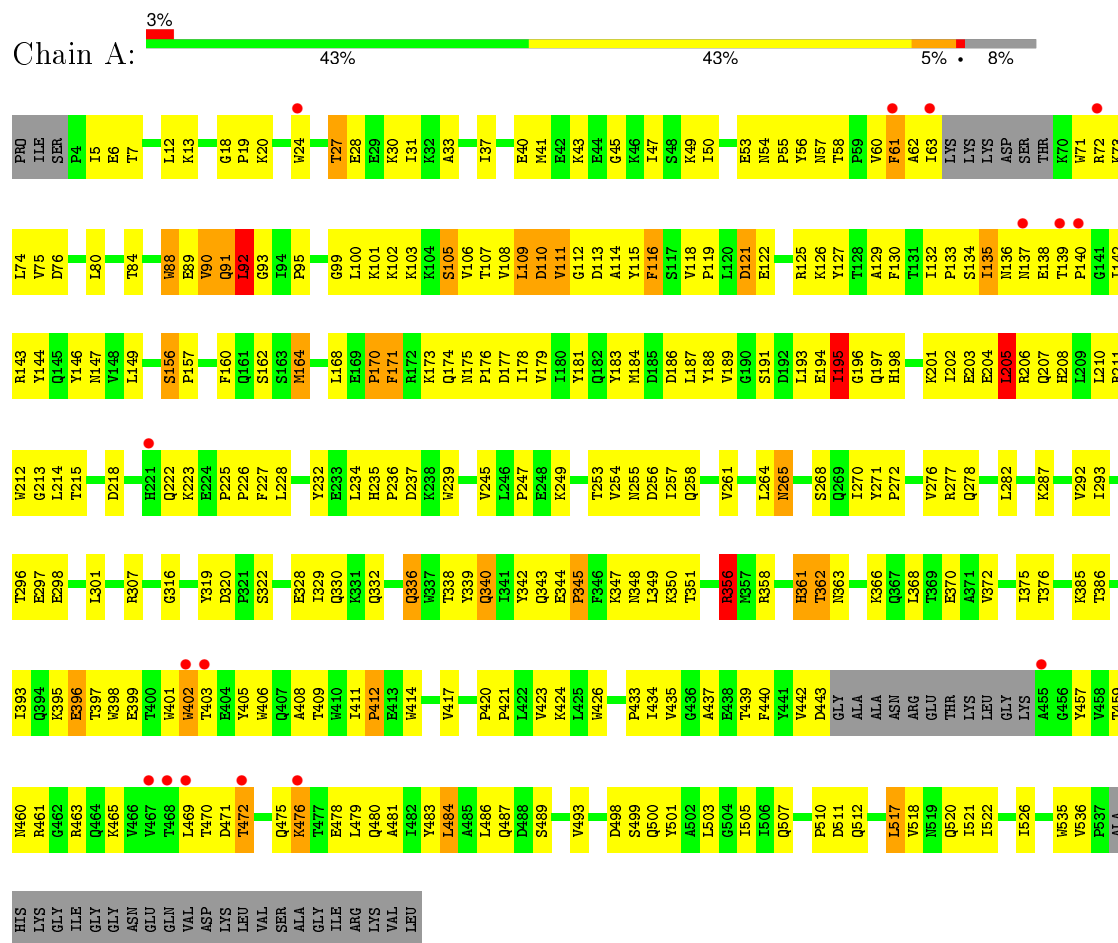


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			22	18	1	1	1	1		

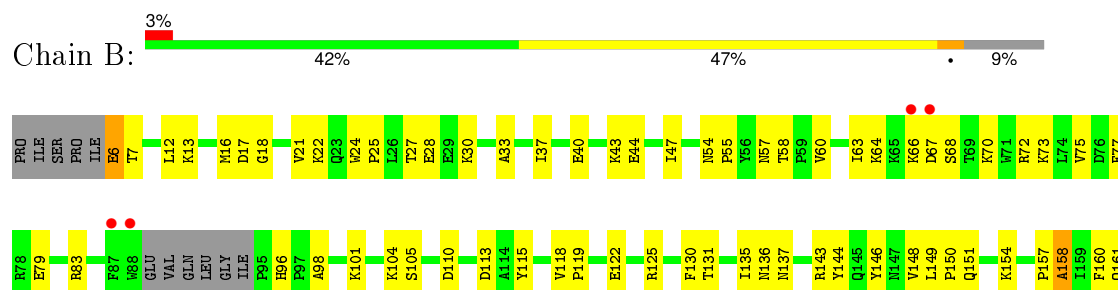
3 Residue-property plots

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: Pol polyprotein, Reverse transcriptase, Chain A



- Molecule 2: Pol polypprotein, Reverse transcriptase, Chain B



THR PHE	V365	K366	Q367	L368	T369	E370	A371	V372											T376	T377	E378	S379	I380	V381	I382	W383	G384	K385	T386	P387	K388	F389	K390											I393	Q394	W398	W401	Y405	T409	W410	W414	N418	T419	P420	P421	L422	V423	K424	L425	W426	Y427	GLN	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU
	A299	E300	L301	E302	L303	T369	A304	E305	R306	R307	E308	I309	L310	K311	E312	P313	V317	D320	K323	D324	L325	I326	A327	E328	I329	Q330	K331	Q332	G333	Q334	G335	Q336	W337	T338	Y342	Q343	E344	P345	F346	K347	N348	L349	K350	T351	G352	K353	Y354	A355	R356	MET	ARG	GLY	ALA	HIS	T362	N363	E237	E298														
	P225	P226	F227	L228	W229	W230	Q231	Y232	E233	L234	H235	P236	W239	T240	V241	Q242	P243	I244	K249	D250	S251	W252	T253	V254	T257	Q258	K259	L260	W266	Q269	I270	Y271	P272	G273	I274	R275	V276	R277	Q278	L279	L283	T286	L289	T290	E291	V292	I293	P294	L295	T296	E297	E298																				
	S162	S163	M164	T165	K166	I167	L168	E169	P170	F171	R172	K173	Q174	N175	P176	D177	I178	Q182	Y183	M184	D185	D186	L187	G190	S191	D192	L193	E194	I195	G196	Q197	H198	R199	T200	K201	L202	E203	E204	L205	R206	Q207	H208	L209	L210	R211	W212	G213	L214	THR	THR	PRO	ASP	LYS	HIS	GLN	LYS	GLU															

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.80 Å 115.20 Å 65.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 2.81 29.81 – 2.81	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.81-2.81) 93.9 (29.81-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.80 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.283 0.199 , 0.214	Depositor DCC
R_{free} test set	1165 reflections (4.79%)	DCC
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 84.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 24363 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7612	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, PO4, H16

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	0.50	0/4352	0.72	3/5918 (0.1%)
2	B	0.50	0/3425	0.70	0/4652
All	All	0.50	0/7777	0.71	3/10570 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	TRP	N-CA-C	-6.47	93.54	111.00
1	A	92	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	205	LEU	CA-CB-CG	5.28	127.44	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4247	0	4275	269	0
2	B	3328	0	3353	209	0
3	A	15	0	0	3	0
4	A	22	0	22	2	0
All	All	7612	0	7650	455	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 30.

All (455) 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:206:ARG:HH12	1:A:218:ASP:HA	1.28	0.98
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.49	0.95
1:A:195:ILE:H	1:A:195:ILE:HD13	1.33	0.94
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.50	0.93
2:B:66:LYS:HE3	2:B:230:MET:HG3	1.50	0.91
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.53	0.89
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.53	0.88
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.55	0.88
1:A:89:GLU:HG2	1:A:90:VAL:HG23	1.56	0.87
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.73	0.86
1:A:257:ILE:O	1:A:261:VAL:HG23	1.76	0.85
1:A:101:LYS:N	1:A:101:LYS:HD2	1.91	0.84
1:A:191:SER:HB3	1:A:198:HIS:ND1	1.93	0.84
1:A:206:ARG:NH1	1:A:218:ASP:HA	1.94	0.82
2:B:193:LEU:HD22	2:B:201:LYS:HD2	1.63	0.81
2:B:40:GLU:HG3	2:B:44:GLU:OE2	1.79	0.81
1:A:500:GLN:NE2	2:B:422:LEU:HD12	1.96	0.81
2:B:227:PHE:HB3	2:B:231:GLY:CA	2.12	0.80
2:B:242:GLN:HG2	2:B:353:LYS:HG2	1.65	0.78
2:B:362:THR:HG22	2:B:366:LYS:HD3	1.62	0.78
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.66	0.78
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.49	0.77
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.20	0.77
1:A:40:GLU:OE2	1:A:43:LYS:HD3	1.84	0.76
1:A:228:LEU:HA	1:A:232:TYR:O	1.86	0.76
2:B:295:LEU:HD12	2:B:295:LEU:N	2.02	0.75
2:B:297:GLU:O	2:B:301:LEU:HG	1.87	0.74
1:A:27:THR:HG23	1:A:30:LYS:HB2	1.69	0.73
2:B:266:TRP:O	2:B:269:GLN:HG2	1.88	0.73
2:B:330:GLN:HB2	2:B:338:THR:OG1	1.88	0.73
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.01	0.73
2:B:295:LEU:HD12	2:B:295:LEU:H	1.53	0.72
2:B:305:GLU:O	2:B:309:ILE:HG13	1.89	0.72
2:B:193:LEU:HD22	2:B:201:LYS:CD	2.20	0.72
2:B:154:LYS:O	2:B:157:PRO:HD2	1.89	0.72
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.19	0.71
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.26	0.71
1:A:476:LYS:HD2	1:A:476:LYS:O	1.90	0.71
2:B:234:LEU:HD21	2:B:377:THR:HG21	1.72	0.71
2:B:66:LYS:HG2	2:B:230:MET:HA	1.73	0.70
2:B:332:GLN:HA	2:B:424:LYS:HE3	1.74	0.70
1:A:125:ARG:HG2	1:A:146:TYR:O	1.92	0.70
1:A:89:GLU:CG	1:A:90:VAL:H	2.04	0.69
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.06	0.69
1:A:181:TYR:HE1	1:A:183:TYR:HB2	1.56	0.69
1:A:253:THR:HG22	1:A:255:ASN:H	1.58	0.69
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.73	0.69
1:A:92:LEU:HD12	1:A:92:LEU:O	1.94	0.68
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.27	0.68
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.74	0.68
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.28	0.68
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.28	0.68
2:B:63:ILE:HD11	2:B:72:ARG:HD3	1.76	0.67
2:B:203:GLU:HG3	2:B:207:GLN:NE2	2.09	0.67
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.76	0.67
1:A:518:VAL:O	1:A:522:ILE:HG13	1.94	0.67
1:A:500:GLN:HE21	2:B:422:LEU:CD1	2.08	0.66
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.77	0.66
2:B:244:ILE:HD13	2:B:266:TRP:HZ3	1.60	0.66
2:B:420:PRO:O	2:B:423:VAL:HG12	1.95	0.66
2:B:205:LEU:O	2:B:209:LEU:HG	1.95	0.66
1:A:347:LYS:O	1:A:347:LYS:HG2	1.94	0.66
2:B:193:LEU:CD2	2:B:201:LYS:HD2	2.26	0.65
1:A:500:GLN:HE21	2:B:422:LEU:HD12	1.59	0.65
1:A:411:ILE:O	1:A:412:PRO:O	2.15	0.65
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.79	0.65
1:A:134:SER:HB3	1:A:140:PRO:O	1.96	0.64
1:A:191:SER:OG	1:A:193:LEU:HG	1.97	0.64
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.32	0.64
2:B:193:LEU:H	2:B:193:LEU:HD12	1.63	0.64
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.62	0.64
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.78	0.64
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.31	0.64
2:B:169:GLU:O	2:B:173:LYS:HG3	1.96	0.64
1:A:296:THR:HG22	1:A:297:GLU:H	1.61	0.64
1:A:28:GLU:OE1	1:A:135:ILE:HG22	1.97	0.64
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.33	0.63
1:A:40:GLU:HA	1:A:40:GLU:OE2	1.99	0.63
1:A:319:TYR:OH	1:A:385:LYS:HE2	1.98	0.63
2:B:195:ILE:HG13	2:B:199:ARG:HE	1.63	0.62
1:A:91:GLN:HE21	2:B:137:ASN:HB3	1.64	0.62
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.34	0.62
1:A:53:GLU:O	1:A:55:PRO:HD3	2.00	0.62
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.82	0.62
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.35	0.62
2:B:13:LYS:HB2	2:B:16:MET:SD	2.40	0.61
1:A:296:THR:HG22	1:A:297:GLU:N	2.15	0.61
2:B:66:LYS:HE3	2:B:230:MET:CG	2.27	0.61
1:A:207:GLN:HE21	1:A:207:GLN:HA	1.63	0.61
1:A:61:PHE:CE2	1:A:74:LEU:HG	2.35	0.61
1:A:27:THR:HG23	1:A:30:LYS:CB	2.30	0.61
1:A:110:ASP:O	1:A:112:GLY:N	2.34	0.61
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.36	0.61
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.65	0.61
1:A:89:GLU:HG2	1:A:90:VAL:H	1.64	0.60
1:A:249:LYS:NZ	1:A:256:ASP:HB3	2.16	0.60
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.37	0.60
1:A:376:THR:HG23	1:A:386:THR:HG22	1.82	0.60
1:A:111:VAL:CG1	1:A:114:ALA:HB2	2.32	0.60
2:B:166:LYS:O	2:B:169:GLU:HG3	2.02	0.59
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.84	0.59
2:B:191:SER:HB2	2:B:193:LEU:CD1	2.32	0.59
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.85	0.59
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.85	0.59
1:A:62:ALA:C	1:A:63:ILE:HD12	2.23	0.59
2:B:254:VAL:HG23	2:B:291:GLU:O	2.03	0.59
2:B:79:GLU:O	2:B:83:ARG:HG3	2.03	0.59
1:A:56:TYR:O	1:A:143:ARG:NH2	2.31	0.59
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.37	0.58
1:A:27:THR:HG23	1:A:30:LYS:CG	2.33	0.58
1:A:178:ILE:HG22	1:A:179:VAL:N	2.19	0.58
1:A:265:ASN:N	1:A:265:ASN:HD22	2.01	0.58
1:A:498:ASP:O	1:A:535:TRP:NE1	2.34	0.58
2:B:33:ALA:O	2:B:37:ILE:HG13	2.02	0.58
2:B:6:GLU:O	2:B:6:GLU:HG2	2.02	0.58
1:A:177:ASP:O	1:A:178:ILE:HD13	2.03	0.58
1:A:136:ASN:OD1	1:A:139:THR:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:ND2	1:A:126:LYS:HB2	2.19	0.58
1:A:522:ILE:O	1:A:526:ILE:HG13	2.04	0.57
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.49	0.57
2:B:113:ASP:OD1	2:B:214:LEU:HD11	2.05	0.57
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.34	0.57
1:A:129:ALA:HA	1:A:144:TYR:O	2.04	0.57
1:A:194:GLU:O	1:A:197:GLN:N	2.38	0.57
1:A:132:ILE:HB	1:A:142:ILE:HG13	1.87	0.57
1:A:195:ILE:HD13	1:A:195:ILE:N	2.12	0.57
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.86	0.57
2:B:239:TRP:HB3	2:B:350:LYS:NZ	2.19	0.57
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.40	0.57
1:A:37:ILE:O	1:A:41:MET:HG3	2.05	0.57
1:A:89:GLU:CG	1:A:90:VAL:N	2.67	0.56
2:B:66:LYS:CG	2:B:230:MET:HA	2.34	0.56
2:B:197:GLN:O	2:B:201:LYS:HG3	2.05	0.56
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.41	0.56
2:B:175:ASN:N	2:B:176:PRO:HD3	2.20	0.56
2:B:175:ASN:HB3	2:B:178:ILE:HD12	1.86	0.56
2:B:203:GLU:CG	2:B:207:GLN:HE22	2.18	0.56
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.88	0.56
1:A:170:PRO:HA	1:A:173:LYS:HE3	1.88	0.56
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.06	0.55
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.53	0.55
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.88	0.55
2:B:193:LEU:N	2:B:193:LEU:HD12	2.20	0.55
1:A:396:GLU:HG3	1:A:397:THR:N	2.20	0.55
1:A:108:VAL:C	1:A:109:LEU:HD23	2.28	0.55
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.42	0.55
2:B:208:HIS:NE2	2:B:212:TRP:HZ3	2.05	0.55
1:A:363:ASN:ND2	1:A:401:TRP:CZ3	2.75	0.54
1:A:226:PRO:HA	1:A:234:LEU:O	2.07	0.54
2:B:66:LYS:CE	2:B:230:MET:HG3	2.30	0.54
1:A:406:TRP:O	2:B:331:LYS:HB3	2.08	0.54
2:B:379:SER:CB	2:B:387:PRO:HD3	2.38	0.54
1:A:116:PHE:CD2	1:A:116:PHE:N	2.73	0.54
1:A:89:GLU:HG2	1:A:90:VAL:N	2.22	0.54
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.38	0.54
1:A:507:GLN:NE2	2:B:421:PRO:HB3	2.23	0.54
2:B:60:VAL:HG11	2:B:130:PHE:CD1	2.43	0.54
1:A:257:ILE:HD13	1:A:282:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:OE1	1:A:135:ILE:CG2	2.56	0.54
1:A:61:PHE:N	1:A:61:PHE:CD2	2.75	0.54
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.42	0.54
1:A:393:ILE:HD12	1:A:423:VAL:HG21	1.90	0.54
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.43	0.53
1:A:340:GLN:CB	1:A:351:THR:HG22	2.39	0.53
1:A:480:GLN:HG2	1:A:517:LEU:HD11	1.88	0.53
1:A:350:LYS:HG2	1:A:351:THR:N	2.23	0.53
2:B:169:GLU:N	2:B:170:PRO:HD2	2.23	0.53
2:B:186:ASP:OD1	2:B:228:LEU:HD12	2.09	0.53
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.22	0.53
1:A:5:ILE:HG13	1:A:6:GLU:N	2.22	0.53
1:A:366:LYS:HE3	1:A:405:TYR:OH	2.09	0.53
2:B:168:LEU:C	2:B:170:PRO:HD2	2.28	0.53
2:B:167:ILE:HG23	2:B:212:TRP:CE3	2.43	0.53
1:A:183:TYR:CD1	1:A:184:MET:HG2	2.43	0.53
1:A:61:PHE:N	1:A:61:PHE:HD2	2.06	0.53
2:B:295:LEU:H	2:B:295:LEU:CD1	2.21	0.53
2:B:118:VAL:HB	2:B:149:LEU:HG	1.91	0.53
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.43	0.52
1:A:278:GLN:HA	1:A:278:GLN:NE2	2.22	0.52
2:B:257:ILE:HG21	2:B:283:LEU:HD13	1.90	0.52
1:A:178:ILE:HD12	1:A:191:SER:HB2	1.89	0.52
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.92	0.52
2:B:276:VAL:O	2:B:277:ARG:C	2.48	0.52
2:B:308:GLU:HA	2:B:311:LYS:HG3	1.91	0.52
2:B:66:LYS:HG2	2:B:230:MET:CA	2.39	0.52
1:A:174:GLN:O	1:A:176:PRO:HD2	2.09	0.52
2:B:183:TYR:OH	2:B:386:THR:HG23	2.10	0.52
2:B:327:ALA:O	2:B:389:PHE:HA	2.09	0.52
1:A:95:PRO:HB3	2:B:136:ASN:O	2.09	0.52
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.92	0.52
1:A:254:VAL:O	1:A:258:GLN:HG3	2.09	0.52
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.92	0.52
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.90	0.52
2:B:170:PRO:HG2	2:B:171:PHE:H	1.74	0.52
2:B:229:TRP:CE3	2:B:229:TRP:HA	2.46	0.52
2:B:270:ILE:O	2:B:272:PRO:HD3	2.10	0.51
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.45	0.51
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.92	0.51
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:O	1:A:417:VAL:HG13	2.10	0.51
2:B:335:GLY:O	2:B:355:ALA:HA	2.11	0.51
2:B:205:LEU:HD22	2:B:209:LEU:HG	1.93	0.51
2:B:195:ILE:HG23	2:B:196:GLY:N	2.26	0.51
2:B:173:LYS:O	2:B:176:PRO:HD3	2.10	0.51
1:A:170:PRO:O	1:A:173:LYS:HG2	2.10	0.51
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.46	0.51
1:A:440:PHE:HZ	1:A:463:ARG:HH21	1.59	0.51
1:A:261:VAL:O	1:A:265:ASN:ND2	2.44	0.51
1:A:116:PHE:HE1	3:A:1302:PO4:O1	1.94	0.51
1:A:109:LEU:N	1:A:109:LEU:HD23	2.26	0.51
2:B:110:ASP:HB3	2:B:226:PRO:HG2	1.93	0.50
2:B:202:ILE:HG21	2:B:227:PHE:HE1	1.75	0.50
1:A:328:GLU:O	1:A:339:TYR:HA	2.11	0.50
1:A:433:PRO:HB3	2:B:289:LEU:HD23	1.93	0.50
2:B:206:ARG:NH2	2:B:226:PRO:HA	2.25	0.50
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.46	0.50
1:A:254:VAL:HG22	1:A:293:ILE:CD1	2.40	0.50
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.76	0.50
1:A:332:GLN:HB3	1:A:336:GLN:HB3	1.92	0.50
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.47	0.50
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.32	0.50
1:A:118:VAL:HB	1:A:149:LEU:HG	1.92	0.50
1:A:108:VAL:HA	1:A:187:LEU:O	2.11	0.50
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.10	0.50
2:B:195:ILE:CG2	2:B:196:GLY:N	2.75	0.50
1:A:102:LYS:HZ3	1:A:237:ASP:HB2	1.77	0.50
1:A:72:ARG:HG2	1:A:73:LYS:N	2.27	0.50
2:B:170:PRO:HA	2:B:173:LYS:NZ	2.27	0.49
1:A:409:THR:O	2:B:364:ASP:HB2	2.12	0.49
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.94	0.49
1:A:424:LYS:HE3	1:A:426:TRP:CE2	2.46	0.49
1:A:178:ILE:HD11	1:A:193:LEU:HD11	1.94	0.49
1:A:115:TYR:HA	1:A:149:LEU:HD12	1.93	0.49
1:A:57:ASN:HA	1:A:129:ALA:O	2.11	0.49
1:A:91:GLN:O	1:A:93:GLY:N	2.44	0.49
1:A:292:VAL:C	1:A:293:ILE:HD12	2.32	0.49
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.47	0.49
1:A:201:LYS:O	1:A:204:GLU:HB3	2.12	0.49
1:A:90:VAL:O	1:A:91:GLN:HB2	2.12	0.49
2:B:195:ILE:HD11	2:B:233:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:CD1	1:A:191:SER:HB2	2.43	0.49
2:B:40:GLU:OE2	2:B:40:GLU:HA	2.13	0.49
2:B:295:LEU:CD1	2:B:295:LEU:N	2.73	0.49
1:A:507:GLN:HE22	2:B:421:PRO:HB3	1.76	0.49
1:A:253:THR:O	1:A:256:ASP:N	2.46	0.49
1:A:368:LEU:O	1:A:372:VAL:HG23	2.13	0.49
1:A:293:ILE:N	1:A:293:ILE:HD12	2.28	0.48
2:B:425:LEU:HD23	2:B:425:LEU:O	2.12	0.48
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.48	0.48
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.13	0.48
1:A:99:GLY:HA3	2:B:136:ASN:ND2	2.28	0.48
2:B:64:LYS:HE2	2:B:68:SER:O	2.13	0.48
1:A:465:LYS:HD2	1:A:484:LEU:CD2	2.44	0.48
1:A:102:LYS:HG2	1:A:103:LYS:N	2.28	0.48
1:A:188:TYR:CD2	4:A:999:H16:HF1	2.49	0.48
1:A:218:ASP:O	1:A:222:GLN:HG3	2.14	0.48
1:A:115:TYR:HB3	1:A:149:LEU:HB2	1.96	0.48
1:A:249:LYS:HZ1	1:A:256:ASP:HB3	1.78	0.48
1:A:460:ASN:OD1	1:A:461:ARG:HG3	2.13	0.48
2:B:105:SER:O	2:B:190:GLY:HA2	2.13	0.48
1:A:194:GLU:O	1:A:195:ILE:C	2.51	0.48
2:B:66:LYS:HD2	2:B:67:ASP:N	2.29	0.48
2:B:193:LEU:HD21	2:B:201:LYS:NZ	2.29	0.48
2:B:254:VAL:O	2:B:258:GLN:HG3	2.13	0.48
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.49	0.48
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.13	0.48
2:B:380:ILE:O	2:B:384:GLY:N	2.46	0.48
1:A:245:VAL:HG23	1:A:245:VAL:O	2.14	0.48
2:B:170:PRO:HA	2:B:173:LYS:HZ3	1.79	0.47
1:A:24:TRP:HZ3	1:A:61:PHE:CG	2.31	0.47
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.29	0.47
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.35	0.47
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.49	0.47
2:B:328:GLU:CG	2:B:390:LYS:HD2	2.45	0.47
1:A:27:THR:HG23	1:A:30:LYS:HG3	1.94	0.47
2:B:379:SER:HB2	2:B:387:PRO:HD3	1.96	0.47
1:A:113:ASP:HB2	1:A:116:PHE:CD2	2.49	0.47
1:A:106:VAL:HA	1:A:189:VAL:O	2.13	0.47
2:B:249:LYS:HD3	2:B:251:SER:O	2.15	0.47
2:B:17:ASP:CG	2:B:18:GLY:H	2.18	0.47
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.44	0.47
1:A:164:MET:O	1:A:168:LEU:HG	2.14	0.47
2:B:172:ARG:O	2:B:176:PRO:HG3	2.14	0.47
2:B:98:ALA:O	2:B:101:LYS:HG2	2.13	0.47
1:A:60:VAL:HG22	1:A:75:VAL:HG22	1.97	0.47
1:A:156:SER:HB2	1:A:157:PRO:CD	2.35	0.47
1:A:399:GLU:HG3	1:A:402:TRP:CZ3	2.49	0.47
1:A:393:ILE:HD12	1:A:423:VAL:CG2	2.44	0.47
1:A:505:ILE:O	1:A:510:PRO:HD3	2.15	0.47
1:A:49:LYS:HA	1:A:143:ARG:O	2.15	0.47
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.47	0.47
2:B:98:ALA:O	2:B:101:LYS:HE3	2.15	0.47
1:A:45:GLY:O	1:A:147:ASN:ND2	2.40	0.47
2:B:66:LYS:NZ	2:B:67:ASP:HB2	2.30	0.47
1:A:93:GLY:O	2:B:137:ASN:HB3	2.14	0.46
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.50	0.46
1:A:470:THR:O	1:A:471:ASP:HB2	2.15	0.46
2:B:331:LYS:O	2:B:424:LYS:HE3	2.15	0.46
2:B:376:THR:O	2:B:377:THR:C	2.54	0.46
1:A:61:PHE:CZ	1:A:74:LEU:HD23	2.50	0.46
1:A:202:ILE:O	1:A:205:LEU:HB3	2.16	0.46
2:B:160:PHE:CD1	2:B:160:PHE:O	2.68	0.46
2:B:163:SER:O	2:B:167:ILE:HG13	2.16	0.46
1:A:116:PHE:HD2	1:A:116:PHE:H	1.58	0.46
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.50	0.46
2:B:96:HIS:CE1	2:B:381:VAL:O	2.69	0.46
2:B:393:ILE:HG12	2:B:394:GLN:N	2.30	0.46
1:A:33:ALA:HB2	1:A:71:TRP:CD1	2.51	0.46
1:A:253:THR:O	1:A:254:VAL:C	2.53	0.46
2:B:167:ILE:O	2:B:208:HIS:HE1	1.98	0.46
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.97	0.46
2:B:344:GLU:HG2	2:B:345:PRO:HD2	1.98	0.46
2:B:227:PHE:CB	2:B:231:GLY:HA2	2.34	0.46
1:A:239:TRP:CZ2	1:A:349:LEU:O	2.69	0.46
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.53	0.46
1:A:63:ILE:HD12	1:A:63:ILE:N	2.31	0.46
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.97	0.46
1:A:108:VAL:HG13	1:A:223:LYS:HB2	1.98	0.46
2:B:40:GLU:OE2	2:B:43:LYS:HD2	2.16	0.45
2:B:208:HIS:CE1	2:B:212:TRP:HZ3	2.34	0.45
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:VAL:HG13	2:B:424:LYS:N	2.31	0.45
1:A:340:GLN:HA	1:A:351:THR:HA	1.98	0.45
1:A:479:LEU:N	1:A:479:LEU:HD12	2.32	0.45
1:A:31:ILE:HD13	1:A:133:PRO:O	2.17	0.45
1:A:30:LYS:CD	1:A:62:ALA:HB3	2.43	0.45
2:B:206:ARG:NH1	2:B:227:PHE:CE2	2.85	0.45
1:A:194:GLU:O	1:A:196:GLY:N	2.49	0.45
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.51	0.45
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.52	0.45
1:A:434:ILE:HB	1:A:437:ALA:HB3	1.99	0.45
1:A:264:LEU:HD13	1:A:276:VAL:HG12	1.99	0.45
2:B:297:GLU:HA	2:B:300:GLU:HB2	1.99	0.45
2:B:257:ILE:O	2:B:260:LEU:HB3	2.17	0.45
1:A:472:THR:CB	1:A:476:LYS:HE3	2.46	0.45
1:A:406:TRP:HH2	2:B:418:ASN:OD1	2.00	0.45
1:A:193:LEU:HD13	1:A:197:GLN:HG3	1.99	0.44
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.73	0.44
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.42	0.44
1:A:479:LEU:HD11	1:A:501:TYR:CE2	2.52	0.44
1:A:457:TYR:C	1:A:457:TYR:CD1	2.91	0.44
1:A:115:TYR:N	1:A:115:TYR:CD2	2.86	0.44
2:B:253:THR:HA	2:B:292:VAL:HA	1.98	0.44
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.99	0.44
1:A:344:GLU:HB3	1:A:347:LYS:HD3	1.99	0.44
2:B:113:ASP:HB2	2:B:214:LEU:HD12	1.99	0.44
1:A:102:LYS:HG3	1:A:237:ASP:HA	1.98	0.44
1:A:228:LEU:N	1:A:228:LEU:HD12	2.32	0.44
1:A:237:ASP:N	1:A:237:ASP:OD2	2.48	0.44
2:B:303:LEU:HD22	2:B:307:ARG:HG3	2.00	0.44
1:A:361:HIS:O	1:A:362:THR:HG23	2.16	0.44
1:A:498:ASP:HA	1:A:536:VAL:O	2.18	0.44
1:A:277:ARG:HH11	1:A:277:ARG:HG3	1.82	0.44
2:B:158:ALA:O	2:B:161:GLN:CB	2.65	0.44
1:A:28:GLU:OE1	1:A:135:ILE:HA	2.18	0.44
1:A:356:ARG:CZ	1:A:358:ARG:HG2	2.48	0.44
1:A:478:GLU:CD	1:A:499:SER:HB2	2.38	0.44
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.53	0.43
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.18	0.43
1:A:58:THR:CG2	1:A:76:ASP:O	2.66	0.43
1:A:19:PRO:HD3	1:A:80:LEU:HD13	2.00	0.43
1:A:178:ILE:CG2	1:A:179:VAL:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:O	1:A:92:LEU:C	2.56	0.43
1:A:270:ILE:HG23	1:A:271:TYR:N	2.34	0.43
1:A:164:MET:HE1	1:A:187:LEU:HD22	2.00	0.43
1:A:116:PHE:CE1	3:A:1302:PO4:O3	2.72	0.43
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.48	0.43
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.99	0.43
2:B:174:GLN:C	2:B:176:PRO:HD3	2.38	0.43
1:A:156:SER:CB	1:A:157:PRO:HD3	2.35	0.43
2:B:320:ASP:OD2	2:B:323:LYS:HG2	2.19	0.43
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.54	0.43
1:A:118:VAL:HG13	1:A:119:PRO:HD2	2.01	0.43
2:B:57:ASN:ND2	2:B:143:ARG:HH11	2.13	0.43
2:B:239:TRP:HB3	2:B:350:LYS:HZ1	1.84	0.43
1:A:503:LEU:HD22	1:A:535:TRP:CB	2.47	0.43
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.19	0.42
2:B:325:LEU:HB3	2:B:387:PRO:HA	2.01	0.42
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.54	0.42
1:A:402:TRP:CG	1:A:403:THR:N	2.87	0.42
2:B:199:ARG:CZ	2:B:233:GLU:OE1	2.67	0.42
2:B:12:LEU:O	2:B:13:LYS:C	2.56	0.42
1:A:320:ASP:OD2	1:A:322:SER:OG	2.36	0.42
1:A:420:PRO:HA	1:A:421:PRO:C	2.40	0.42
1:A:194:GLU:OE1	1:A:194:GLU:HA	2.19	0.42
1:A:115:TYR:O	1:A:149:LEU:HB2	2.19	0.42
1:A:489:SER:HB2	1:A:493:VAL:HG22	2.01	0.42
1:A:106:VAL:O	1:A:225:PRO:HD3	2.19	0.42
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.54	0.42
1:A:207:GLN:HE21	1:A:207:GLN:CA	2.29	0.42
1:A:116:PHE:HE1	3:A:1302:PO4:P	2.42	0.42
1:A:439:THR:O	1:A:459:THR:HA	2.20	0.42
2:B:345:PRO:O	2:B:346:PHE:HB2	2.20	0.42
2:B:229:TRP:HE3	2:B:229:TRP:HA	1.81	0.42
1:A:465:LYS:HD2	1:A:484:LEU:HD21	2.01	0.42
1:A:88:TRP:HB2	2:B:54:ASN:O	2.20	0.42
2:B:389:PHE:CD1	2:B:389:PHE:N	2.88	0.42
2:B:21:VAL:HG12	2:B:22:LYS:O	2.19	0.42
1:A:100:LEU:C	1:A:101:LYS:HD2	2.38	0.42
2:B:193:LEU:H	2:B:193:LEU:CD1	2.29	0.42
2:B:148:VAL:HG23	2:B:149:LEU:N	2.34	0.42
2:B:161:GLN:O	2:B:164:MET:HB3	2.20	0.42
1:A:483:TYR:CZ	1:A:520:GLN:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:VAL:HG11	2:B:313:PRO:HG3	2.02	0.42
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.42	0.42
2:B:278:GLN:HB3	2:B:299:ALA:HB2	2.02	0.42
2:B:233:GLU:HG2	2:B:233:GLU:H	1.66	0.42
2:B:348:ASN:HD22	2:B:351:THR:HG22	1.82	0.41
2:B:58:THR:HG21	2:B:77:PHE:CD2	2.55	0.41
2:B:332:GLN:HB2	2:B:336:GLN:O	2.19	0.41
1:A:136:ASN:OD1	1:A:139:THR:CG2	2.68	0.41
1:A:171:PHE:CE2	1:A:175:ASN:ND2	2.89	0.41
1:A:91:GLN:C	1:A:93:GLY:N	2.72	0.41
1:A:93:GLY:O	2:B:137:ASN:CB	2.68	0.41
1:A:249:LYS:HZ3	1:A:256:ASP:HB3	1.85	0.41
1:A:160:PHE:C	1:A:160:PHE:CD2	2.94	0.41
1:A:134:SER:OG	1:A:139:THR:O	2.37	0.41
1:A:61:PHE:HE2	1:A:74:LEU:HG	1.84	0.41
1:A:247:PRO:O	1:A:307:ARG:NH2	2.48	0.41
1:A:253:THR:HG22	1:A:255:ASN:N	2.31	0.41
1:A:160:PHE:CE2	1:A:164:MET:HG2	2.55	0.41
2:B:298:GLU:CD	2:B:298:GLU:H	2.24	0.41
2:B:259:LYS:HE2	2:B:259:LYS:HB3	1.95	0.41
2:B:330:GLN:HB2	2:B:338:THR:HG1	1.84	0.41
1:A:203:GLU:O	1:A:207:GLN:HG2	2.20	0.41
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.55	0.41
1:A:210:LEU:O	1:A:213:GLY:N	2.54	0.41
1:A:340:GLN:HE21	1:A:340:GLN:HB3	1.65	0.41
1:A:73:LYS:HZ3	1:A:75:VAL:HG23	1.85	0.41
2:B:7:THR:HG22	2:B:119:PRO:HG2	2.02	0.41
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.20	0.41
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.56	0.41
1:A:236:PRO:HA	4:A:999:H16:H9	2.02	0.41
2:B:125:ARG:HG2	2:B:146:TYR:O	2.21	0.41
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.50	0.41
2:B:66:LYS:HZ2	2:B:67:ASP:HB2	1.85	0.41
1:A:362:THR:O	1:A:512:GLN:HG2	2.21	0.41
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.54	0.41
1:A:476:LYS:HD3	1:A:517:LEU:HD12	2.04	0.40
2:B:276:VAL:O	2:B:279:LEU:N	2.54	0.40
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.56	0.40
1:A:270:ILE:O	1:A:272:PRO:HD3	2.20	0.40
1:A:212:TRP:O	1:A:214:LEU:N	2.53	0.40
2:B:278:GLN:NE2	2:B:298:GLU:CB	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLN:HG3	1:A:298:GLU:HB3	2.03	0.40
1:A:270:ILE:HG23	1:A:271:TYR:CD2	2.57	0.40
1:A:208:HIS:O	1:A:211:ARG:HB2	2.21	0.40
1:A:13:LYS:HE3	1:A:84:THR:O	2.22	0.40
1:A:7:THR:HG21	1:A:121:ASP:HA	2.04	0.40
1:A:109:LEU:CD2	1:A:109:LEU:N	2.83	0.40
2:B:208:HIS:CE1	2:B:212:TRP:CZ3	3.10	0.40
2:B:368:LEU:O	2:B:371:ALA:HB3	2.21	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	510/560 (91%)	453 (89%)	42 (8%)	15 (3%)	6	19
2	B	393/440 (89%)	338 (86%)	49 (12%)	6 (2%)	13	38
All	All	903/1000 (90%)	791 (88%)	91 (10%)	21 (2%)	8	25

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	91	GLN
1	A	92	LEU
1	A	137	ASN
1	A	156	SER
1	A	412	PRO
1	A	472	THR
1	A	111	VAL
1	A	195	ILE
1	A	402	TRP

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Mol	Chain	Res	Type
1	A	268	SER
1	A	345	PRO
2	B	250	ASP
2	B	286	THR
1	A	121	ASP
1	A	170	PRO
1	A	356	ARG
2	B	166	LYS
2	B	158	ALA
2	B	277	ARG
2	B	167	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	466/499 (93%)	433 (93%)	33 (7%)	18	45
2	B	366/400 (92%)	349 (95%)	17 (5%)	33	67
All	All	832/899 (92%)	782 (94%)	50 (6%)	24	55

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	27	THR
1	A	61	PHE
1	A	92	LEU
1	A	105	SER
1	A	107	THR
1	A	109	LEU
1	A	110	ASP
1	A	116	PHE
1	A	135	ILE
1	A	138	GLU
1	A	162	SER

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Mol	Chain	Res	Type
1	A	164	MET
1	A	171	PHE
1	A	195	ILE
1	A	205	LEU
1	A	215	THR
1	A	265	ASN
1	A	287	LYS
1	A	301	LEU
1	A	336	GLN
1	A	340	GLN
1	A	345	PRO
1	A	348	ASN
1	A	356	ARG
1	A	361	HIS
1	A	362	THR
1	A	396	GLU
1	A	443	ASP
1	A	476	LYS
1	A	484	LEU
1	A	487	GLN
1	A	517	LEU
2	B	6	GLU
2	B	55	PRO
2	B	70	LYS
2	B	122	GLU
2	B	194	GLU
2	B	205	LEU
2	B	210	LEU
2	B	212	TRP
2	B	232	TYR
2	B	233	GLU
2	B	240	THR
2	B	250	ASP
2	B	295	LEU
2	B	303	LEU
2	B	394	GLN
2	B	410	TRP
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	182	GLN
1	A	207	GLN
1	A	222	GLN
1	A	265	ASN
1	A	278	GLN
1	A	336	GLN
1	A	407	GLN
1	A	475	GLN
1	A	480	GLN
1	A	500	GLN
1	A	507	GLN
1	A	509	GLN
1	A	520	GLN
2	B	57	ASN
2	B	175	ASN
2	B	207	GLN
2	B	269	GLN
2	B	278	GLN
2	B	336	GLN
2	B	348	ASN
2	B	394	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	0.83	0	3,8,10	4.18	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	7.00	117.06	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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	1300	-	4,4,4	1.04	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	1301	-	4,4,4	1.11	0	6,6,6	0.27	0
3	PO4	A	1302	-	4,4,4	1.15	0	6,6,6	0.27	0
4	H16	A	999	-	22,24,24	2.01	7 (31%)	25,33,33	1.74	3 (12%)

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
3	PO4	A	1302	-	-	0/0/0/0	0/0/0/0
4	H16	A	999	-	-	0/7/15/15	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	H16	C4-C3	-2.86	1.39	1.43
4	A	999	H16	C7-C8	2.01	1.40	1.36
4	A	999	H16	CF-CA	2.42	1.60	1.51
4	A	999	H16	C2-N1	2.45	1.39	1.35
4	A	999	H16	C10-C9	3.04	1.43	1.36
4	A	999	H16	C6-N1	4.20	1.40	1.33
4	A	999	H16	C4-S4	4.86	1.83	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	H16	C3-C2-N1	-3.31	120.42	123.45
4	A	999	H16	C4-C3-C2	2.30	120.20	117.59
4	A	999	H16	C6-N1-C2	6.96	120.93	116.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1302	PO4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	H16	2	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	516/560 (92%)	-0.21	16 (3%)	52 40	25, 63, 107, 131	0
2	B	401/440 (91%)	-0.07	12 (2%)	54 41	25, 62, 110, 135	0
All	All	917/1000 (91%)	-0.15	28 (3%)	52 40	25, 62, 108, 135	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	LEU	6.4
2	B	88	TRP	4.5
1	A	455	ALA	4.2
1	A	63	ILE	4.2
2	B	356	ARG	3.9
1	A	467	VAL	3.8
2	B	67	ASP	3.5
1	A	468	THR	3.5
2	B	294	PRO	3.4
1	A	72	ARG	3.4
2	B	362	THR	3.2
1	A	402	TRP	3.1
2	B	334	GLN	2.8
1	A	472	THR	2.8
1	A	137	ASN	2.7
2	B	66	LYS	2.7
1	A	476	LYS	2.5
1	A	221	HIS	2.4
2	B	292	VAL	2.4
2	B	87	PHE	2.4
1	A	403	THR	2.3
2	B	186	ASP	2.3
1	A	140	PRO	2.2
1	A	61	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	139	THR	2.2
1	A	24	TRP	2.2
2	B	409	THR	2.2
2	B	242	GLN	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, 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
1	CSD	A	280	8/9	0.97	0.13	-	48,54,61,78	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(Å ²)	Q<0.9
3	PO4	A	1301	5/5	0.87	0.19	2.35	121,133,134,136	0
3	PO4	A	1302	5/5	0.83	0.26	1.77	145,147,149,149	0
3	PO4	A	1300	5/5	0.81	0.23	1.62	123,128,130,133	0
4	H16	A	999	22/22	0.97	0.19	0.86	26,48,56,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.